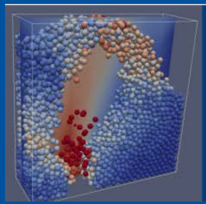

LIGGGHTS: An example of a real-world scientific code

ICTP Workshop, March 2014

Richard Berger

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

Department of Particulate Flow Modelling, JKU Linz, Austria

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/

* 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.

LIGGGHTS+CFDEMcoupling
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 behavior**, 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/

* 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.

LIGGGHTS+CFDEMcoupling
The Framework

Professional Base: DCS Computing GmbH

Scientific Base:

CFDEM project

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

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

Sandia National Laboratories — LAMMPS

OpenFOAM — esi get it right®

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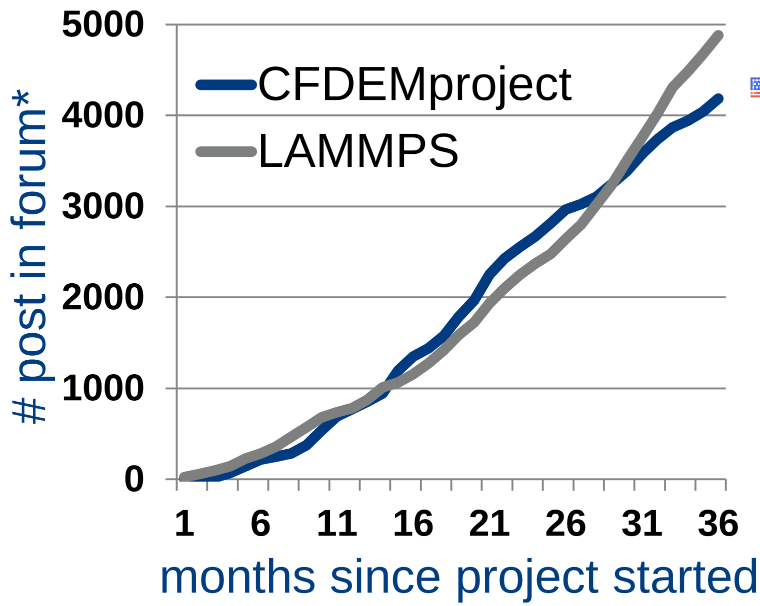
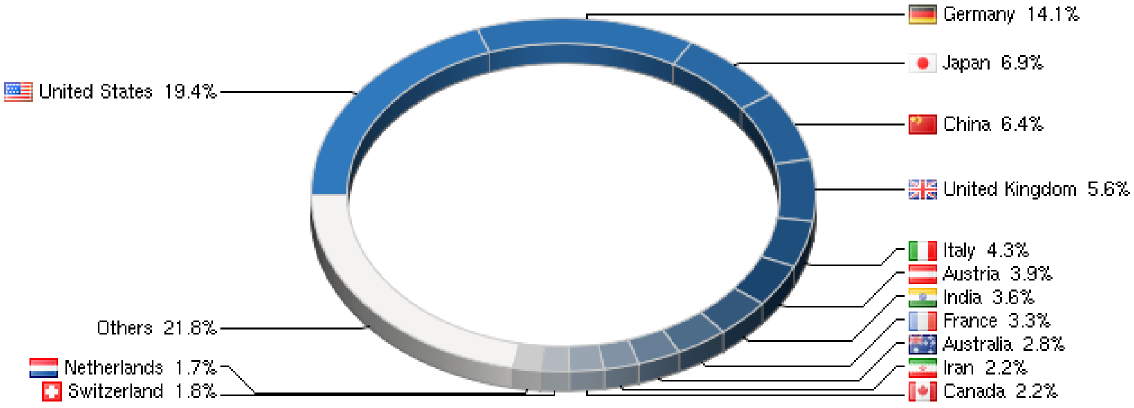
CFDEM Community after 3 yrs

