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Granular Simulations in LAMMPS

New Key Features and Perspectives

LAMMPS User Workshop, February 2010

Christoph Kloss and Christoph Goniva

Christian Doppler Laboratory on Particulate Flow Modelling
Johannes Kepler University Linz
www.cfdem.com (to be launched soon) | **www.particule-flow.at**

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Part I

Our Laboratory

CD – Lab. on Particulate Flow Modelling
Introduction

Founded in 2009 by **Dr. Stefan Pirker** at the **Johannes Kepler University, Linz, Austria.**

Governmental funding (50-70%) for application oriented fundamental research based on existing knowledge on particulate flows at the Institute of Fluid Mechanics and Heat Transfer of the JKU.

Our **research focus** covers:

(a) solids charging,
(b) offgas scrubbing,
(c) industrial dust recycling,
(d) sedimentation & erosion and
(e) trickling beds

Current Industrial partners:

Siemens VAI Metals Technologies,
voestalpine Stahl,
voestalpine Donawitz,
Polysius (ThyssenKrupp group)

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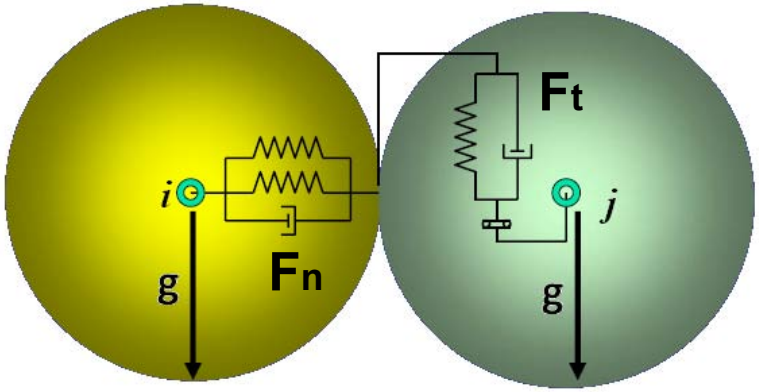
Part II

Simulation of Granular Materials

Principles of MD-Like Granular Material Simulation: DEM (Discrete Element Method)

DEM manages information about each individual particle (mass, velocity,...) and the forces acting on it. Every single particle is tracked in Lagrangian Frame. The force balance is integreated explicitely.

Normally, soft-sphere pair potentails are used where particles are allowed to slightly overlap (<0.5% d). The soft-sphere approach allows for handling equilibrium states.



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

DEM can also take into account the particle's shape, rather than assuming that all particles are spherical.

Principles of DEM

In it's simplest form (**linear spring-dashpot model**), the force balance is

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

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 is 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

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Part III

The Current “Granular” Package in LAMMPS

LAMMPS GRANULAR Package
The Current Implementation

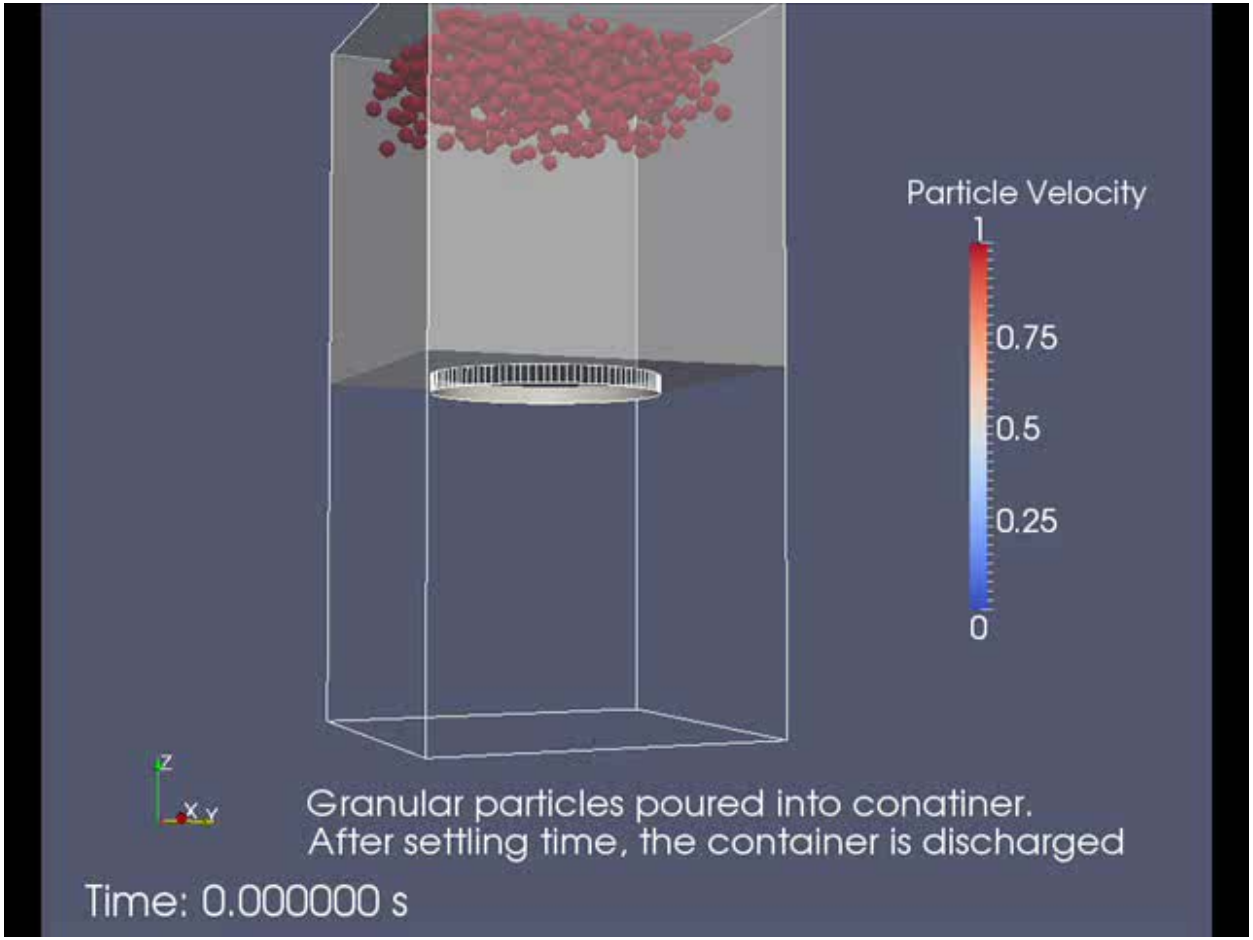
Currently, LAMMPS offers a **fast and efficient "GRANULAR" package** .

The **key functionalities** of this package are

- Pair Styles for Hooke and Hertz contact laws [e.g. pair gran/hooke]
- Shear history for pair style (Integral term on slide #6) [e.g. pair gran/hooke/history]
- Granular walls (Hooke and Hertz) for geometric primitives (box, cylinder) [fix wall/gran]
- A function to pour a stream of material into a geometrical region [fix rigid]
- Fixes to introduce gravity [fix gravity], freeze particles [fix freeze] and exert Stokes drag [fix viscous]
- The [fix rigid] command allows multibody dynamics
- With pair style "hybrid/overlay", other LAMMPS functionalities can be added (e.g. adding bonds, point charges, dipole moments,...)

