LIGGGHTS OPEN SOURCE DEM:
COUPLING TO DNS OF TURBULENT CHANNEL FLOW

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I. The LIGGGHTS Code

An Introduction

A definition of bulk solids*:

A bulk solid (granular material) consists of many particles (granules) of different sizes (and possibly different chemical compositions, densities, shapes) randomly grouped together to form a bulk. The “nature” of such a material (...) is thus dependent on many factors (...).“

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

* Woodcock, C. R., Mason, J. S. (1987): Bulk Solids Handling: An Introduction To The Practice And Technology, Technology & Engineering.

The Importance of Bulk Solid Handling:

- **More than 50% of all products** sold are either granular in form or involve granular materials in their production.*
- **About 40% of the value added in chemical industry** is linked to particle technology.**
- Despite this importance, the **mechanics** of granular materials is **not well understood at present.*****

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.

*** Campbell, C. S. (2006): Granular Material Flows - An Overview", Powder Technology, 162, 208-229.

Motivation and Background
Examples of Granular Materials

Geomechanics, Construction: Sand, gravel, stone, asphalt

Mining and Mineral Processing, Metals: Coal, Ores of all kinds

Agricultural Machinery: Crops of all kinds, sugar, flour, fruits, wood pellets

Pharmacy: Tablets (pills), powders

Chemical industry: Chemical powders and bulk materials, plastic pellets

Consumer goods: “PEZ”, bonbons, cosmetic powder, detergent, cornflakes,...

Motivation and Background
Discrete Element Method

- DEM manages information about **each individual particle** (mass, velocity, ...) and the forces acting on it.
- Each particle is tracked in **Lagrangian Frame**, the force balance

  $$m_p \ddot{\vec{x}}_p = \sum_i \vec{F}_i$$

  is integrated using an appropriate integration scheme.
- DEM can take into account the particle‘s shape

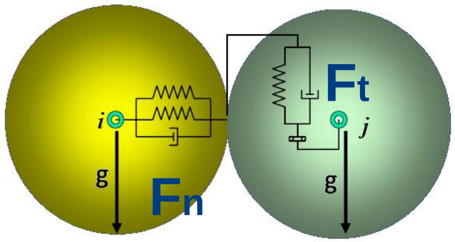
Examples of forces $\vec{F}_i$ that can be included:

- Contact forces (particle-particle, particle-wall)
- Gravity
- Fluid drag force

Motivation and Background
Discrete Element Method

Soft sphere approach (Classical DEM, constant time-stepping)

$$m_p \ddot{\vec{x}}_p = \vec{F}_n + \vec{F}_t + m\vec{g}$$



A simple soft-sphere contact model: Linear spring-dashpot

A **small overlap δ between particles** is allowed

The **normal force** tending to repulse the particles is

$$\vec{F}_n = -k_n \vec{\delta} + c_n \overrightarrow{\Delta v_n}$$

δ: spatial overlap, Δv_n: normal relative velocity at the contact point.

The **tangential force** F_t (representing elastic tangential deformation) can be written as

$$\vec{F}_t = k_t \underbrace{\left| \int_{t_{c,0}}^{t} \Delta v_t(\tau)\, d\tau \right|}_{"\delta_t"} \vec{t} + c_t \overrightarrow{\Delta v_t}\ , \qquad \max\left(\left| \vec{F}_t \right| \right) = \left| \mu \vec{F}_n \right|$$

Δv_t: relative tangential velocity, t: contact point tangential vector

$t_{c,0}$: time when the contact between the particles started

The LIGGGHTS Code
Overview

- **LIGGGHTS = An Open Source, C++, MPI parallel DEM code**
- **LAMMPS IMPROVED FOR GENERAL GRANULAR AND GRANULAR**
- **HEAT TRANSFER SIMULATIONS**
- **WWW.LIGGGHTS.COM | WWW.CFDEM.COM**

- Based on the popular MD code **LAMMPS (Sandia National Labs, USA)**
- **LAMMPS** = **L**arge-Scale **A**tomic/**M**olecular **M**assively **P**arallel **S**imulator
  A **massively parallel, widely used, C++, Open Source MD code**
  More generally, it is a **parallel particle simulator**
- **CFDEM: Coupling to CFD code OpenFOAM®**

The LIGGGHTS Code
The LAMMPS Code

- **LAMMPS** =
  Large-Scale Atomic and Molecular Massively Parallel Simulator

- **OpenSource MD code under GPL**, provided by **Sandia National Laboratories** since the mid 90‘s (http://lammps.sandia.gov/). **Widely used** (over **500 journal publications** 2000-2009 using LAMMPS, http://lammps.sandia.gov/papers.html)