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

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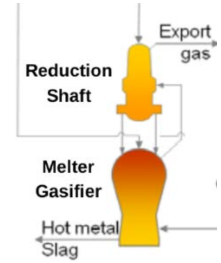
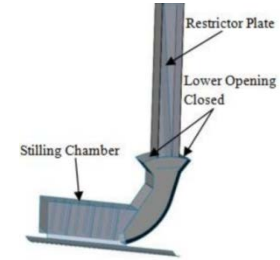
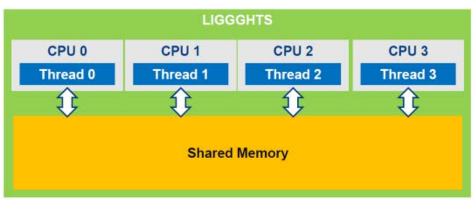
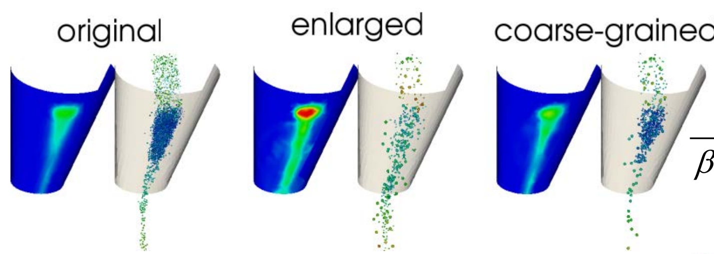
- Open source simulation software is **driven by the applications,** rules of market apply





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

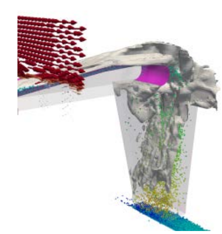


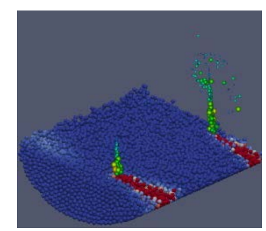


parcel size correction — fluid grid size correction — particle volume fraction correction

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

- **Most applications are multi-phase flow**
  (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

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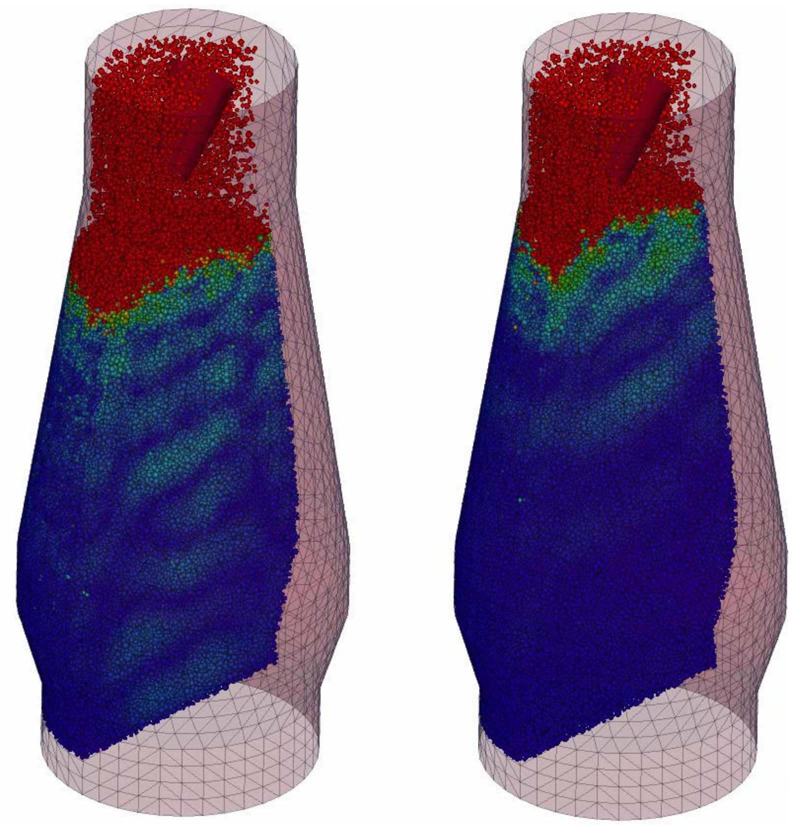
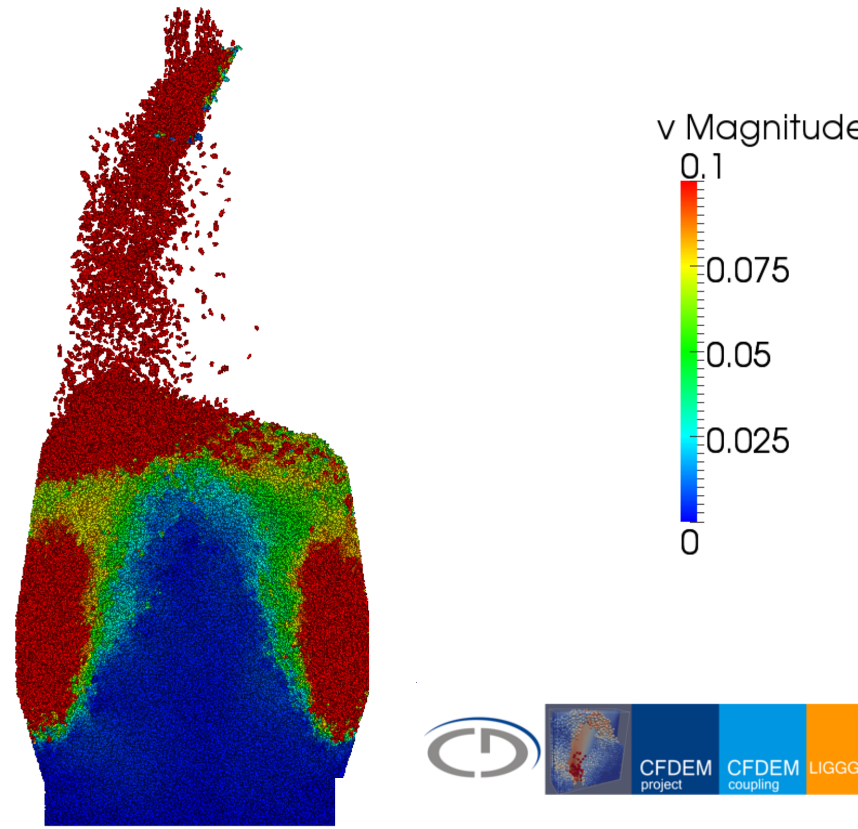
Blast Furnace