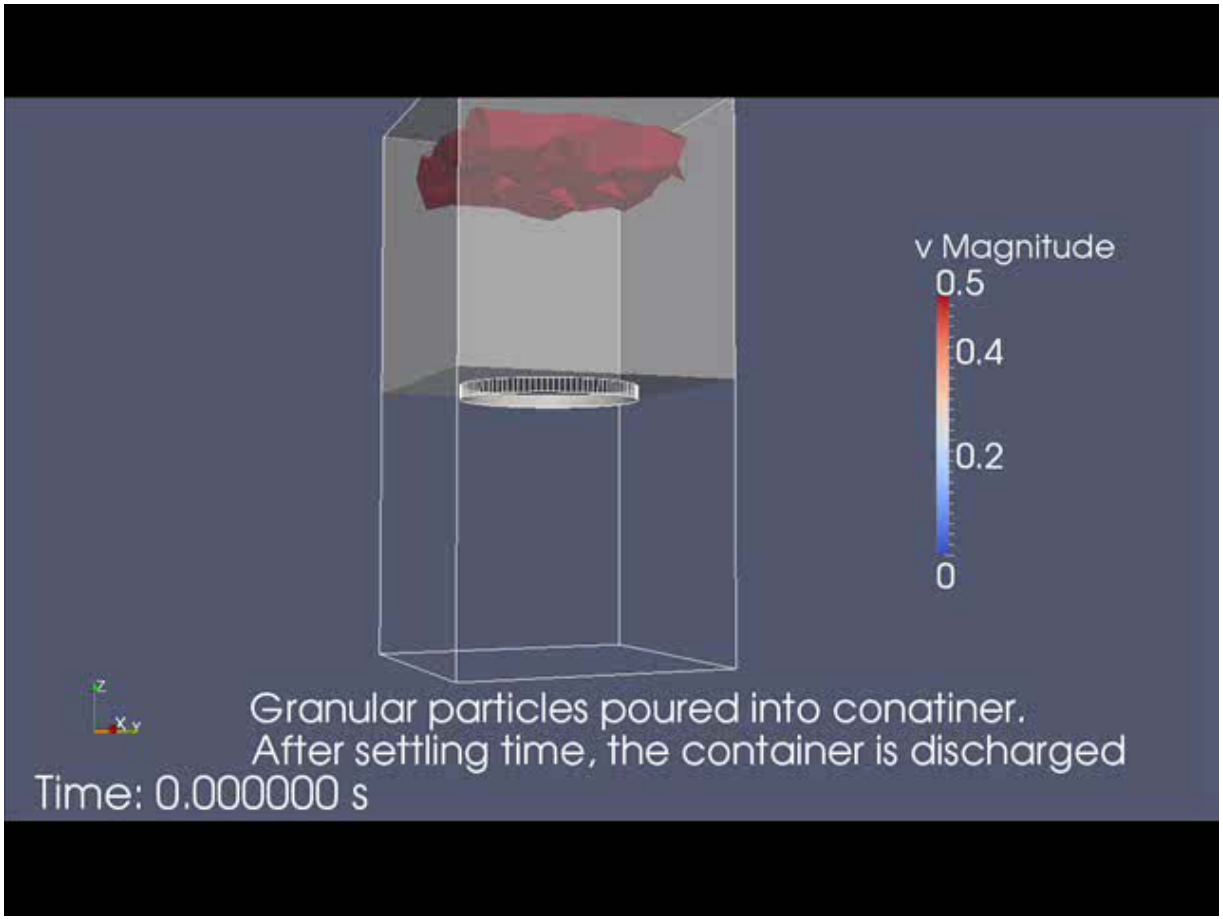
Current LAMMPS GRANULAR Package
Application Examples

Hopper Discharge



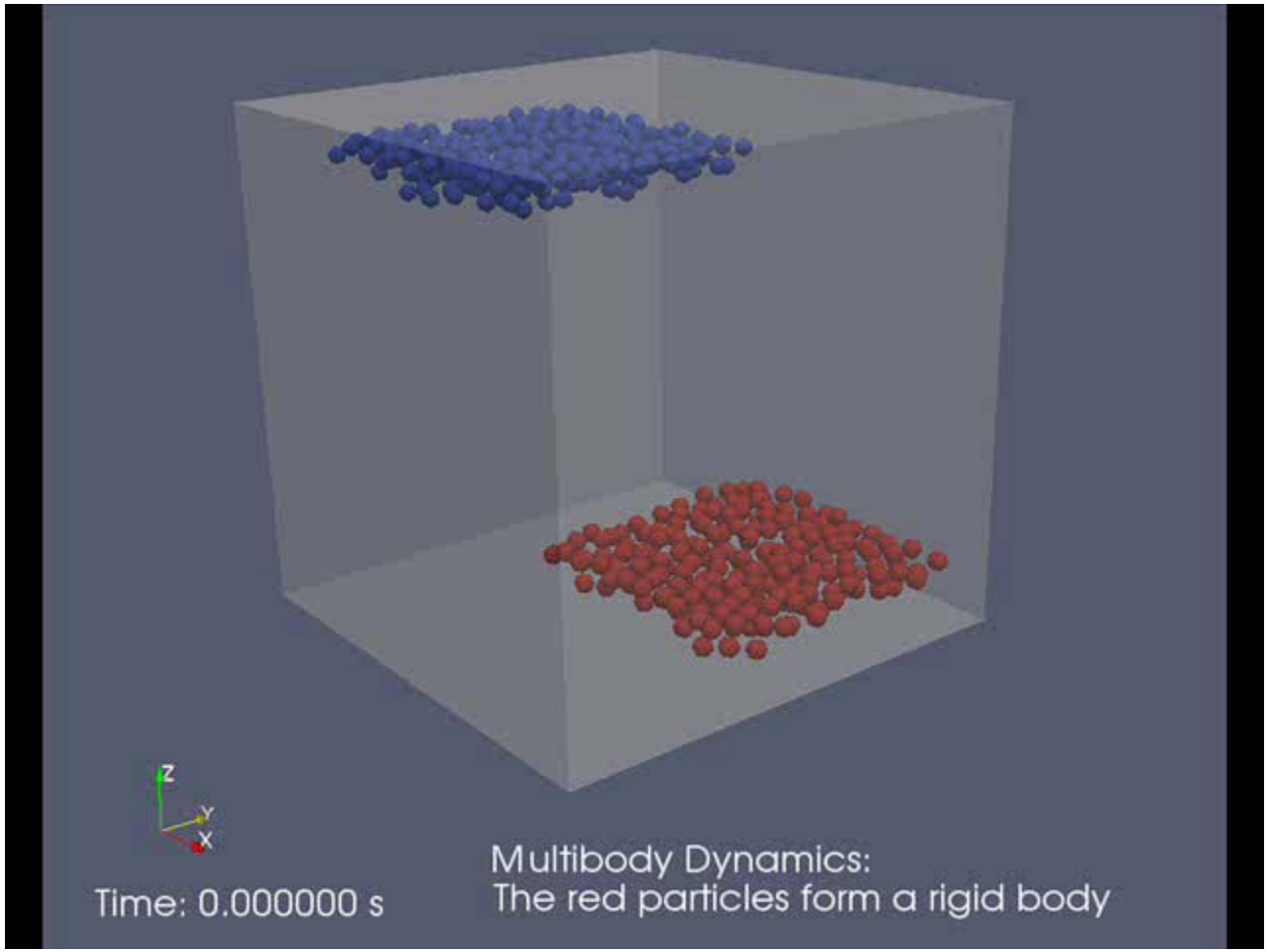
Current LAMMPS GRANULAR Package
Application Examples

Hopper Discharge (with Delaunay triangulation)



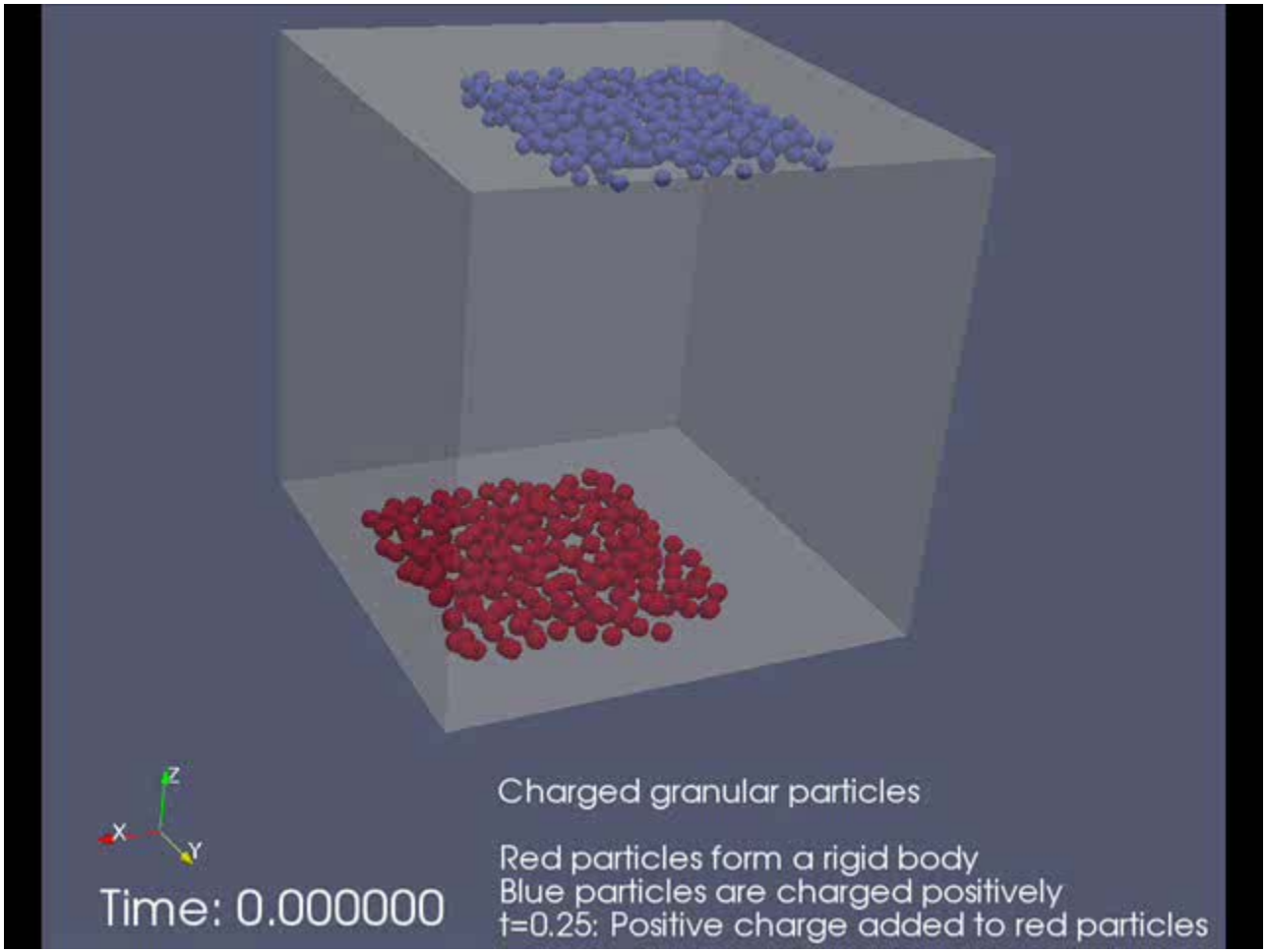
Current LAMMPS GRANULAR Package
Application Examples

