XDEM: Extended Discrete Element Method

Workshop on HPC Collaboration between Europe and Latin America

July 16, 2015

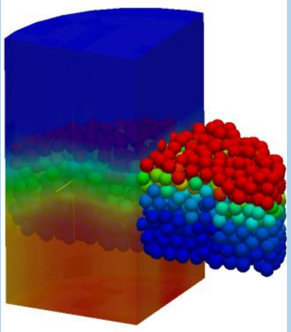
Luxembourg XDEM Research Centre

http://luxdem.uni.lu/

Bernhard Peters Xavier Besseron

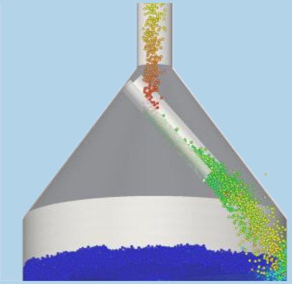
Strategic Competency

Computational Process Engineering



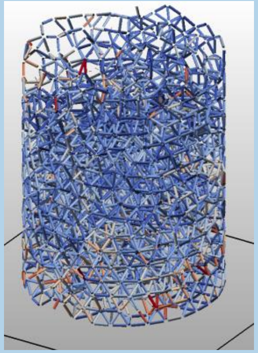
- Thermal conversion of packed/moving beds
- Conjugate heat/mass transfer
- Reactor design

Computational Dynamics



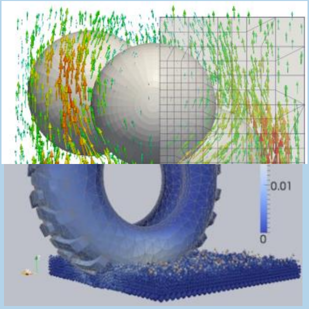
- Transport and storage of granular media
- Impact of granular media on structures

Computational Material Science



- Advanced materials
- Material processing
- Fracture

CFD / FEA



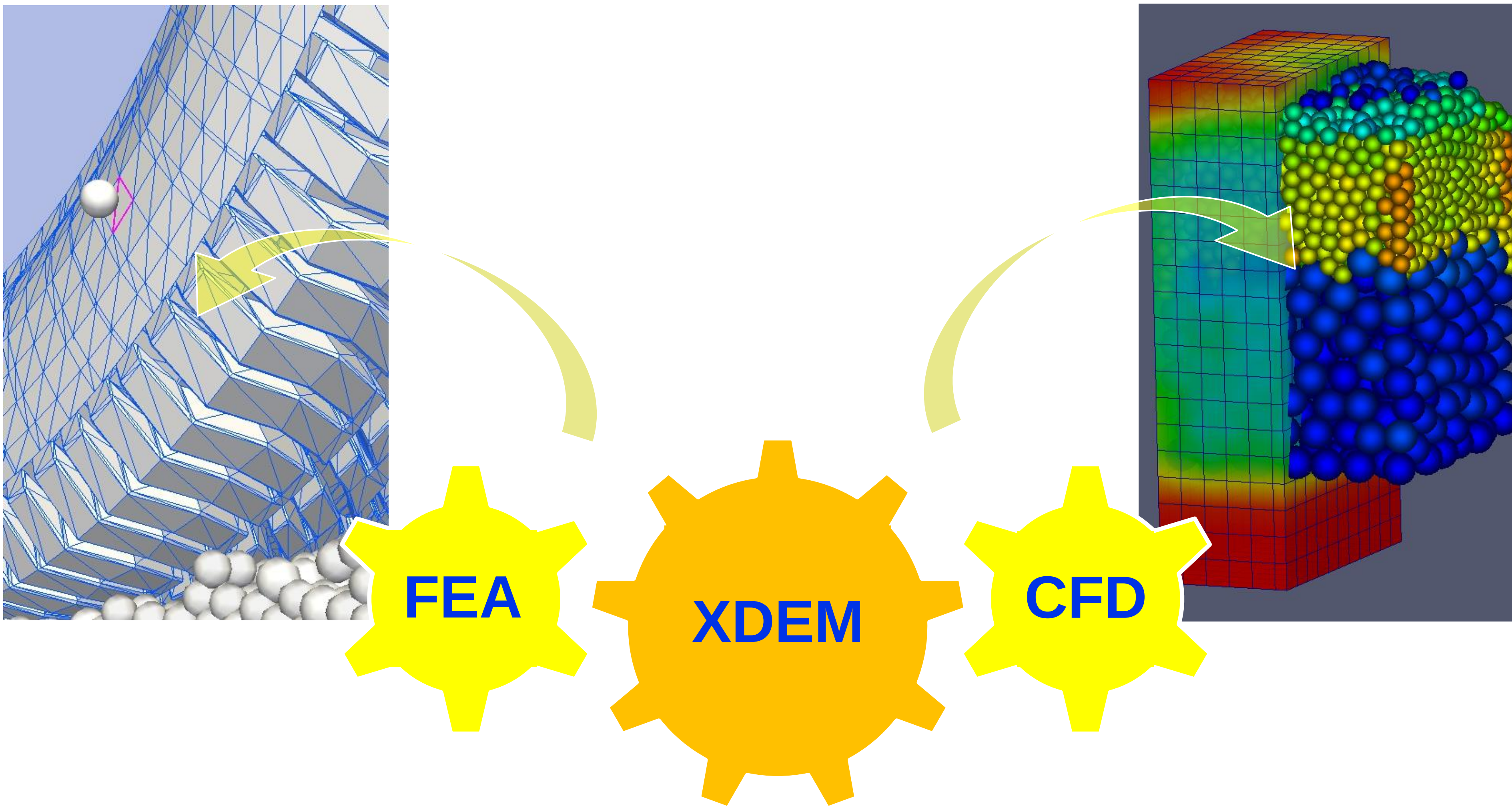
- Single/multi-phase reacting flow
- Emissions
- Simultaneous FEA/CFD analysis