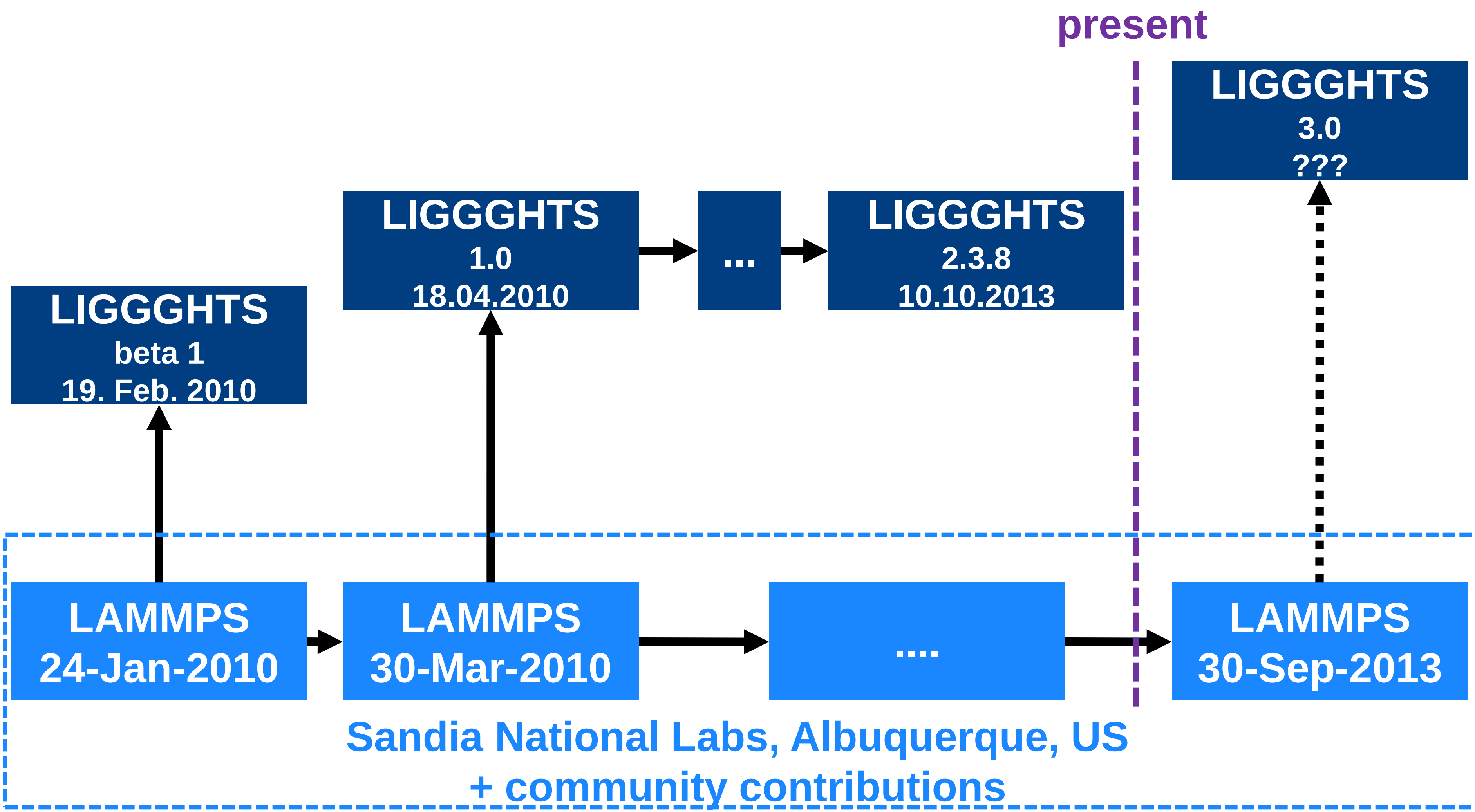
- LAMMPS has potentials for soft materials (biomolecules, polymers), solid-state materials (metals, semiconductors) and **coarse-grained systems**. It can be used to model atoms or, more generically, as a **parallel particle simulator** at the atomic, meso, or continuum scale.

- LAMMPS is a **C++** code, it runs on single processors or in parallel using **message-passing** techniques and a **spatial-decomposition of the simulation domain**.

