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

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

- Share and exchange modelling ideas
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.
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.
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

**Fundament**: Technology development with customers, 2 EU FP7 projects

**Impact**: CFDEM®coupling workbench (FFG)

**Pre-Development** outside DCS

- 2009 PhD
- 2010
- 2011
- 2012 DCS founded Group leaders at JKU
- 2013
- 2014 Founders Full-time
- 2015
- 2016
- 2017
- 2018
- 2019
- 2020
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

\[
\frac{\partial \alpha_f \rho_f}{\partial t} + \nabla \cdot (\alpha_f \rho_f \mathbf{u}_f) = 0
\]

\[
\frac{\partial (\alpha_f \rho_f \mathbf{u}_f)}{\partial t} + \nabla \cdot (\alpha_f \rho_f \mathbf{u}_f \mathbf{u}_f) = -\alpha_f \nabla p + \nabla \cdot (\alpha_f \mathbf{\tau}) + \alpha_f \rho_f \mathbf{g} - K_{fs} (\mathbf{u}_f - \mathbf{u}_s)
\]

Lagrangian Particle Trajectory for Parcels

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

Scaling laws from dimensional analysis

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

- \(l\): size ratio of colliding particles, \(k_n\): stiffness, \(R\): radius, \(\rho\): 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
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
What needs to be modelled?

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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

- Intra-phase transport processes
- Intra-Particle heat transfer
- Intra-Particle chemical reactions
CFDEM® project latest news

Eco-system is growing!

Mastermind
(right hand side)

New! First release was a new year gift
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- Intra-phase transport processes
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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.
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
CFDEM®project latest news

Testing: LIGGGHTS®

- liggghts-src-unstable-3.0.x
  - Show version consistency compared to liggghts-src-unstable-3.0.2
    - examples
      - ✔️ 175
      - ✗ 2
      - ⚠️ 15
    - local
      - ✔️ 3
      - ✗ 0
      - ⚠️ 145

- pascal-master-0.x
  - pascal-examples
    - ✔️ 3
    - ✗ 1
    - ⚠️ 0

KinEng

DSC Computing @ PFAU X Graz, July 2015 | www.dcs-computing.com | www.cfdem.com
Testing: CFDEM® coupling

Comparison

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

Consistency: None
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)
Moving bed reactor with convective heat transfer

Time: 0.000000

Particle Temperature, Particle Heatflux, Void fraction, Ufluid, Tfluid, Red/Green: Decomp. CFD, Black Lines: Decomp. DEM
CFDEM® project latest news

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

**All-To-All**

**DEM:** one global array for all particles

\[ X_1 X_2 X_3 X_4 \quad \cdots \quad X_n \]

**CFD:** each processor gets a copy and locate his particles

\[ X_1 X_2 X_3 X_4 \quad \cdots \quad X_n \]

\[ X_1 X_2 X_3 X_4 \quad \cdots \quad X_n \]

**Many-To-Many**

**DEM:** the same arrays as for the last time step

\[ x_2 x_7 x_8 x_9 \quad \cdots \quad x_n \]

\[ x_1 x_3 x_4 x_6 \quad \cdots \quad x_u \]

**CFD:** only communicate moved particles

\[ x_2 x_7 x_8 x_9 \quad \cdots \quad x_n \]

\[ x_1 x_3 x_4 x_6 \quad \cdots \quad x_u \]
## ManyToMany Communication

<table>
<thead>
<tr>
<th>Test Case</th>
<th>Purpose</th>
<th>Machine used</th>
<th>Version of “many2many” used</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elongated Packed Bed #1</td>
<td>Show feasibility of the approach and its scalability</td>
<td>JKU cluster “MACH” (512 CPUs)</td>
<td>Very early feasibility version</td>
</tr>
<tr>
<td>Elongated Packed Bed #2</td>
<td>Show scalability of the final stable version and applicability across clusters</td>
<td>JKU cluster “LISE” (128 CPUs)</td>
<td>Stable version 1.0</td>
</tr>
<tr>
<td>Thermal Packed Bed</td>
<td>Compare results to physical lab-scale test-case where experimental data is available</td>
<td>Local workstation and JKU cluster “Gollum” (one blade with 32 cores)</td>
<td>Stable version 1.0</td>
</tr>
</tbody>
</table>
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 $n_P=20.48\times 10^6$.  

![Elongated packed Bed #1 diagram and performance scaling graph](image)
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
cylindrical fixed bed \( (d_{\text{cyl}}=0.1\text{m}, h_p=0.1\text{m}) \) 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 macroscopic result.
Result

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

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

Non zero – WRONG!
Hybrid IB Models

- 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
  \[ C_{d,D} = C_{d,sphereD}(1 + 2.632 y) \]
- 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
- Liquid Source Detection
- Droplet-Particle Transfer

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

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

**Literature:**
Spray modelling

- **Equation of Motion**
  \[
  \frac{dV_D}{dt} = g (\rho_D - \rho_G) V_D + C_{d,D} A_D \frac{\rho_G (v_G - v_D) |v_G - v_D|}{2}
  \]

- **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**

- a) Liquid Source Detection
- b) Droplet-Particle Transfer

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Recent Developments on LIGGGHTS®
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
Latest Dev. & Outlook

Liquid Bridge Models

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

<table>
<thead>
<tr>
<th>Washino Kimiaki</th>
<th>Easo</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Liquid properties required</strong></td>
<td><strong>Surface tension</strong></td>
</tr>
<tr>
<td>• Surface tension</td>
<td>• Contact angle</td>
</tr>
<tr>
<td>• Contact angle</td>
<td>• Viscosity</td>
</tr>
<tr>
<td>• Viscosity</td>
<td>• Min separation distance</td>
</tr>
<tr>
<td>• Minimum separation distance ratio for viscosity calculations (~1.0% of smallest particle size); prevents viscous force from becoming exceedingly large</td>
<td>• Maximum separation distance ratio, needed because neighbor lists need a cut-off</td>
</tr>
<tr>
<td>• Maximum separation distance ratio</td>
<td></td>
</tr>
</tbody>
</table>

| **Volume of liquid involved** | **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** |
| 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 |

| **Capillary force** | **Semi-empirical solution to the Young-Laplace equation (Soulie et al, 2006)** |
| Approximate theoretical solution using minimum energy approach (Rabinovitch, 2005) | |

| **Viscous force** | **Nase et al as quoted in Shi&Mccarthy** |
| Nase et al as quoted in Shi&Mccarthy | |

| **Formation distance** | **Contact distance** |
| Rupture distance (see below) | Lian et al, 1993 |

| **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)

| **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 | |

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Particle Breakage

- Particles can break when being processed – usually problem for process
- Breakage processes consume ~2-10% of world's energy
- Spheres can be replaced by a conglomerate of daughter spheres
Latest Dev. & Outlook
Simple Breakage Case
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, \( dt = 1 \times 10^{-5} \) s Fine (right) vs coarse (left)
  (2nd col = position, last col = averaged Temperature)

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