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



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

Case Study: Chute Abrasion

Chute Abrasion with deformation

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

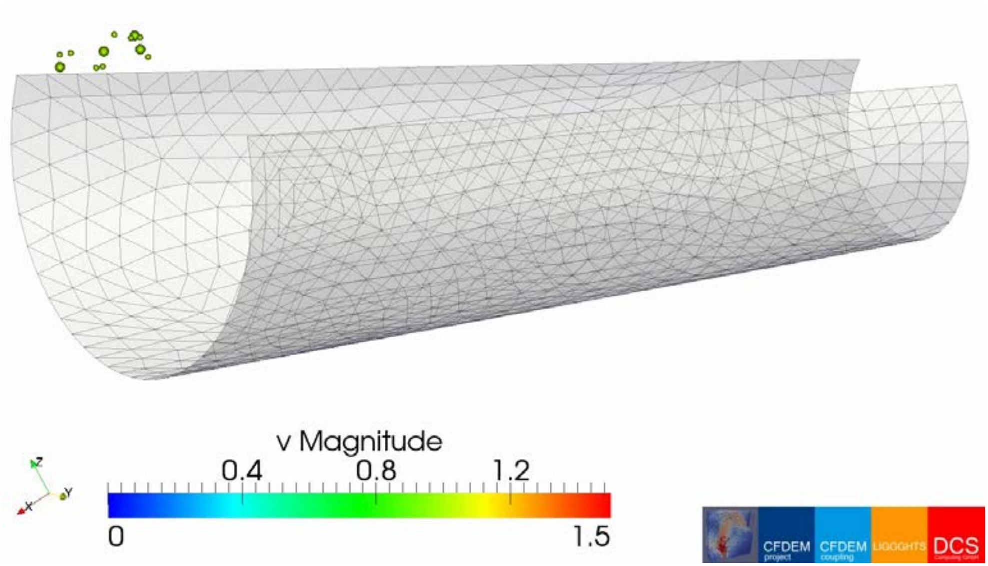
$$E = k_f \left|\mathbf{u_p}\right|^2 f(\gamma_i),$$