Extended Discrete Element Method (XDEM)

Extended Discrete Element Method:

- based on the classical Discrete Element Method (DEM) to describe motion of granular materials (discrete phase)
- extended by
  - thermodynamics for particles
  - an interface to Computational Fluid Dynamics (CFD) and Finite Element Analysis (FEA)
- Coupling to external commercial/OpenSource software

Technology Concept



XDEM: Extended Discrete Element Method

Benefits

- Appropriate solution strategy for discrete and continuous phase
- High resolution of both discrete and continuous phase
- No empirical correlations
- No expensive experiments, sometimes even not feasible
- Retains individual inputs
- Common post-processing preferred, although individual post-processing feasible

Combination of expert tools for maximum synergy by coupling continuous and discrete phases in physical and numerical space

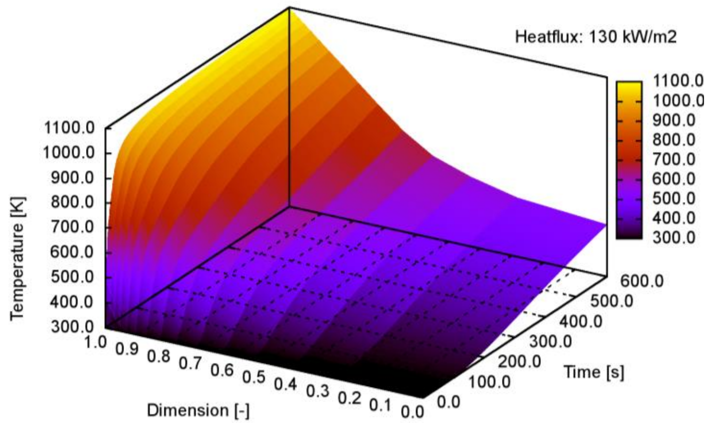
Applications

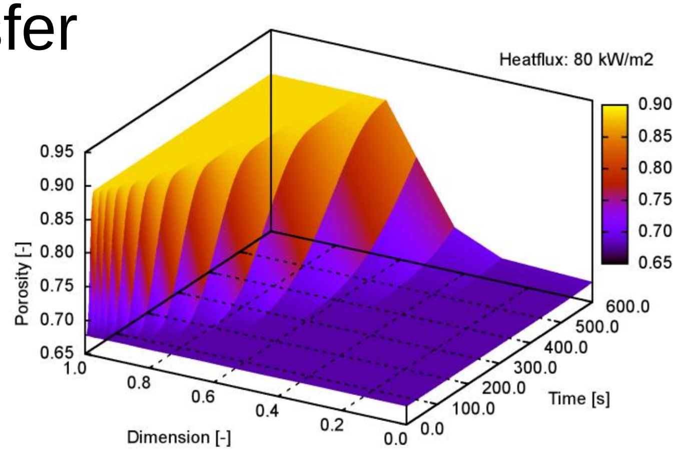
- Storage and transport of granular material
- Mining and its machinery
- Agriculture and its machinery
- Processing industry: Fluidised beds, fixed and moving bed reactors for
  - Drying
  - Thermal conversion (combustion, gasification)
  - Processing of raw materials
- Pharmaceutical industry e.g. coating, drug production
- Food industry (transport, coating, processing)
- Material science