Multibody Dynamics with fix rigid



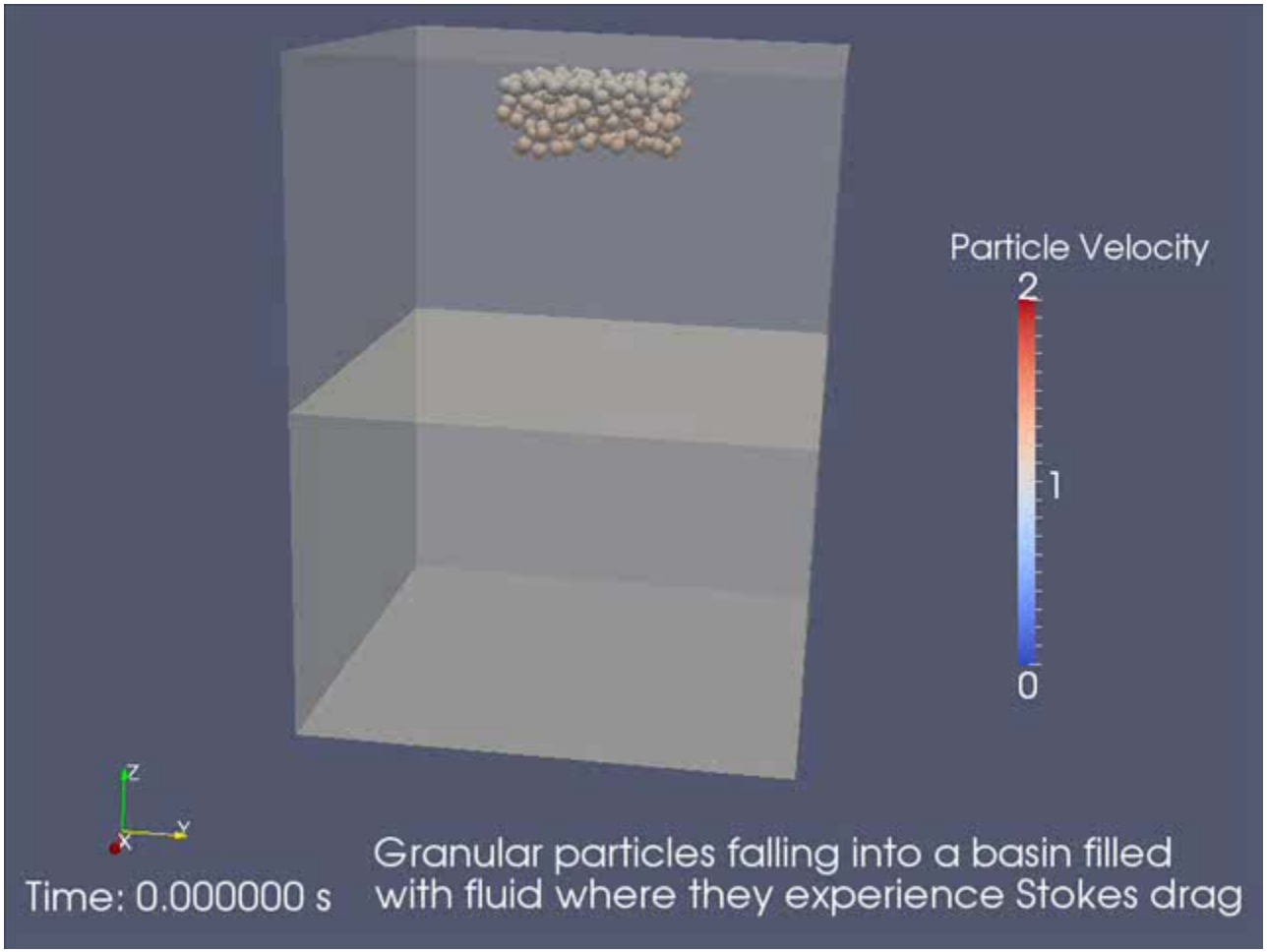
Current LAMMPS GRANULAR Package
Application Examples

Multibody Dynamics coupled with electrostatics



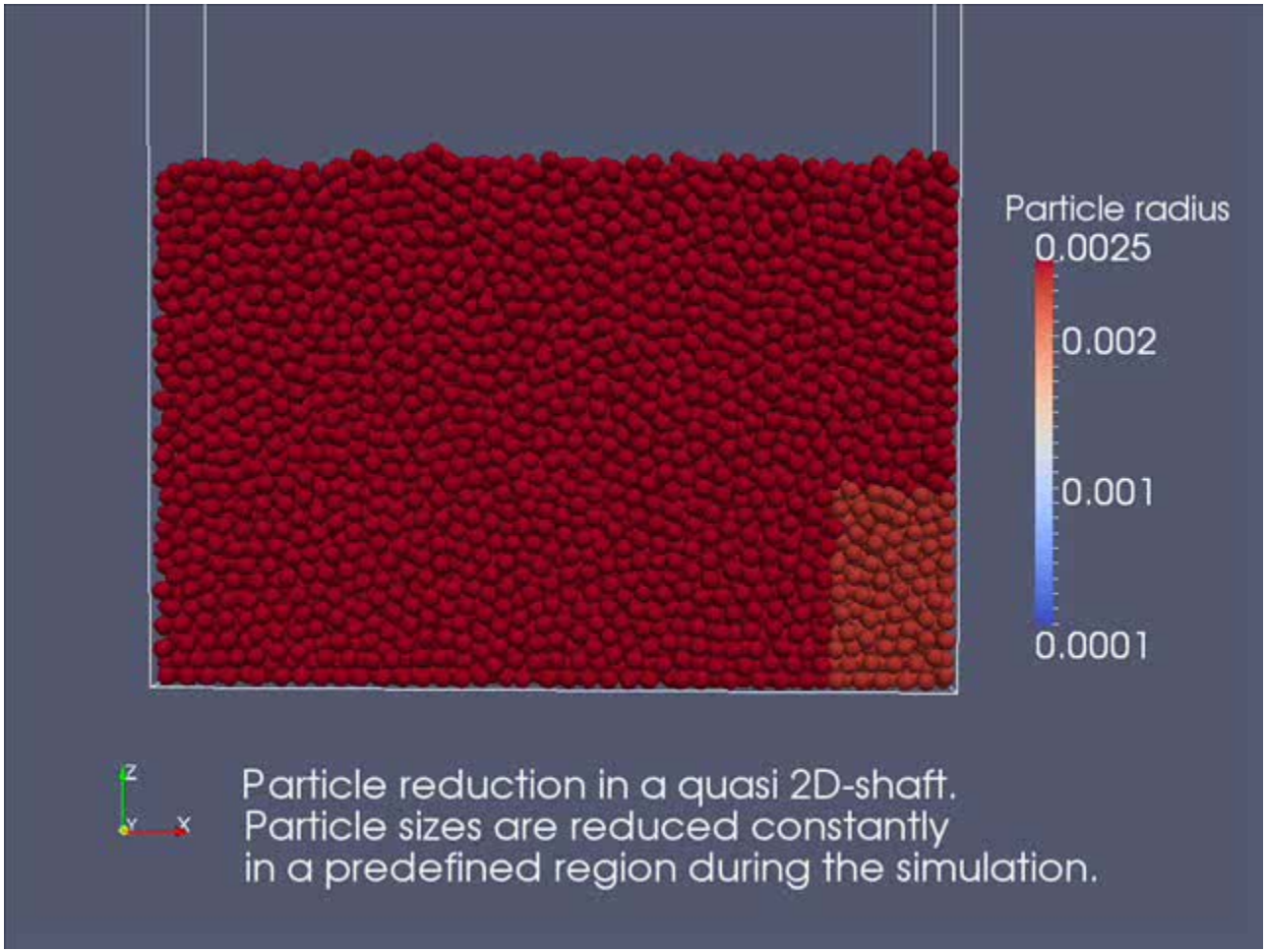
Current LAMMPS GRANULAR Package
Application Examples

Particles with Stokes drag



Current LAMMPS GRANULAR Package
Application Examples

Particles size reduction (e.g. due to chemical reaction)



LAMMPS GRANULAR Package
Why need a better package?