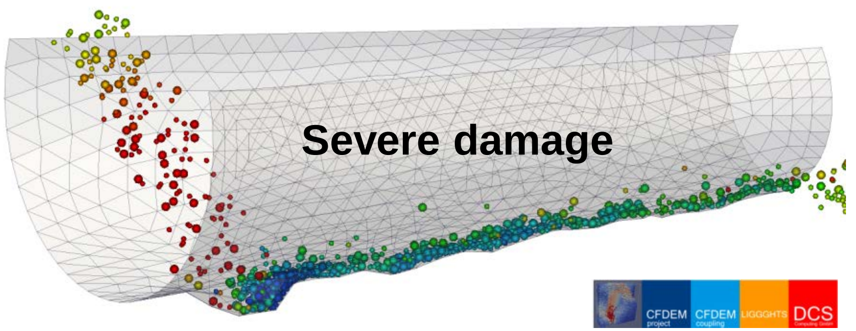
$$f(\gamma_i) = 1/3\cos^2(\gamma_i) \ , \ \tan(\gamma_i) \geq 1/3,$$

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

$$EM = 2k_f \int_{tc,0}^{tc,1} hs(\mathbf{u_p}\,\mathbf{c_n})\sin(2\gamma_i)\mathbf{u_p}\,\mathbf{f_{p\text{-}w}}\, f(\gamma_i)\, dt.$$

- 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-w}	**particle-wall contact force**
c_n	**particle-wall distance vector**

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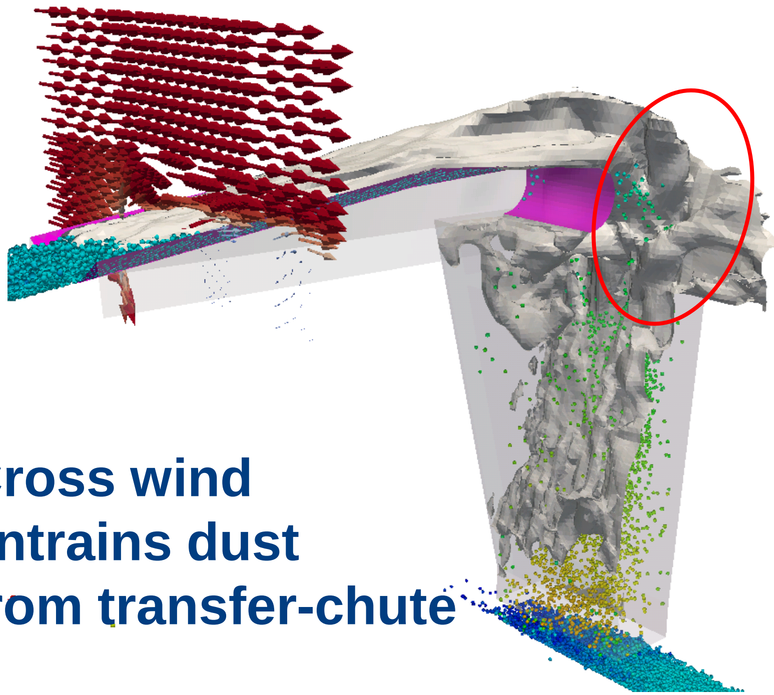
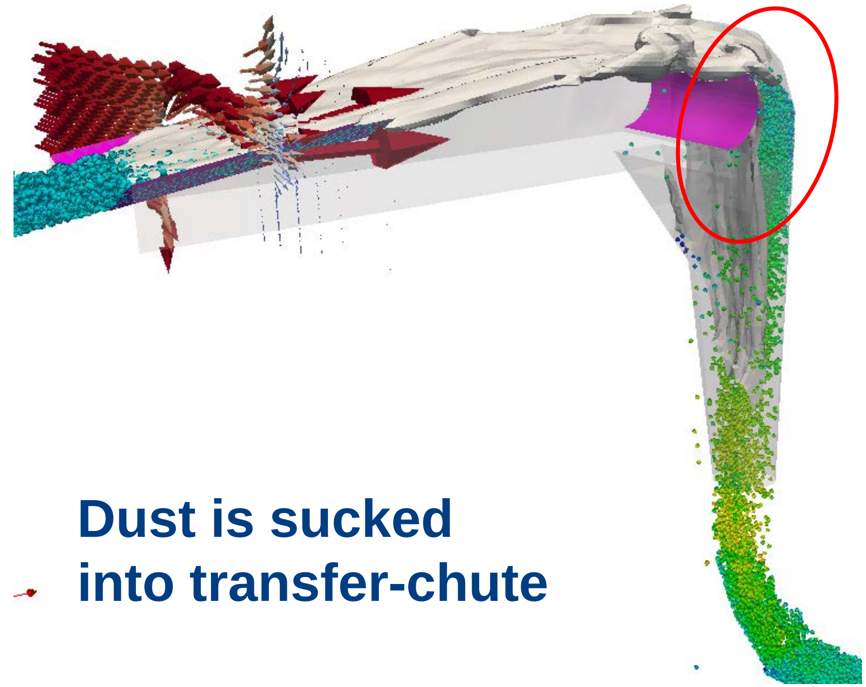
Transfer Chute Dust Emission