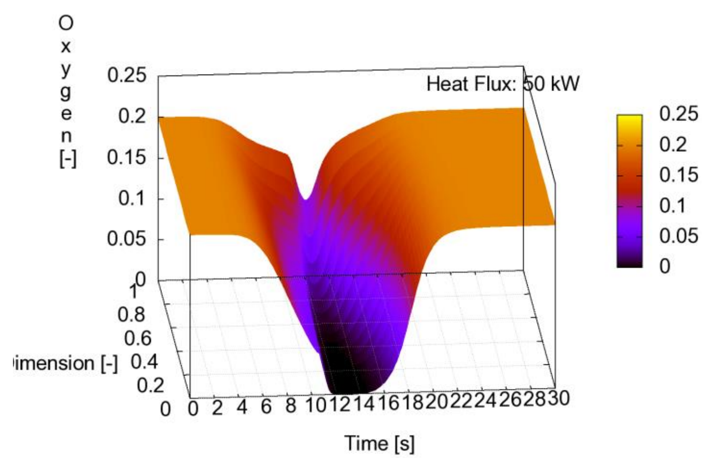
XDEM

Computational Process Engineering

- Generic model to describe particle processes:
  - Temperature distribution
  - Flow inside pore space
  - Chemical conversion
  - Distribution of reactands and products
- Interface to CFD via heat and mass transfer