- It is **fast and efficient** and also used on huge clusters (e.g. on Sandia Red Storm with 16k Quadcore nodes, simulations with billions of particles performed)

- **GPU / CUDA** acceleration packages for NVIDIA hardware

The LIGGGHTS Code
Relation to LAMMPS



II. LIGGGHTS Features and Models

An Overview

The LIGGGHTS Code
Feature Overview

Features added to LAMMPS
Hertz / Hooke pair styles w/ shear history incl. closure contact law to material params
Particle insertion improved
Mesh import from CAD (for walls)
Moving mesh
Multisphere method
Macroscopic cohesion model
Heat transfer model
Particle bonds with torques
Wall stress analysis
6 dof solver
Dynamic Load Balancing

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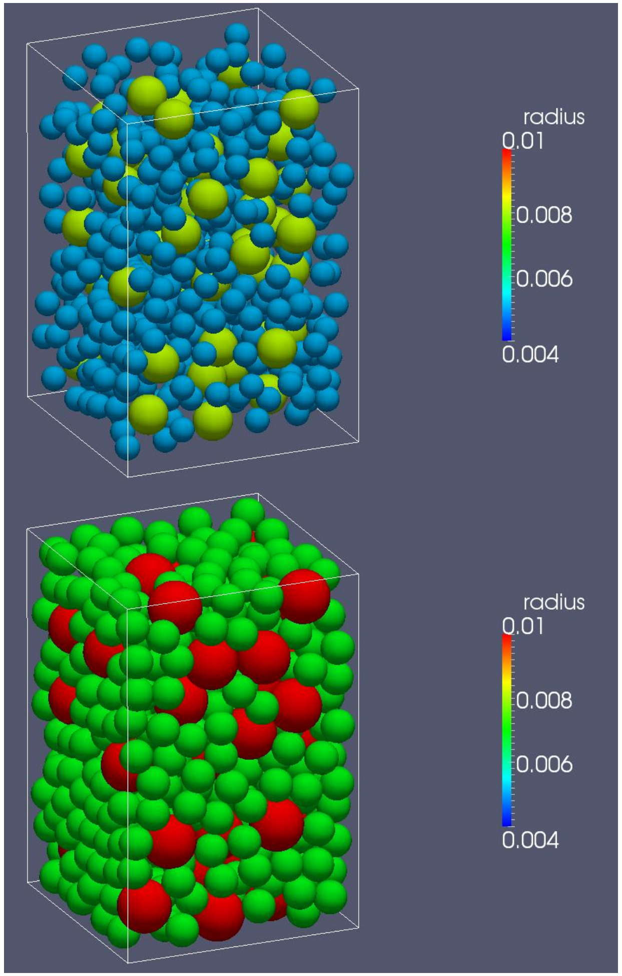

Packing by particle growth

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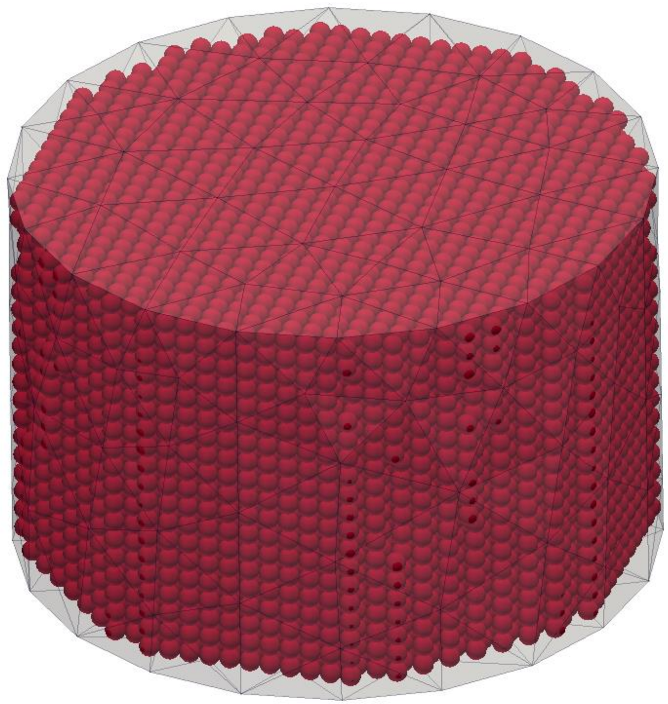