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

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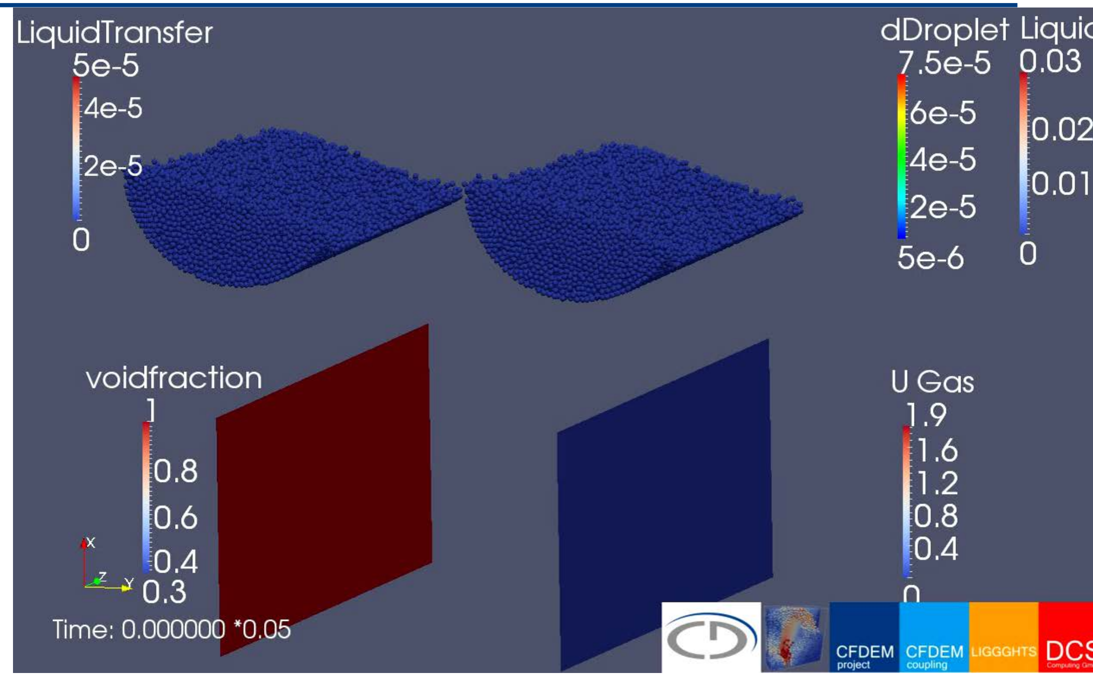
Spray Coating