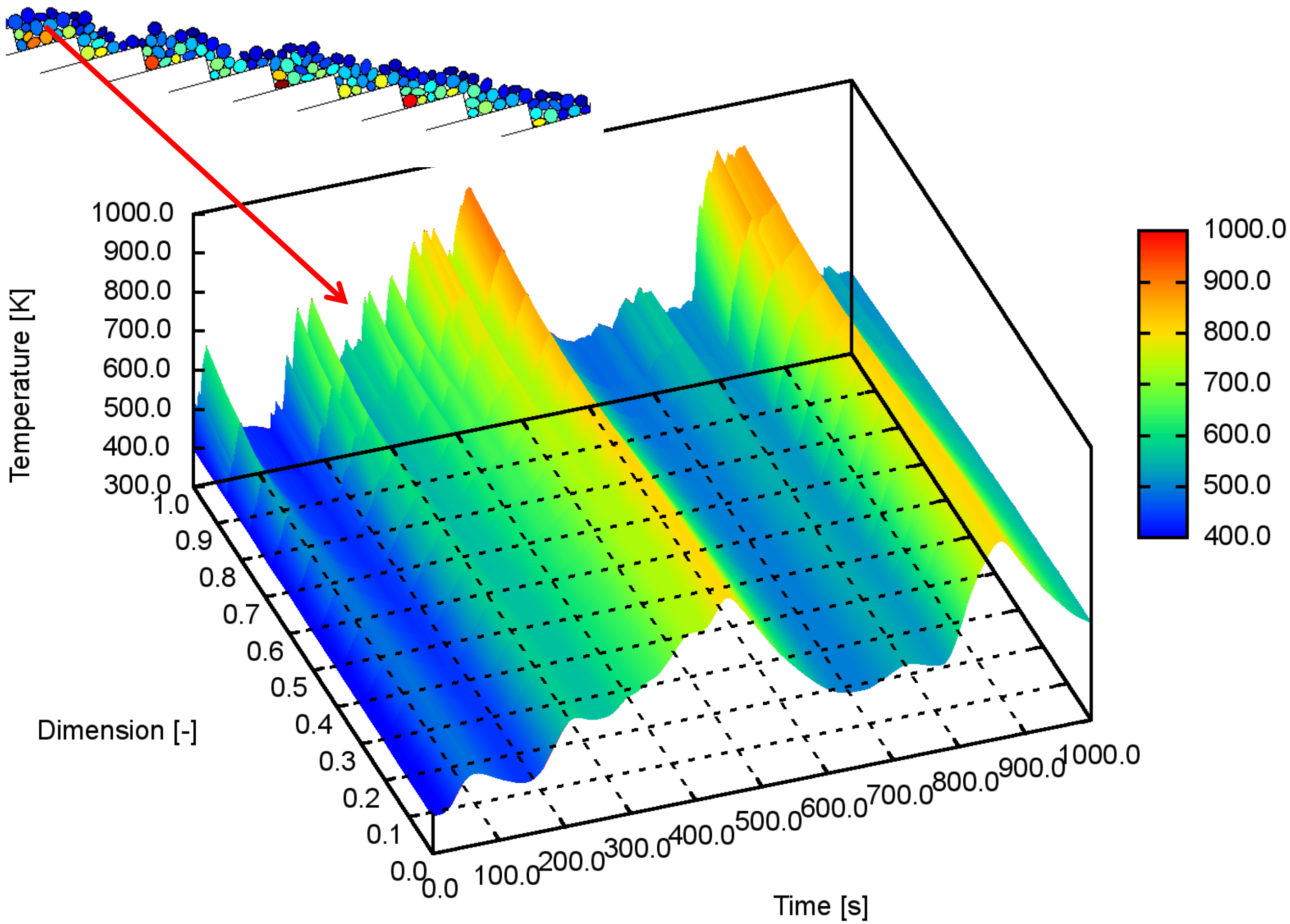




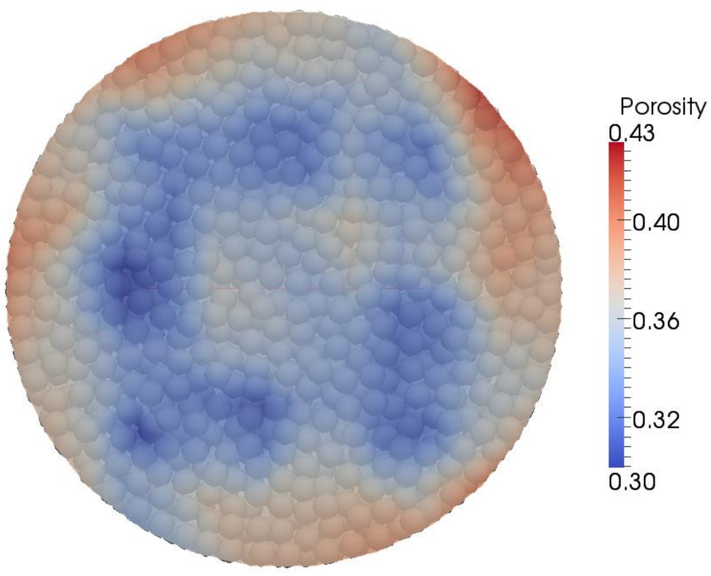


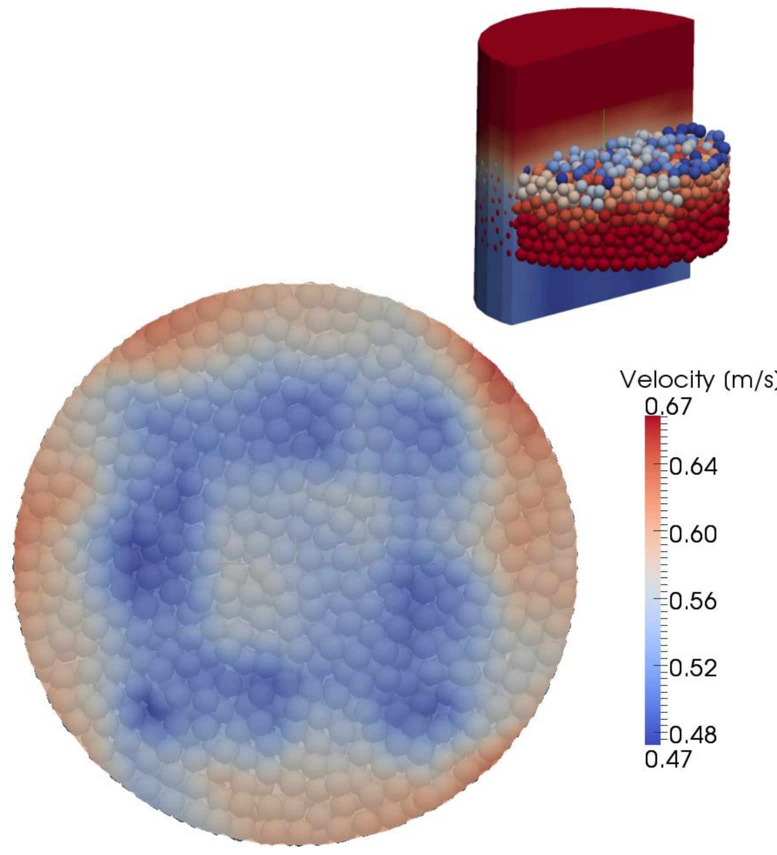
Forward Acting Grate