Packing in tetrahedral mesh

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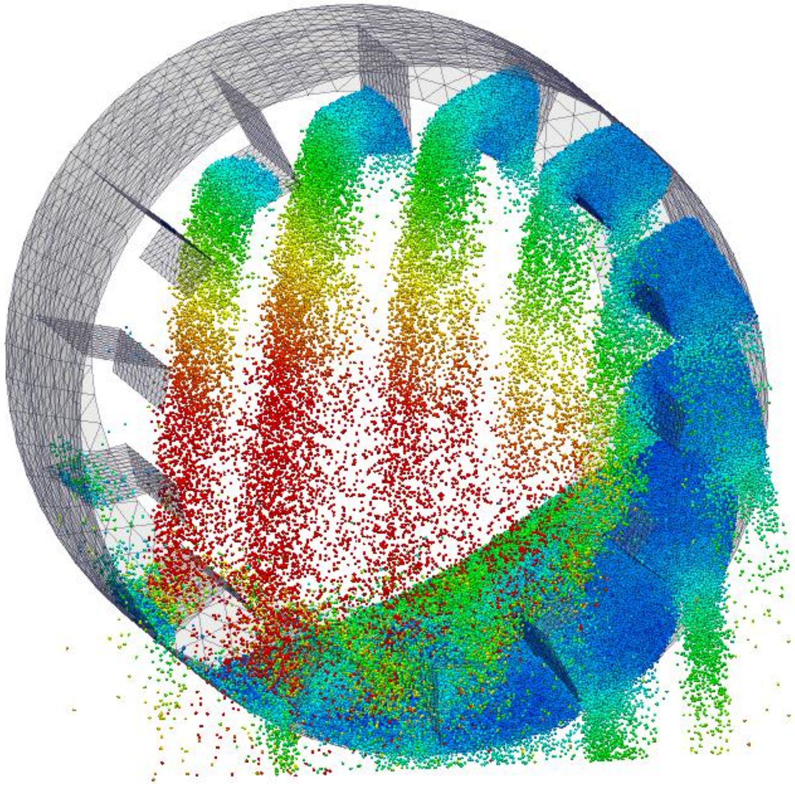

Simulation of a rotary dryer ~1.000.000 particles

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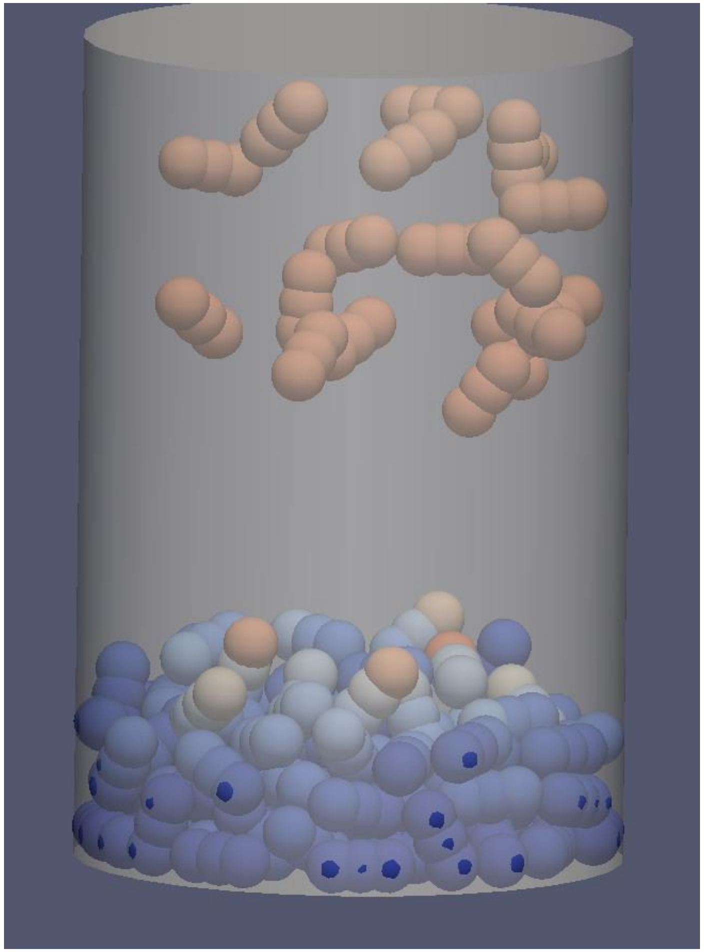

Each body is described by center of mass, mass and inertia tensor.

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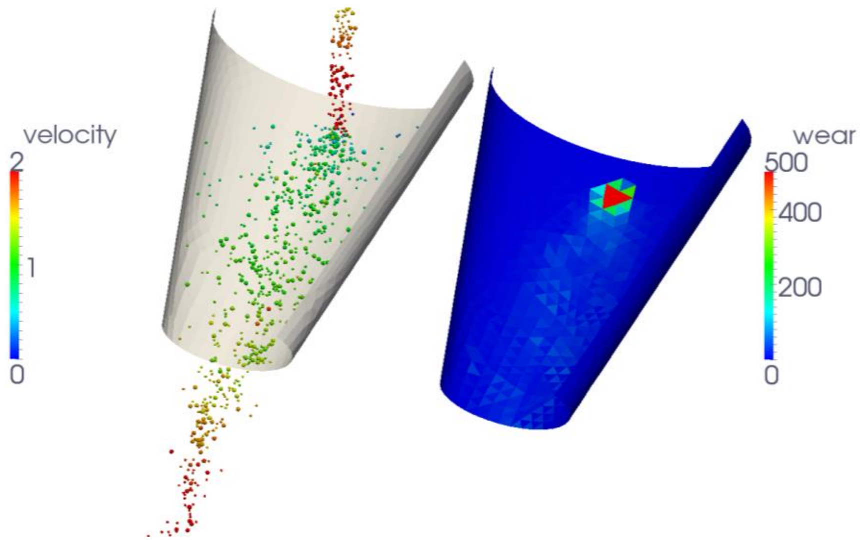