Physics to be covered

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



Spray modelling

- **Equation of Motion**

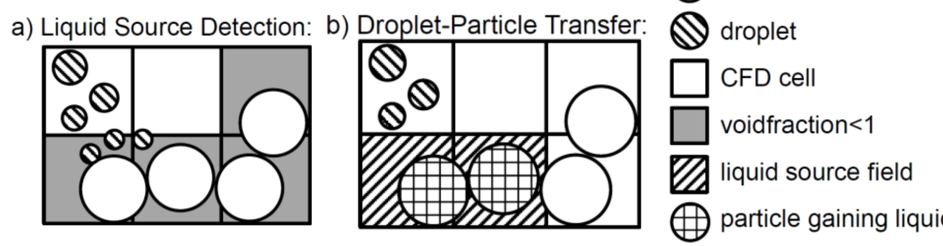
$$m_D \frac{dv_D}{dt} = g\,(\rho_D - \rho_G) V_D + C_{d,D} A_D \frac{\rho_G (v_G - v_D) |v_G - v_D|}{2}$$

- **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

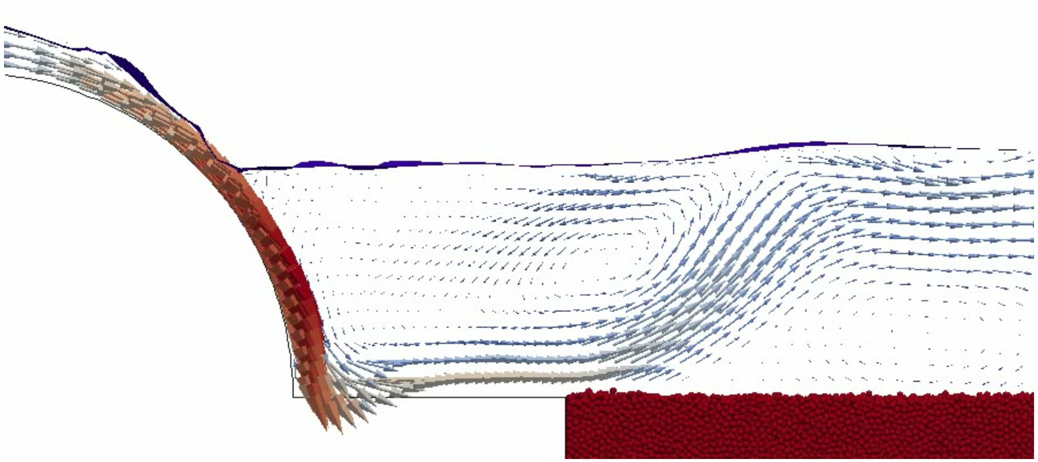


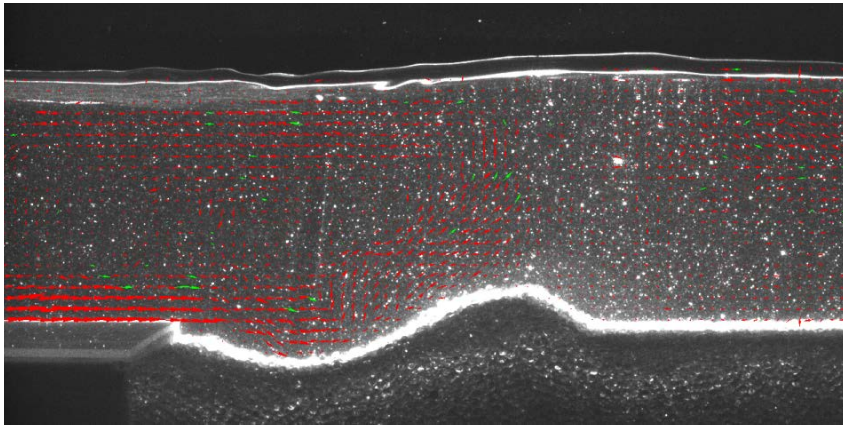
C. Goniva, J. Kerbl, S. Pirker, C. Kloss: Modelling Spray Particle Interaction by a Coupled CFD-DEM Method, Proc. Computational Modelling Conference 2013