Spatial and Temporal Temperature Distribution

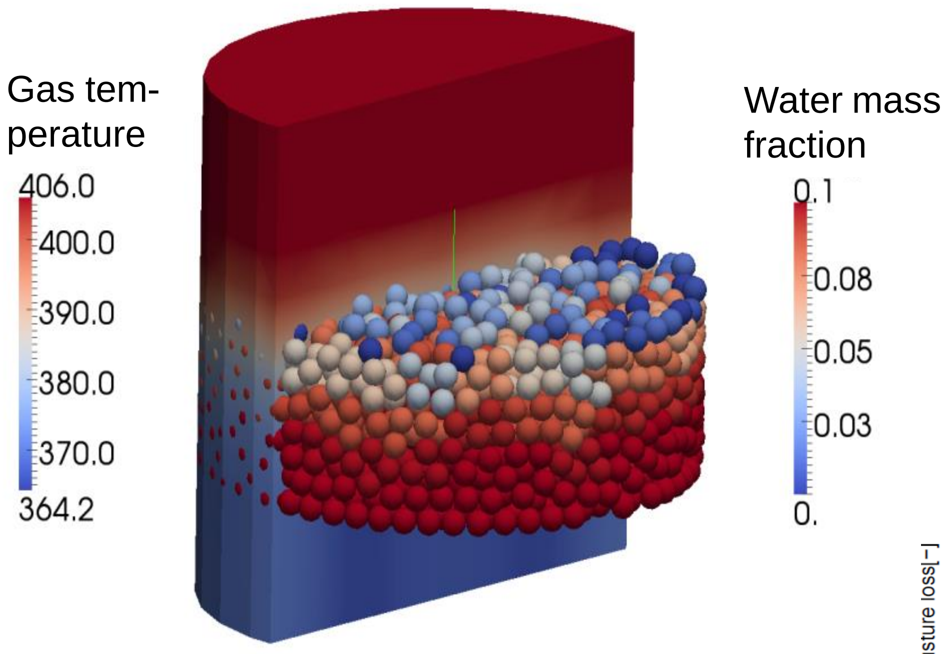


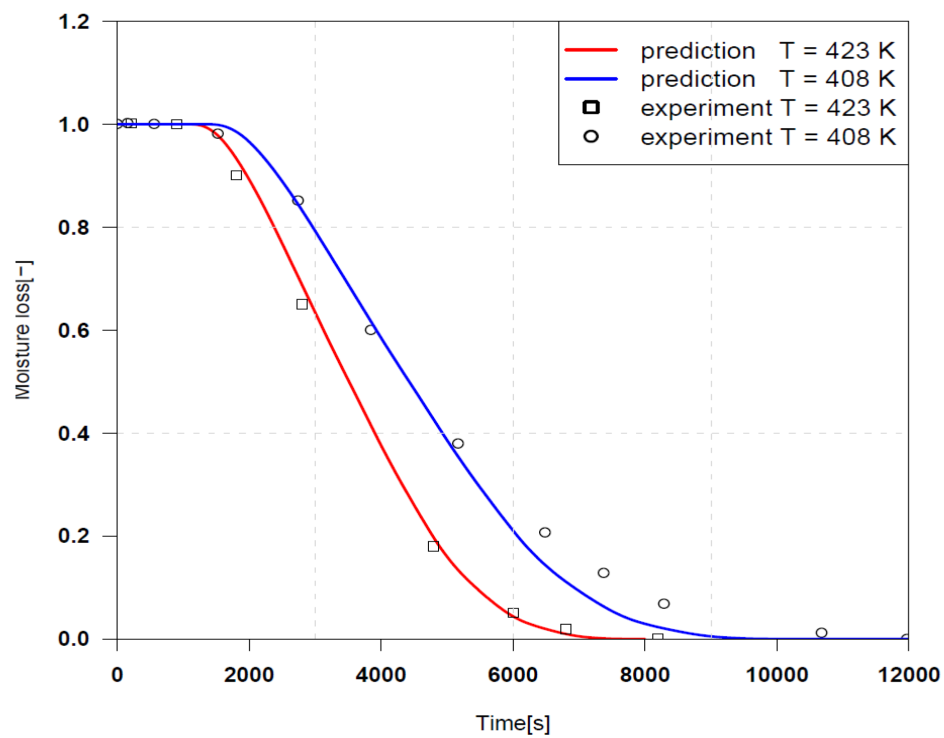
Void Space and Gas Velocity