Wear prediction (Finnie model)

The LIGGGHTS Code
Feature Overview

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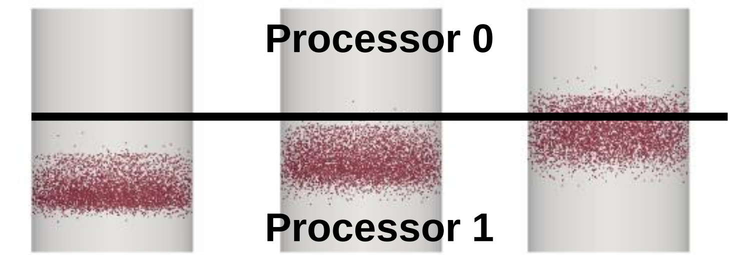
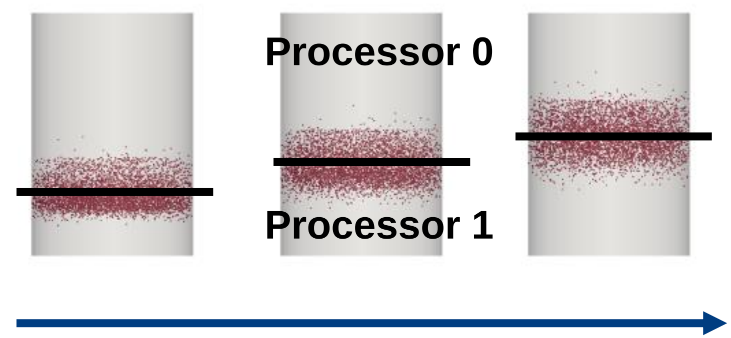
  incl. closure contact law to material params
- **Particle insertion improved**
- **Mesh import from CAD (for walls)**
- **Moving mesh**
- **Multisphere method**
- **Macroscopic cohesion model**
- **Heat transfer model**
- **Particle bonds with torques**
- **Wall stress analysis**
- **6 dof solver**
- **Dynamic Load Balancing**

How to distribute load between processors?

Without dynamic load balancing:



With dynamic load balancing:



advancing simulation time

III. DNS + LIGGGHTS

One-Way Coupling

Establish A One-Way Coupling
Coupling to LIGGGHTS

LIGGGHTS already designed to allow it to be coupled to other codes.

At least 3 ways to handle coupling

- **LIGGGHTS is the driver code** (other code is called during time-stepping)
- **LIGGGHTS and the other code are** on a more **equal** footing (other code is called every few time steps)
- **Use LIGGGHTS as a library** called by another code.

Establish A One-Way Coupling
Tasks (Spherical Particles)

Direct Numerical Simulation gives

- **fluid velocity field** in spectral space (in terms of Fourier/Chebyshev coefficients)

LIGGGHTS

- **read data** from DNS
- **transform data** into velocity field in physical space
- **interpolate data** at particle position using Lagrange polynomials
- **apply Schiller-Naumann drag force to spherical particles***

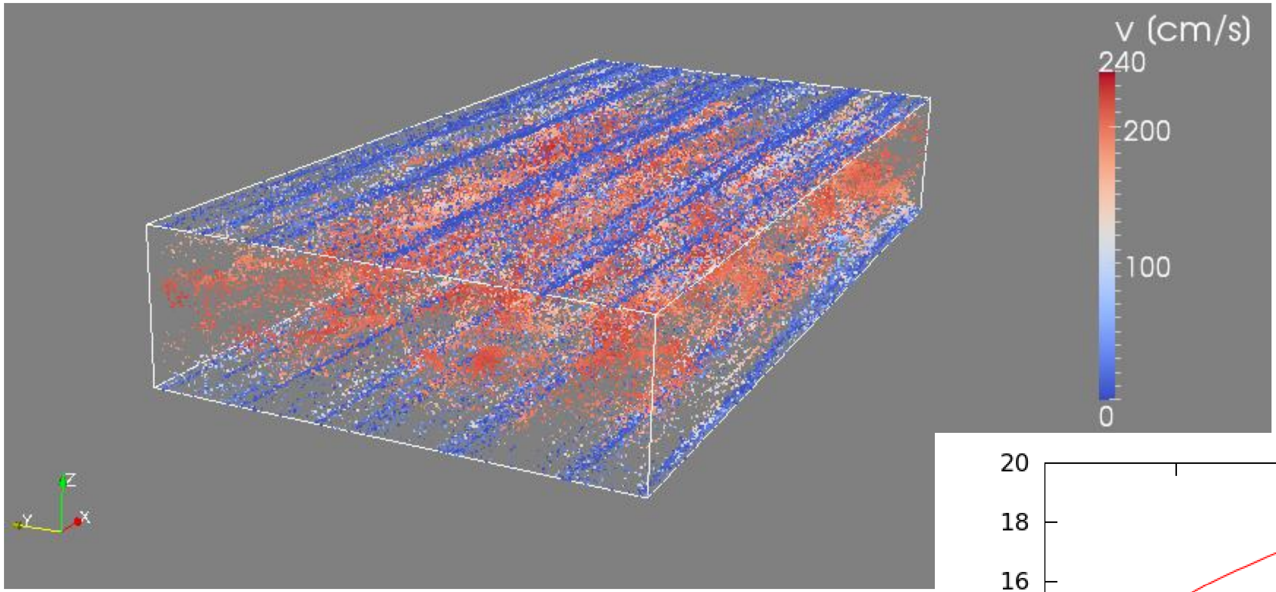
$$\frac{F}{\rho_f U^2 A} = \frac{12}{\mathrm{Re}}\left(1 + 0.15\mathrm{Re}^{0.687}\right) .$$