The following **functionalities** are readily available in commercial DEM software, but missing in LAMMPS.

Category I:
Missing of these features is a killing criterion for most industrial applications

- Import of complex geometry from CAD
- Connection of pair style parameters (stiffness, damping) to material properties that can be identified/derived from experiments (density, Young's modulus, coefficient of restitution)

LAMMPS GRANULAR Package
Why need a better package?

The following **functionalities** are readily available in commercial DEM software, but missing in LAMMPS.

Category II:

These features are not essential, but a good DEM code should have them

- Moving mesh capability for complex walls
- Ability to pour a continuous stream of granular particle clumps
- A macroscopic model for cohesion of granular particles
- Heat transfer model for granular particles
- Particle bonds (that can also take torque)
- For an Open Source code, it would be nice to enable a C++ novice to implement a new granular pair style by changing just a few lines of code

LAMMPS GRANULAR Package
Why take LAMMPS?

There are other Open Source DEM codes available (Esys, YADE) that have already implemented most or all of these features. Why not take them?

The strengths of LAMMPS

- LAMMPS is easy to use (good scripting language)
- LAMMPS source code is easy to read, understand and modify
- The LAMMPS documentation is good
- LAMMPS has a large user community
- LAMMPS is fast and has a scope for massively parallel computing
- GPU acceleration efforts are underway right now
- LAMMPS offers a great MPI coupling interface

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Part IV

A New “GRANULAR” Package For LAMMPS

An New Granular Package for LAMMPS
Scope

The following challenges have been tackled:

Category I Challenges:

Challenge	Tackled
Complex wall import	Yes
Better calculation of pair style parameters	Yes

An New Granular Package for LAMMPS
Scope

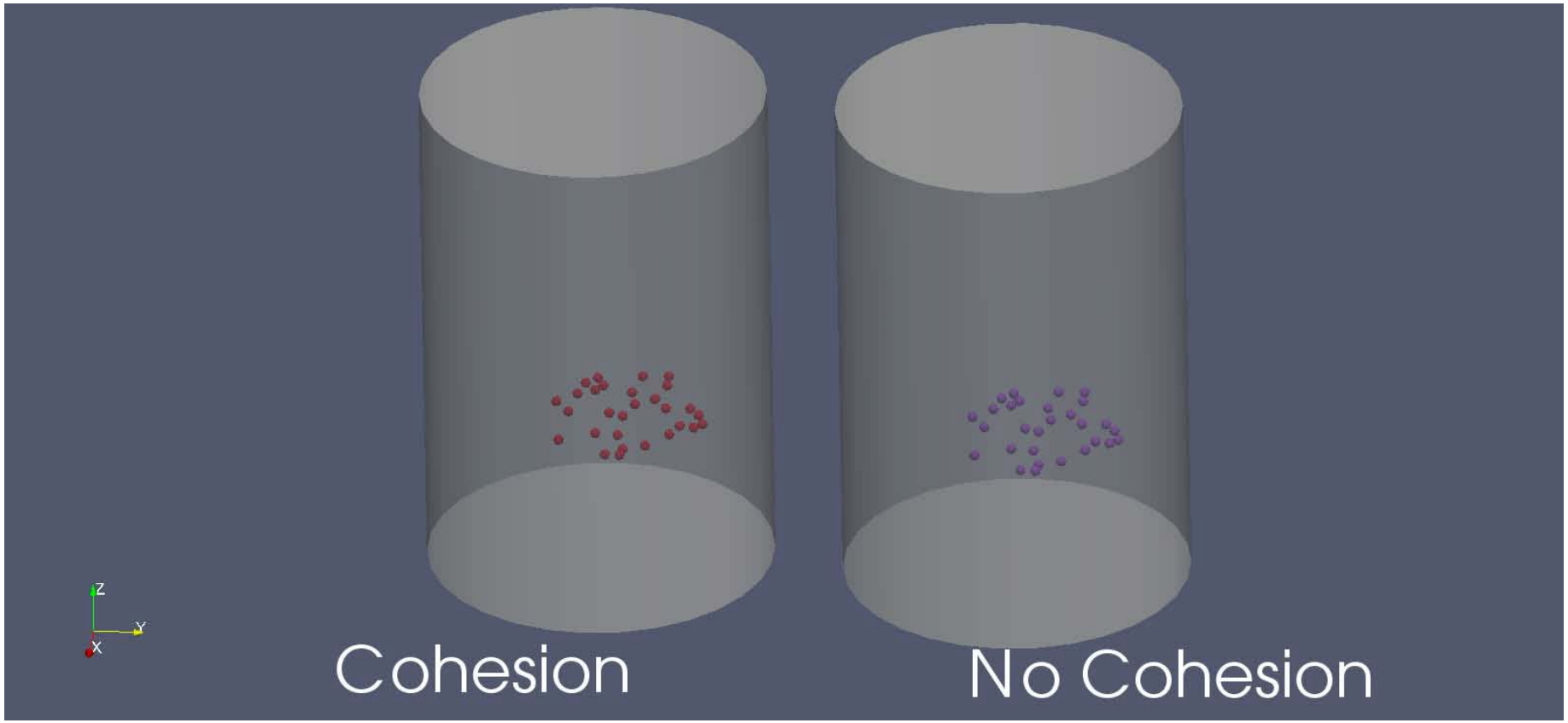
The following challenges have been tackled:

Category II Challenges:

Challenge	Tackled
Moving mesh	**Yes** (yet serial)
Pour nonspherical clumps	**Not yet**
Macroscopic cohesion model	**Yes**
Heat transfer model	**Yes** (simple model)
Particle bonds with torques	**Not yet**

New LAMMPS GRANULAR Package
Application Examples

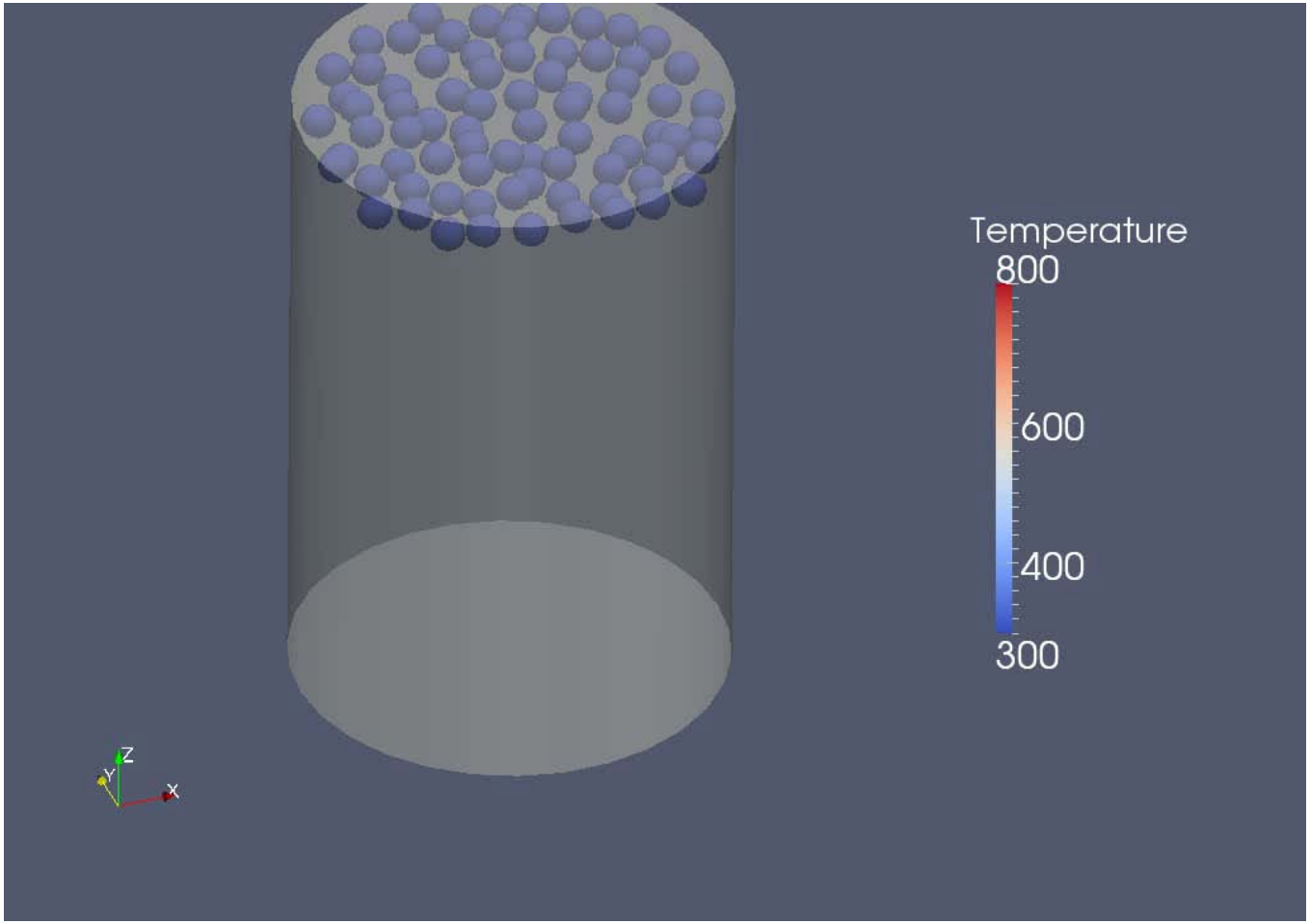
Cohesion Model



New LAMMPS GRANULAR Package
Application Examples

Heat Conduction Model:

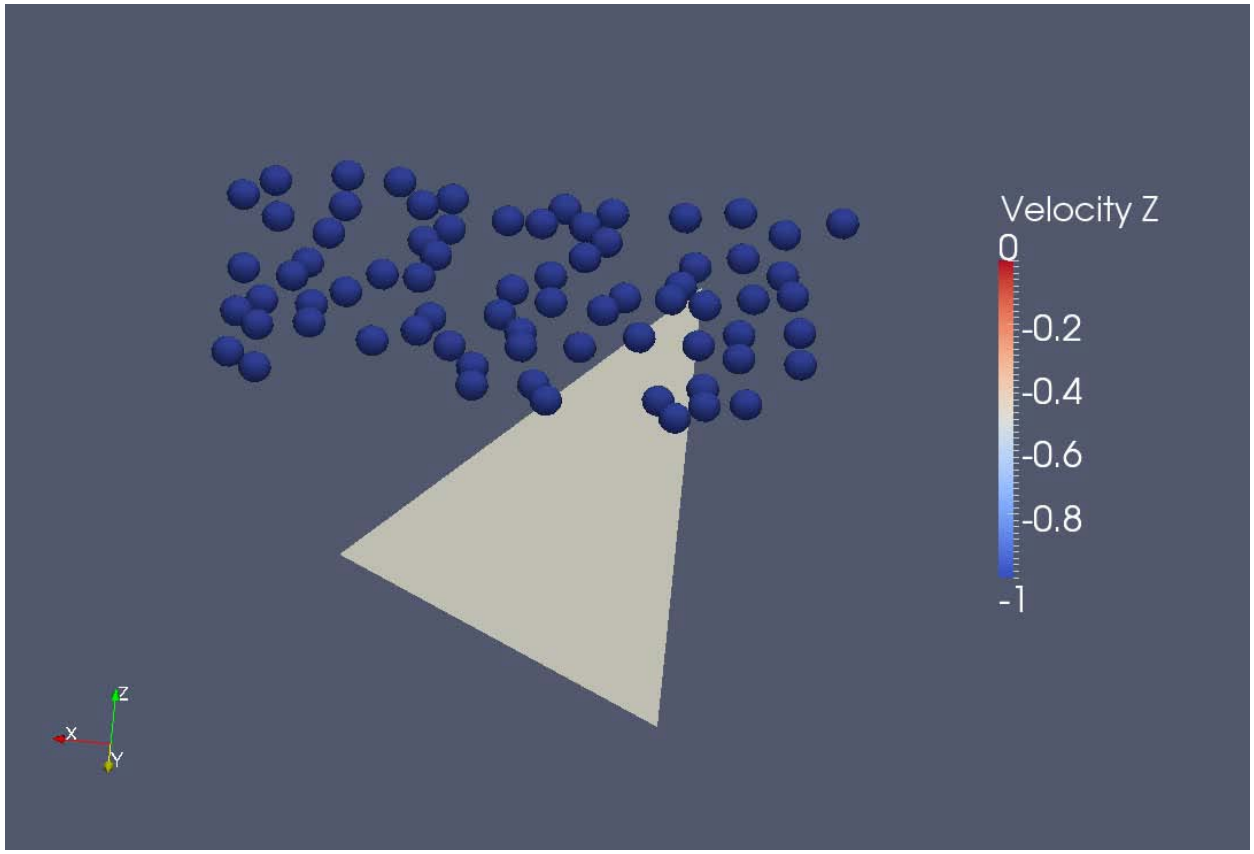
After filling, particle temperature is set. It subsequently levels over time



New LAMMPS GRANULAR Package
Application Examples

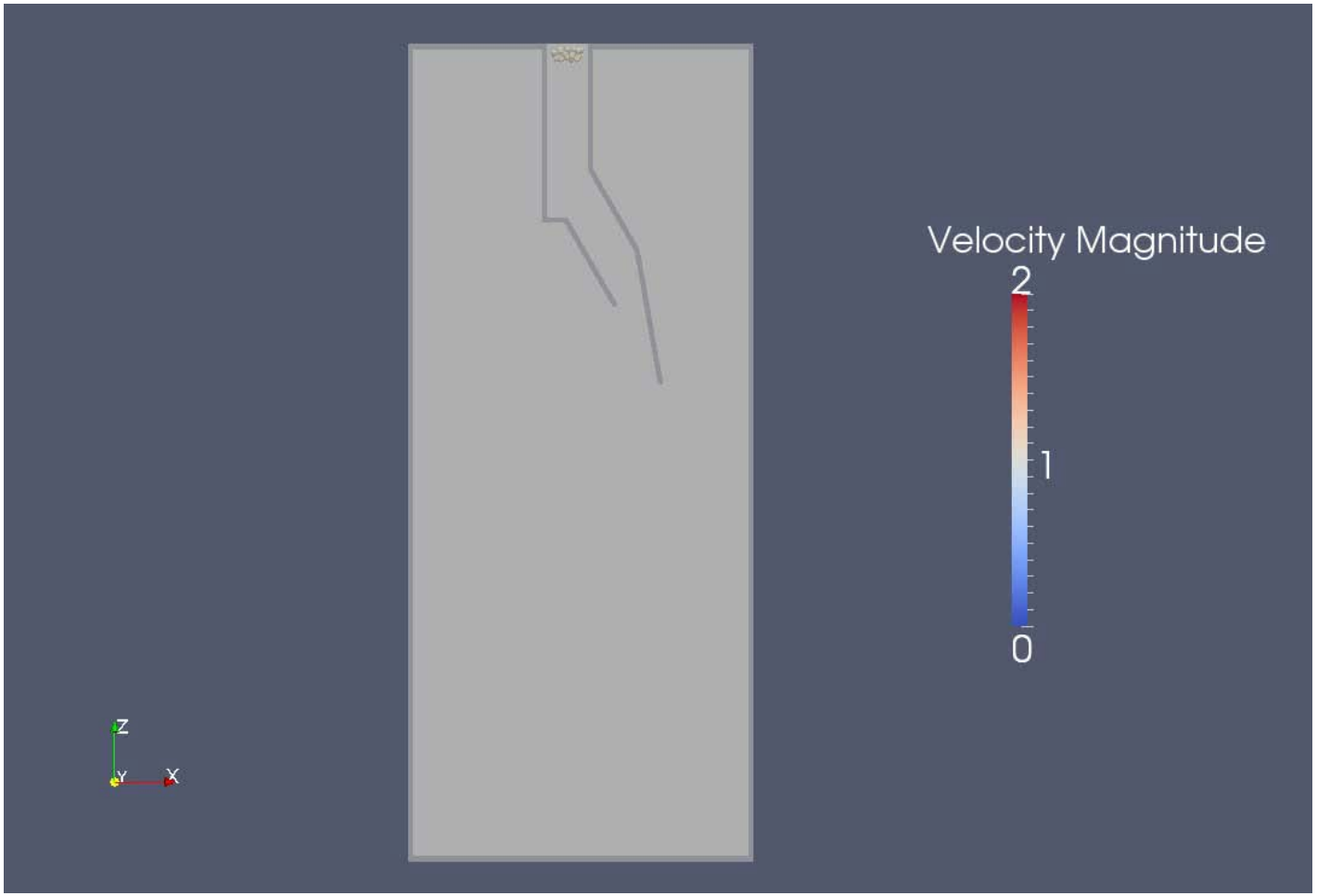
Granular potential for triangle-sphere interaction:

Reference: “A method for representing boundaries in discrete element modelling - part I: Geometry and contact detection”, International Journal for Numerical Methods in Engineering, Volume 51 Issue 12, Pages 1407 - 1421