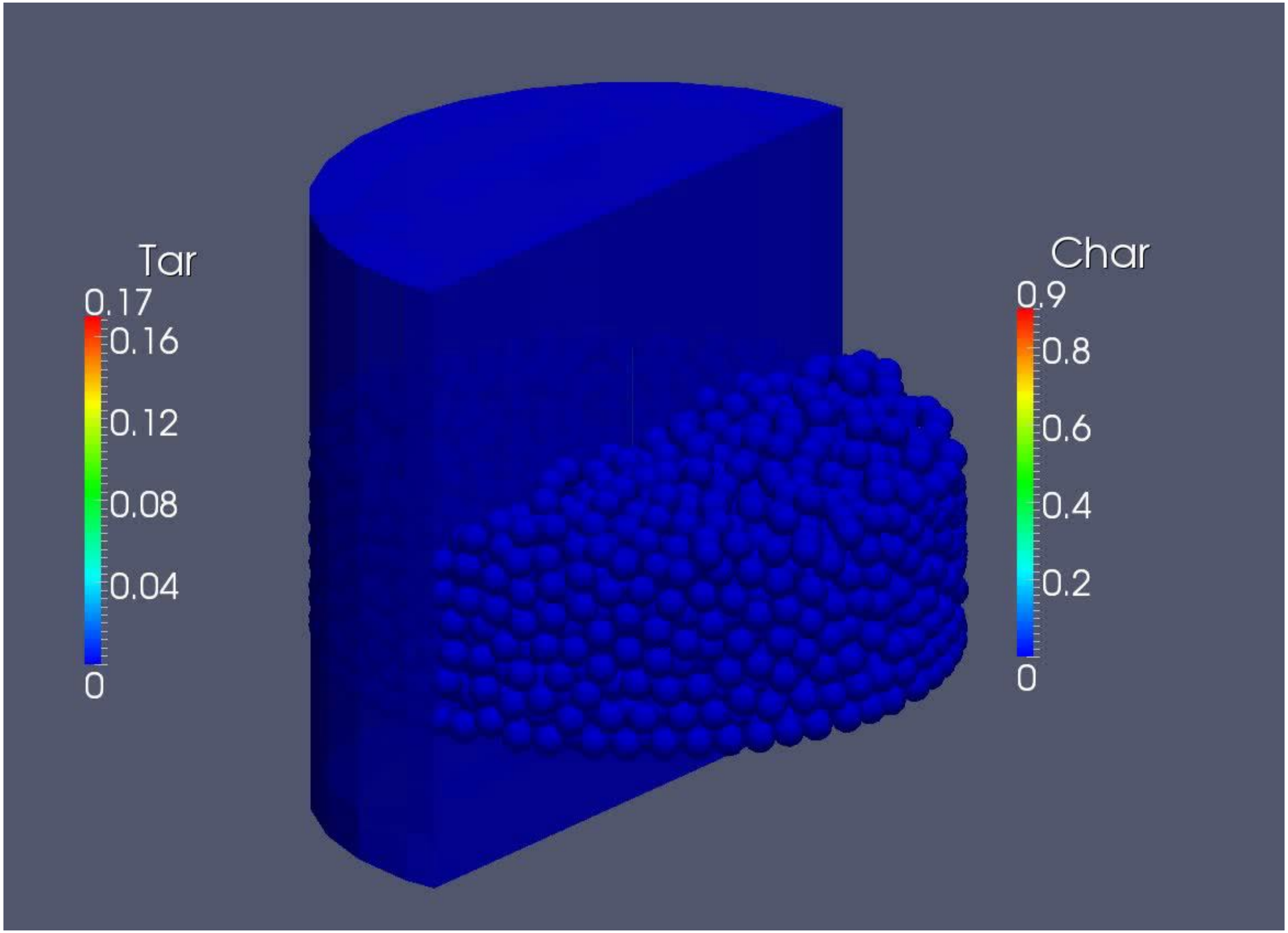


Drying


Gas tem-
perature
406.0
400.0
390.0
380.0
370.0
364.2
Water mass
fraction
0.1
0.08
0.05
0.03
0.