* L. Schiller and A. Naumann, Fundamental calculations in gravitational processing. Zeitschrift des Vereines Deutscher Ingenieure, 77(12), 318-320 (1933).

Establish A One-Way Coupling
Tasks (Ellipsoidal Particles)

- **modify force** to take into account particle shape
- **apply torque** according to Euler equations

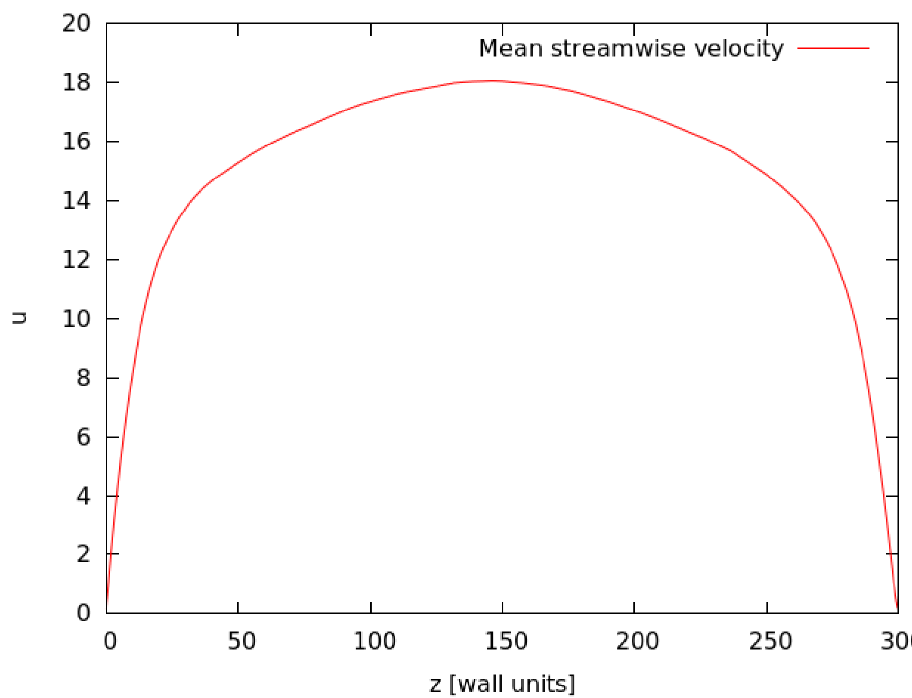
Results
Spherical Particles



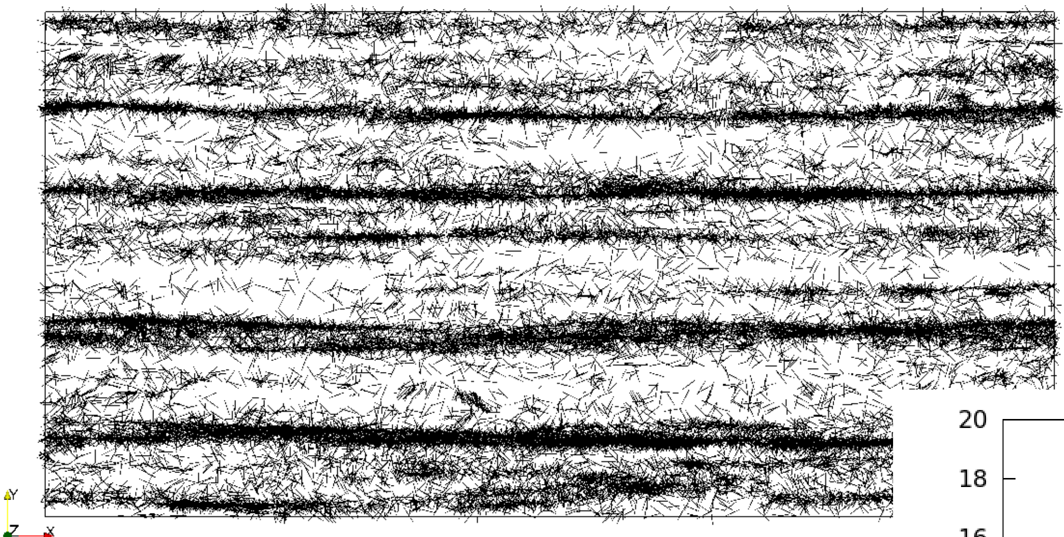
100.000 particles in simulation

6000 DNS output files read

(~1 s of simulated time)