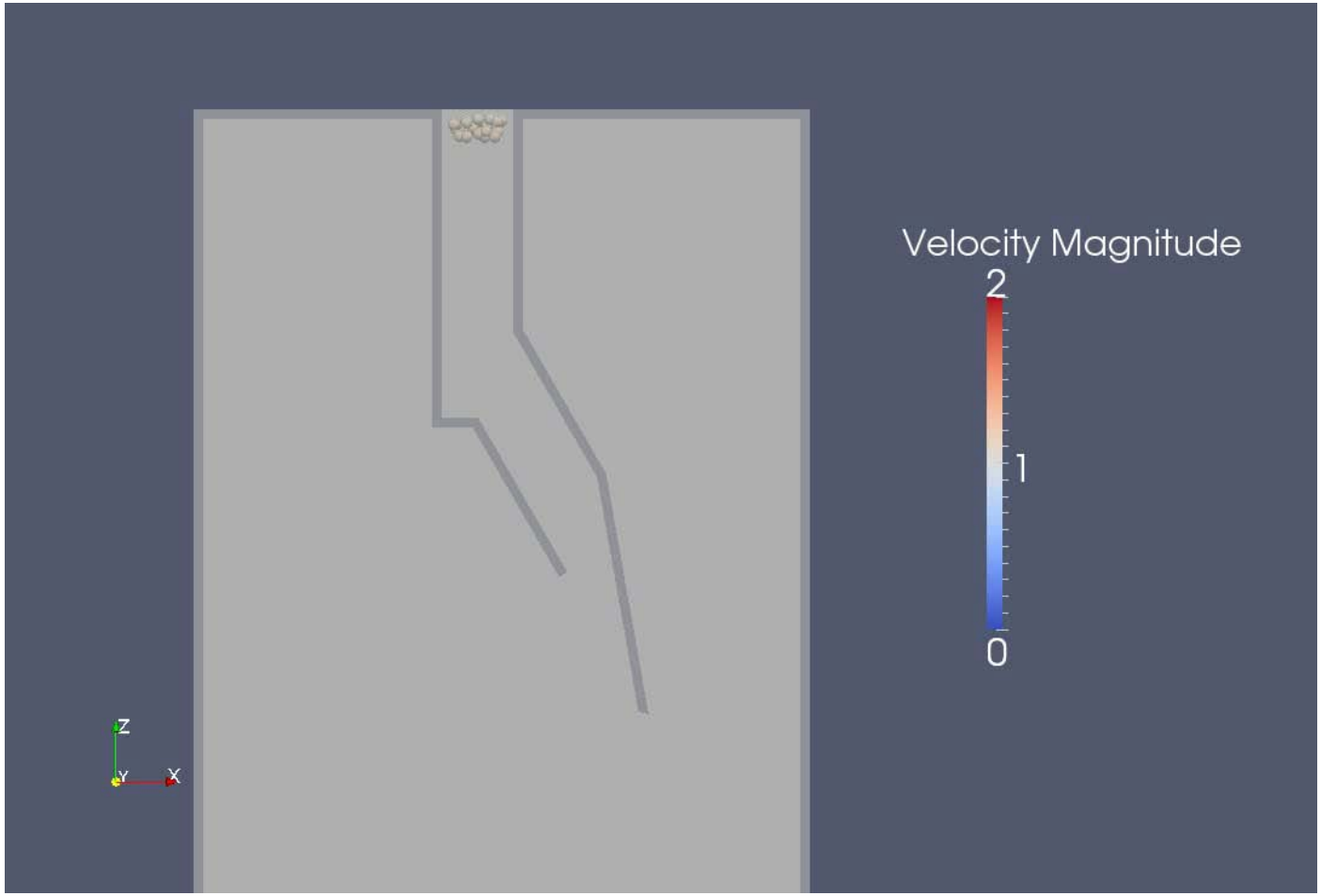
New LAMMPS GRANULAR Package
Application Examples

Import of complex wall geometry from CAD STL files



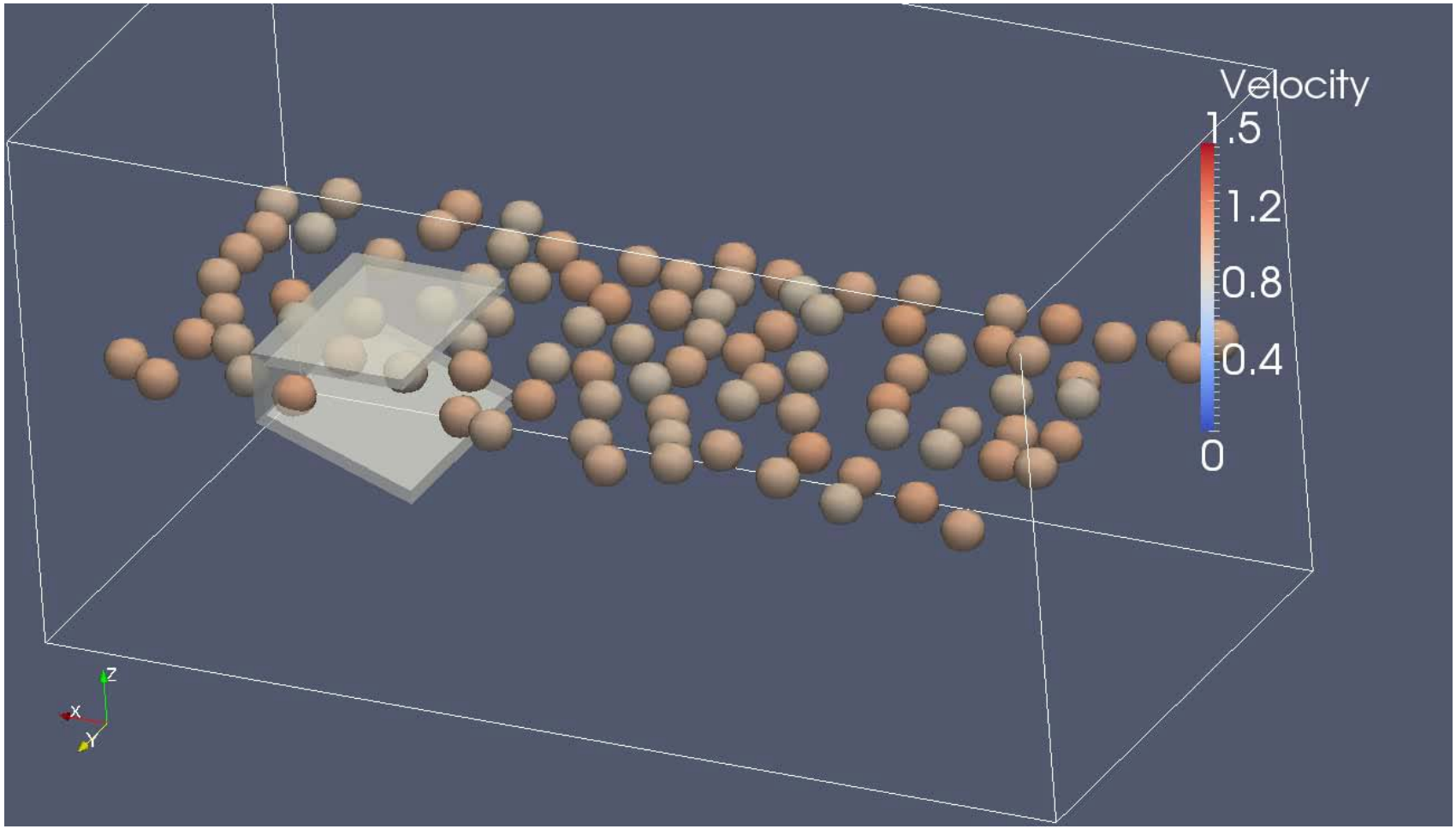
New LAMMPS GRANULAR Package
Application Examples

Import of complex wall geometry from CAD STL files



New LAMMPS GRANULAR Package
Application Examples

Moving mesh feature for complex walls



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Part V

Future Perspective – Coupling With CFD
The Project “CFDEM”

An Open-Source CFD – DEM Perspective
Motivation

***Many* applications require coupled CFD-DEM simulations !**

Unfortunately, the CFD-DEM Approach is **CPU intensive** …

An **efficient CFD-DEM solver is on need**

- Fast solver (both CFD and DEM)
- Efficient parallelisation
- Low license fees
- Open access to source code
- GPU acceleration for DEM is desirable to handle industrial scale processes

OpenFoam is already established as leading Open Source CFD toolbox...

For DEM, LAMMPS is ideal because it is parallel, efficent, and easy to use.