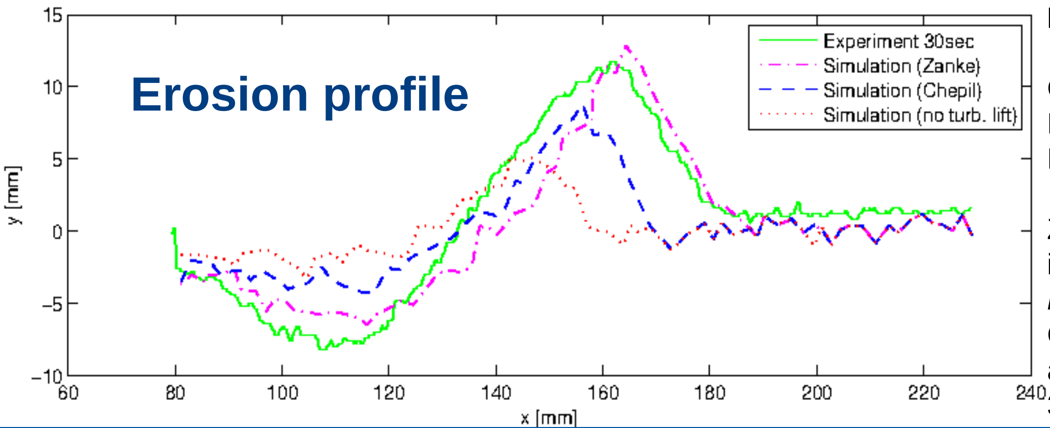
River Bed Erosion

VOF –DEM Modelling of River Bed Erosion

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







Publications:

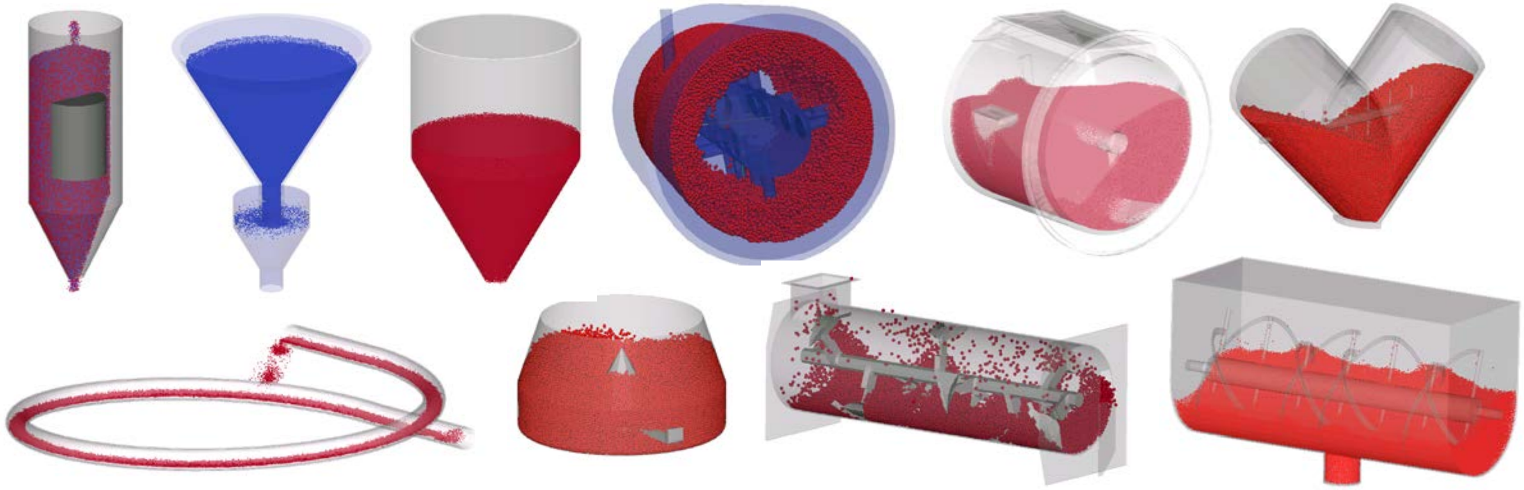
Gruber, K., Kloss, C., Goniva, C: NUMERICAL AND EXPERIMENTAL STUDY OF EROSION IN OPEN CHANNEL FLOW; Proc. IHAR 2012

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

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

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