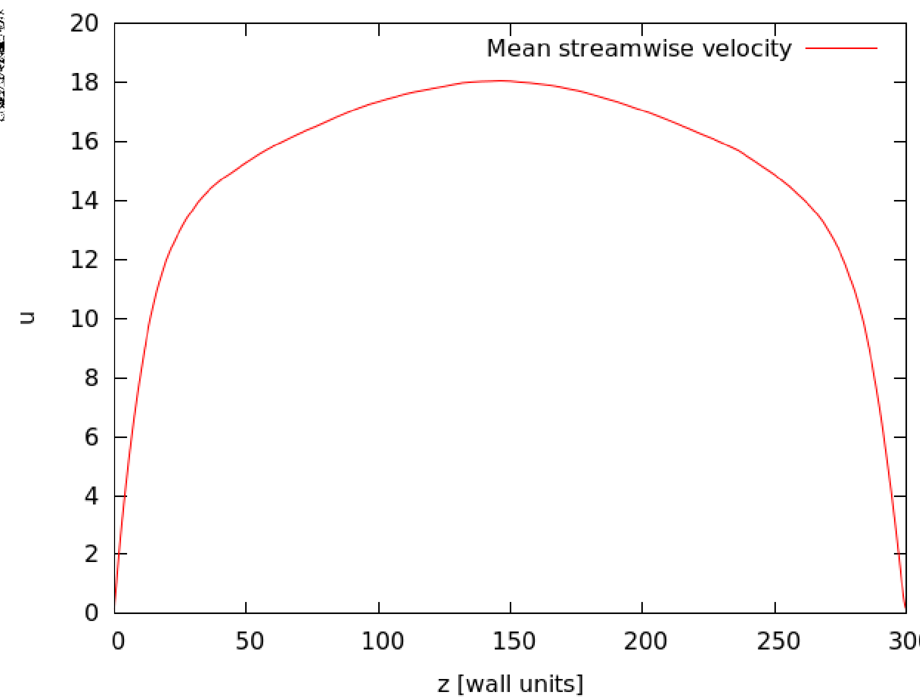
Results
Ellipsoidal Particles



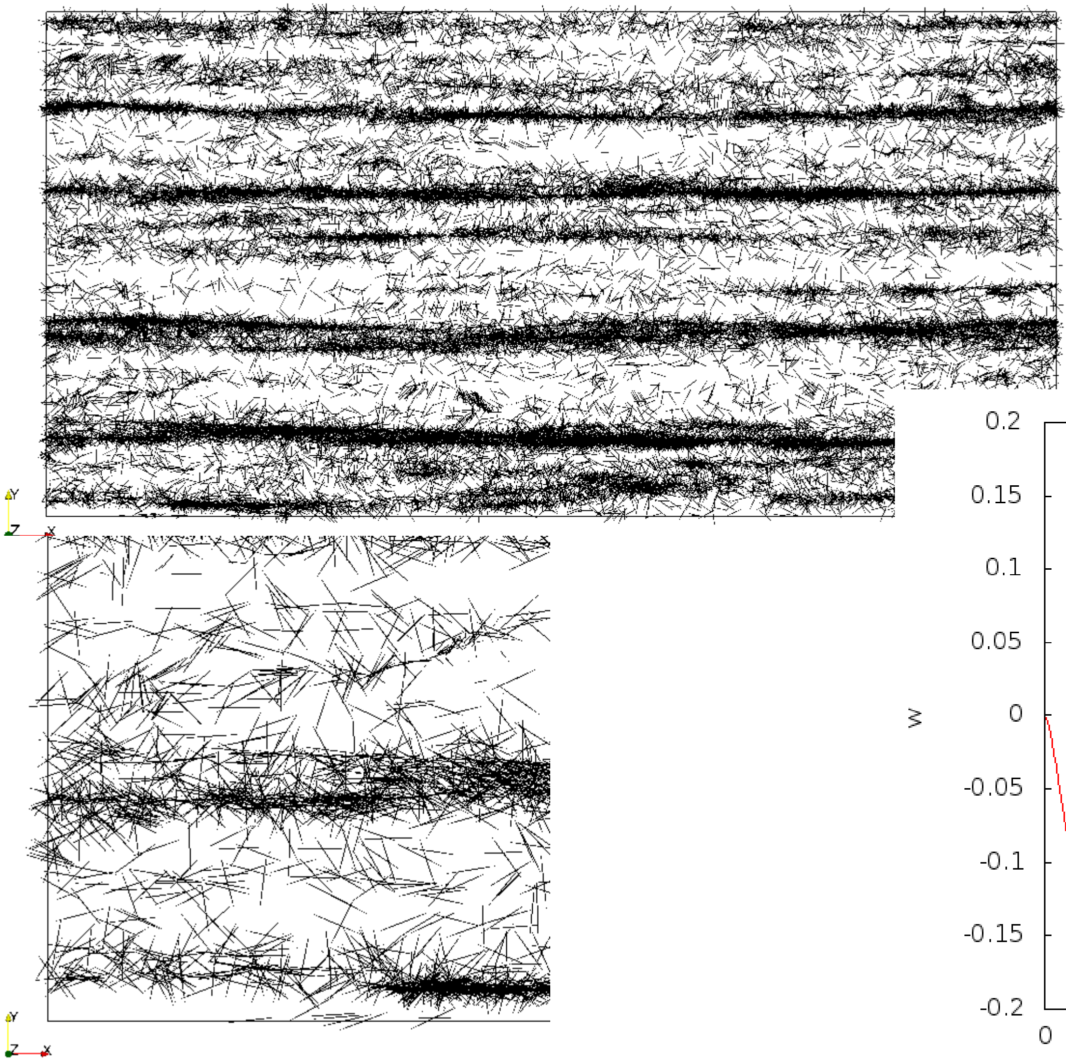
100.000 particles in simulation (b/a = 50)

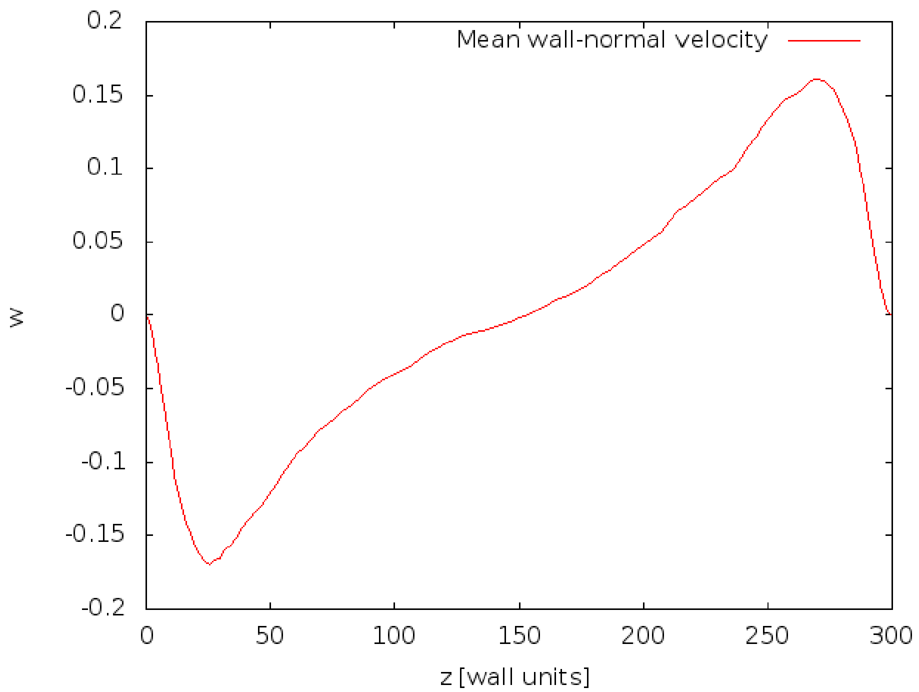
6000 DNS output files read

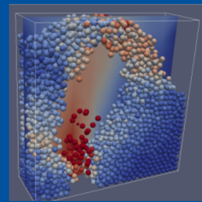
(~1 s of simulated time)



Results
Ellipsoidal Particles







CFDEM project | CFDEM coupling | LIGGGHTS | DCS Computing GmbH

Thank you for your attention!
Questions?

www.cfdem.com | www.particulate-flow.at

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