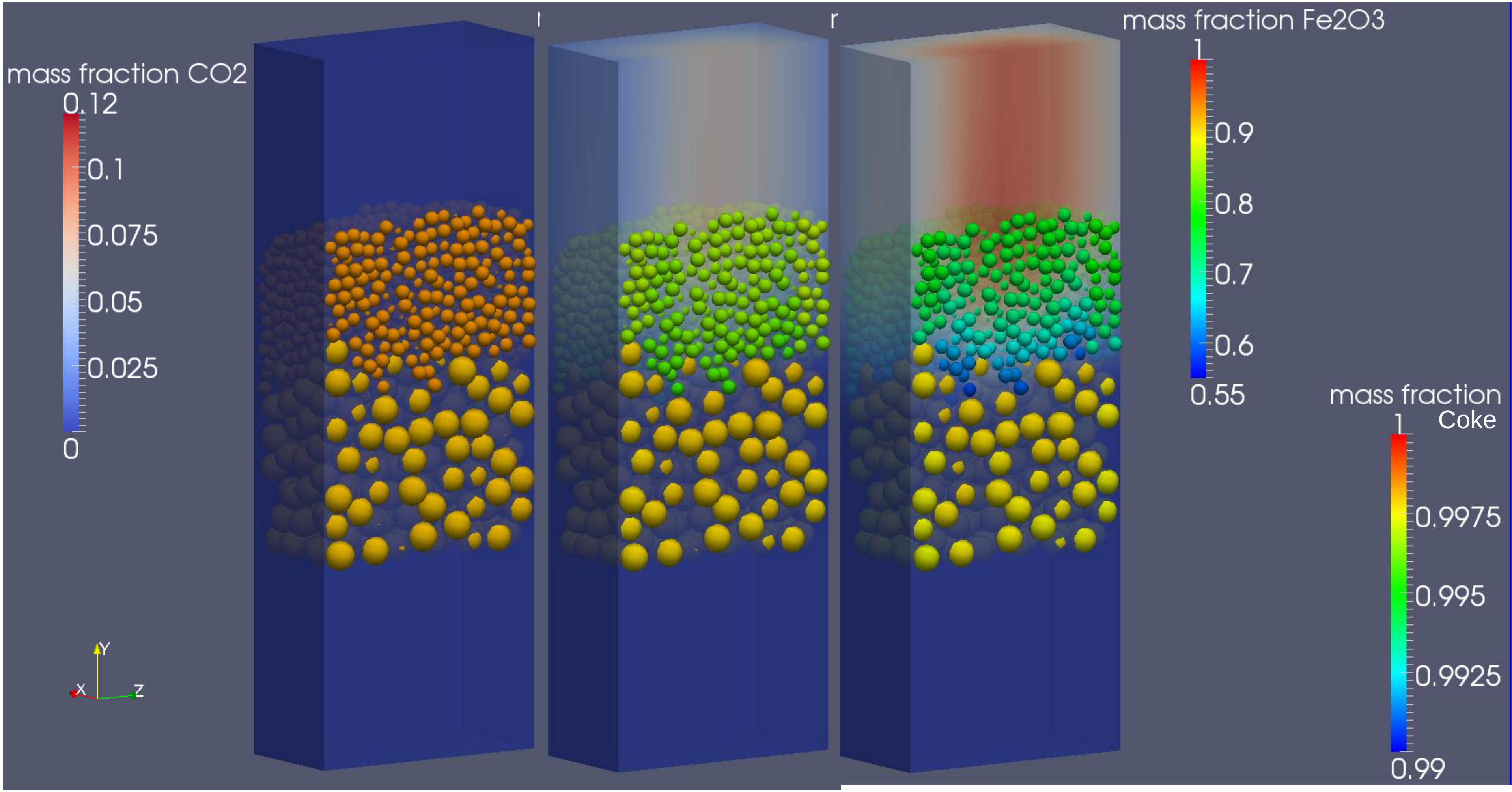

prediction T = 423 K
prediction T = 408 K
experiment T = 423 K
experiment T = 408 K
Moisture loss[−]
Time[s]
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0
2000
4000
6000
8000
10000
12000