An Open-Source CFD – DEM Perspective
Motivation

CFD-DEM simulations are and will be a key focus at our Lab:

KLOSS, C. (2010): “LAMMPS - An Open Source DEM Code”, Invited Lecture at Delft University of Technology, scheduled for March 15

KLOSS, C., AICHINGER, G. and PIRKER, S. (2010):
"COMPREHENSIVE MULTI-SCALE DEM-DPM-CFD SIMULATIONS - MODEL SYNTHESIS, EXPERIMENTAL VALIDATION AND SCALABILITY”, Int. J. Multiscale Com. Eng., Invited for publication

KLOSS, C. (2010): “Making DEM-CFD simulations feasible by switching to Discrete Phase Model (DPM) in dilute regions – model synthesis and validation”, Proceedings of the WCPT6, Nürnberg, April, Accepted for publication

KLOSS, C. (2009): “Coupling of DEM and CFD - Simulation and Experiment”, Invited Lecture at the DANSIS Meeting on DEM, Kopenhagen, March 25

GONIVA, C., KLOSS, C., and PIRKER, S. (2009):
“Towards fast parallel CFD-DEM: An Open-Source Perspective”, Proc. Open Source CFD International Conference, Barcelona, November 12-13.

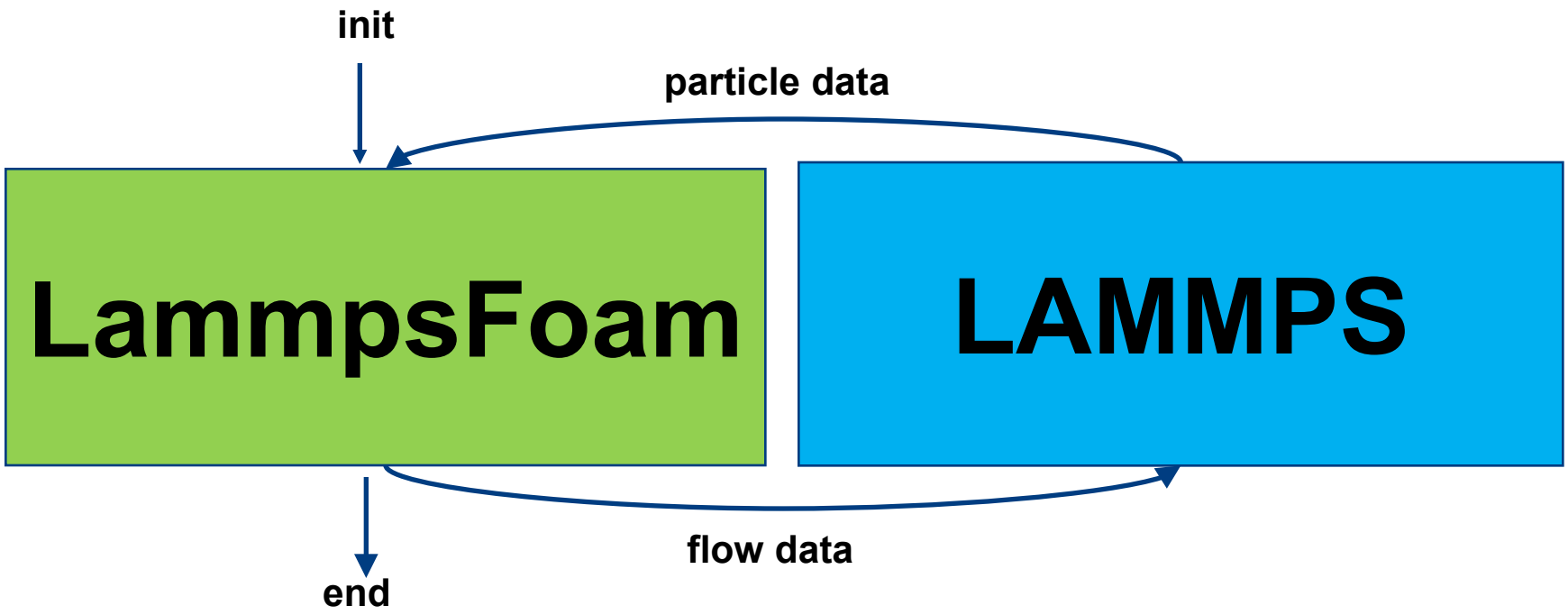
KLOSS, C., GONIVA, C., AICHINGER, G. and PIRKER, S. (2009a):
“Comprehensive DEM-DPM-CFD simulations: Model synthesis, experimental validation and scalability”, Proc. Seventh International Conference on CFD in the Minerals and Process Industries, CSIRO, Melbourne, December 9-11

KLOSS, C., HERRAN-ONTOSO, L., AICHINGER, G. and PIRKER, S. (2009b):
“Accelerating Coupled DEM-CFD Simulations”, Proc. of the International Conference on Particle-Based Methods, CSIRO, Melbourne, November 25-27

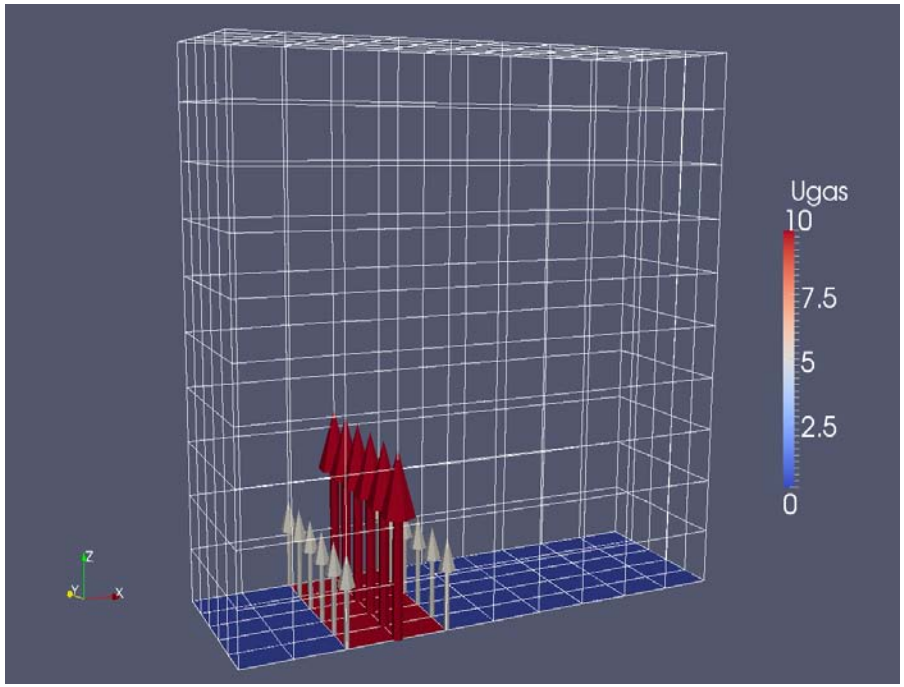
KLOSS, C., AICHINGER, G. and PIRKER, S. (2009c):
"Multiscale Modelling of Particle Motion by Means of DEM and DPM", Proc. of the symposium on Multi-scale Modelling for Industrial Flow Systems, CSIRO, Melbourne, Dec. 8-9

An Open-Source CFD – DEM Perspective
„LammpsFoam“

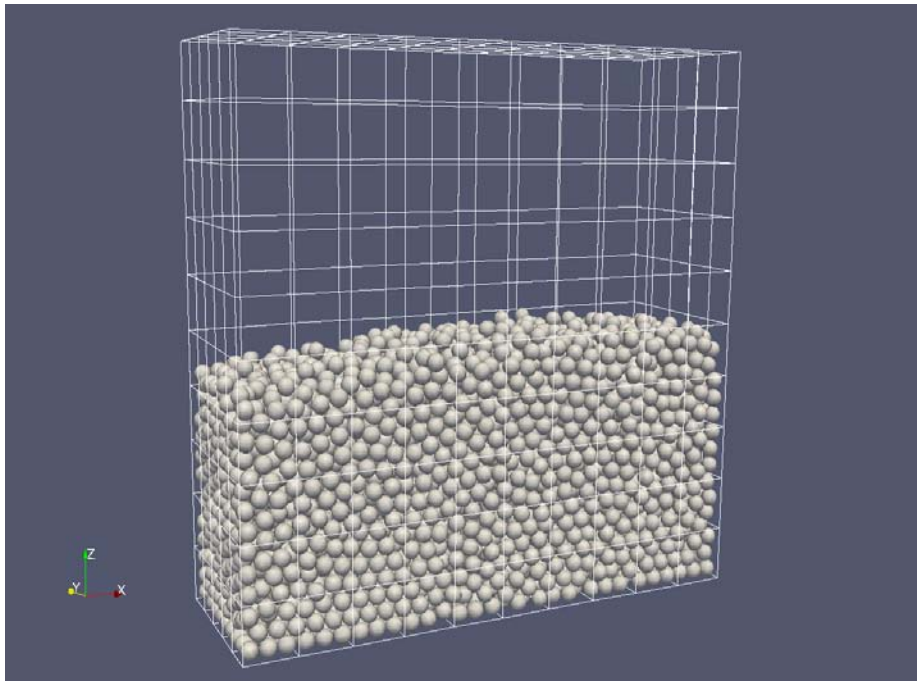
A first version of a **fully MPI parallel coupled CFD-DEM** solver has been developed in 2009 based on LAMMPS and OpenFoam(R)



An Open-Source CFD – DEM Perspective
Partly Fluidized Bed with „LammpsFoam“



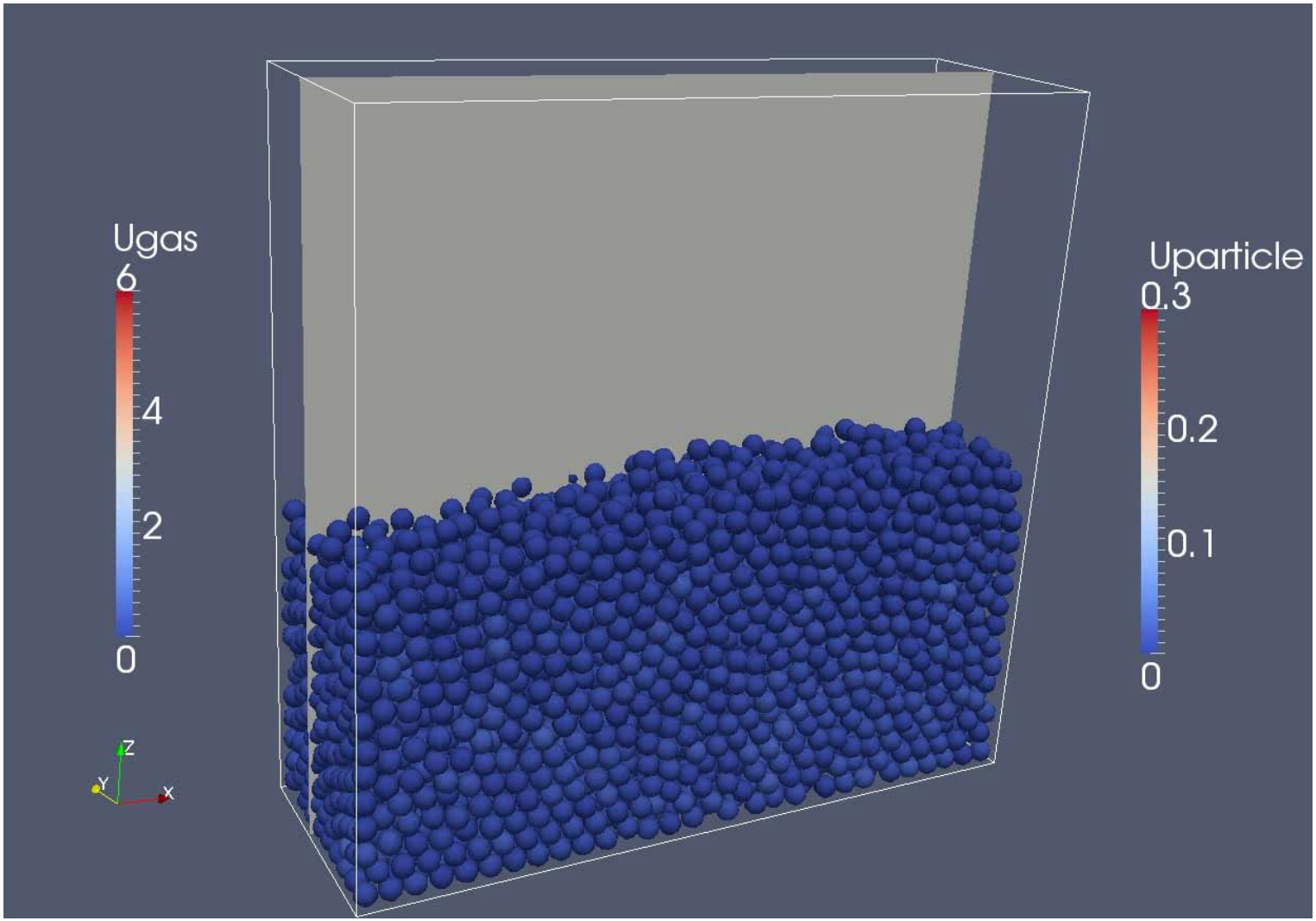
Fluid boundary conditions



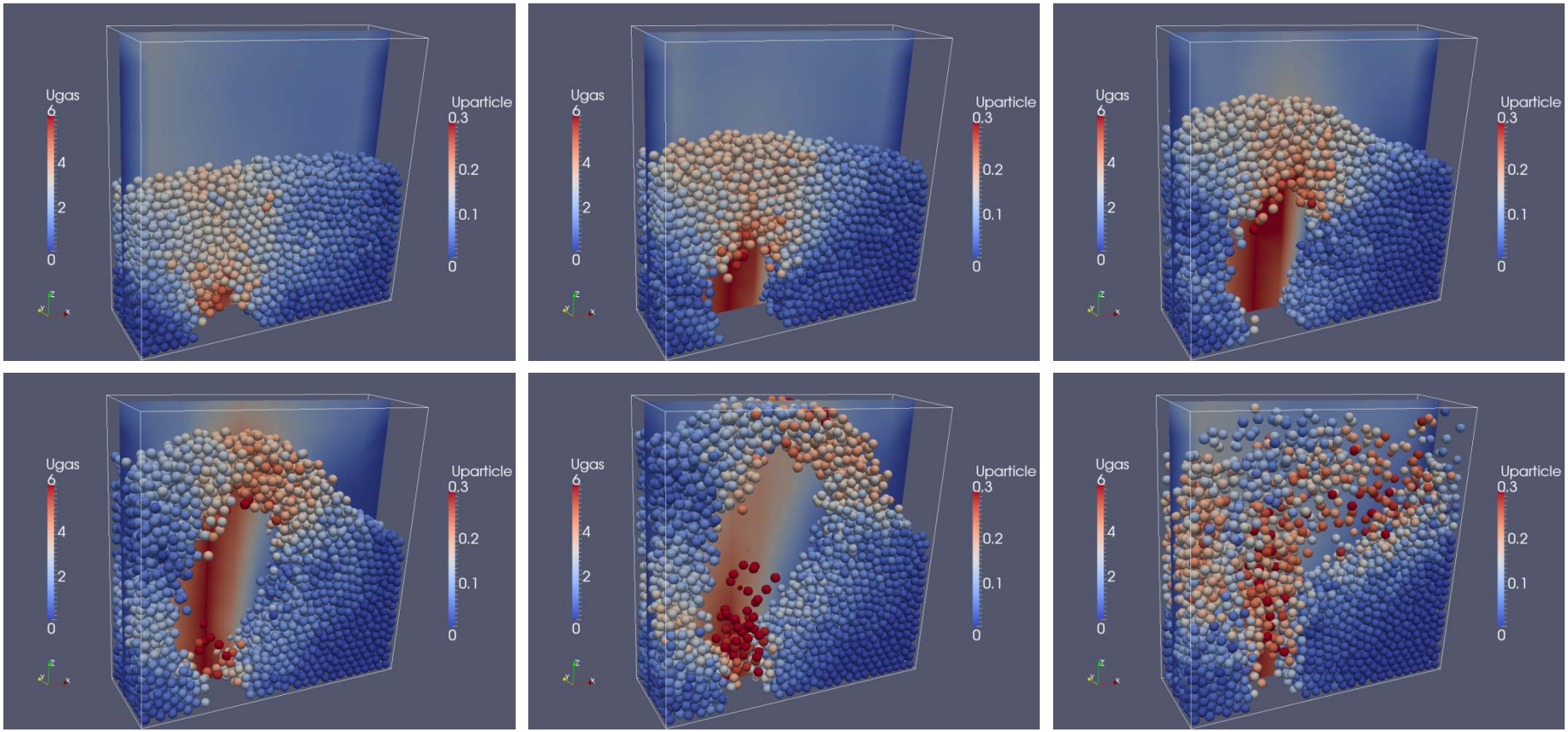
Inital particle packing

An Open-Source CFD – DEM Perspective

Partly Fluidized Bed with „LammpsFoam“



An Open-Source CFD – DEM Perspective
Fluidized Bed with „LammpsFoam“



Further work on DEM with LAMMPS and LammpsFoam in 2010...

An Open-Source CFD – DEM Perspective
LAMMPS - Open Source DEM

- Website dedicated to
  Open Source CFD and Open Source DEM with LAMMPS
  www.cfdem.com

- **Website should start by end of march, containing documentation, forums, and downloads**

- **Features shall then be released as a new branch, called LIGGGHTS – LAMMPS Improved for General Granular and Granular Heat Transfer Simulations**

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Thank you for your attention

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