Packed Bed Conversion



Thermal Conversion: Reduction

t=10s t=300s t=700s

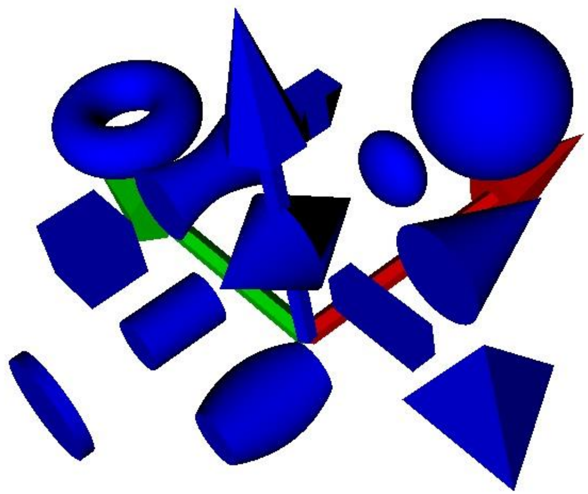


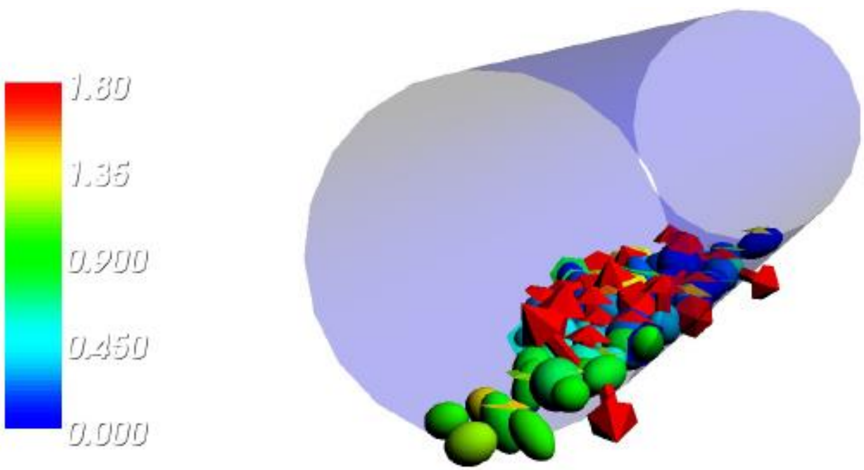
XDEM

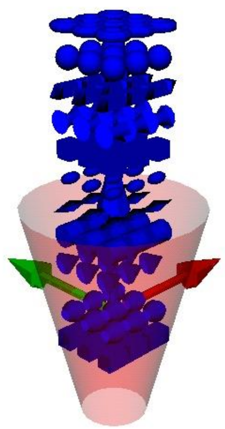
Computational Dynamics

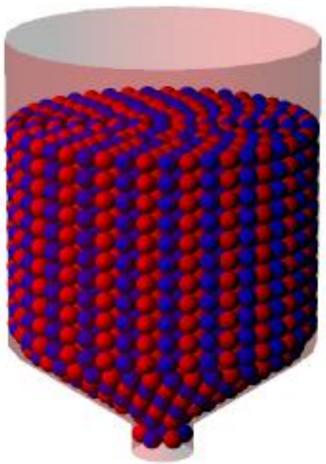
Computational Dynamics

- Prediction of motion of granular material for industrial applications
- Based on the Discrete-Element Method Dynamics
- Integration of Newtonian dynamics to yield position and orientation
- Interface to FEM for mechanical load

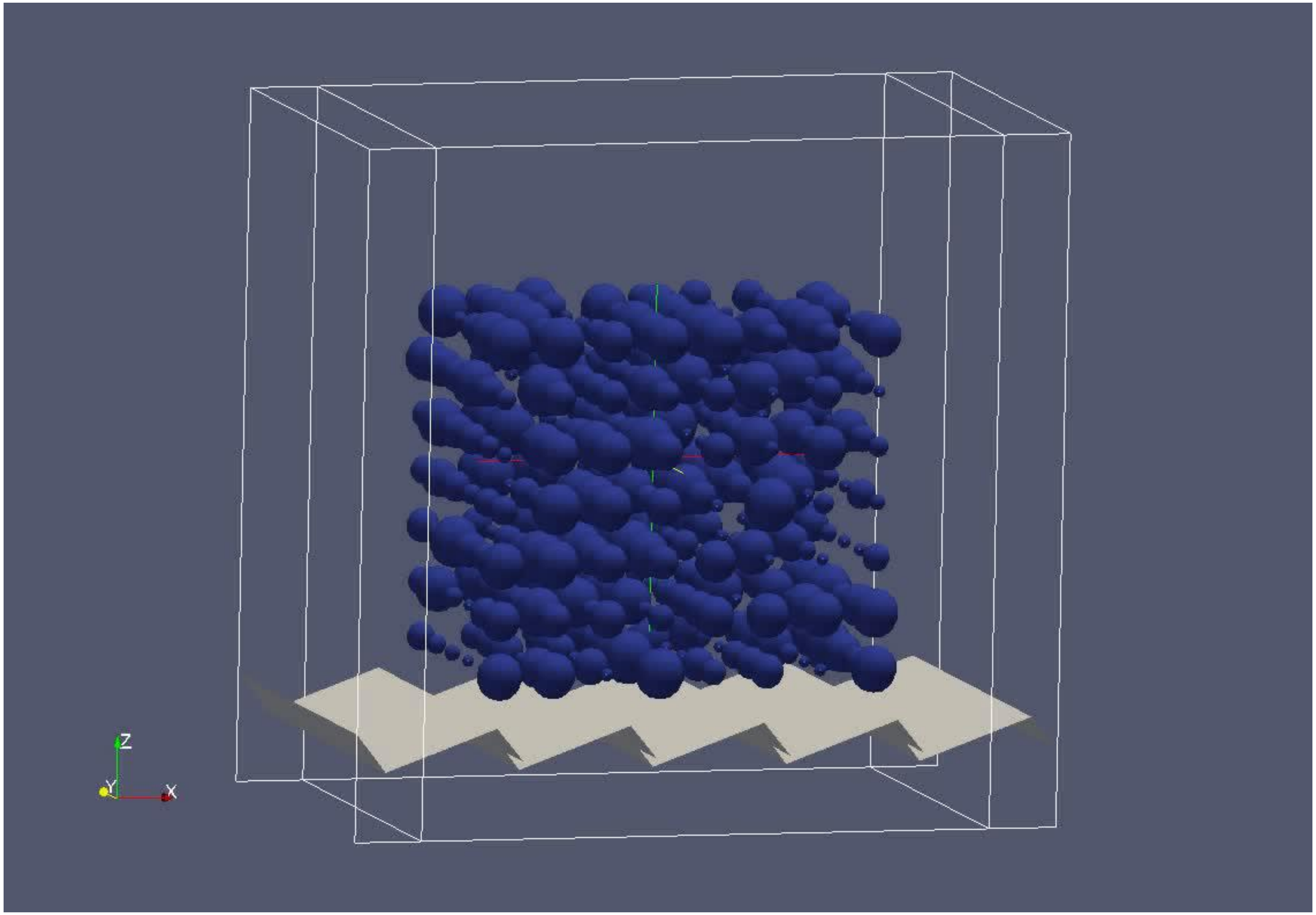




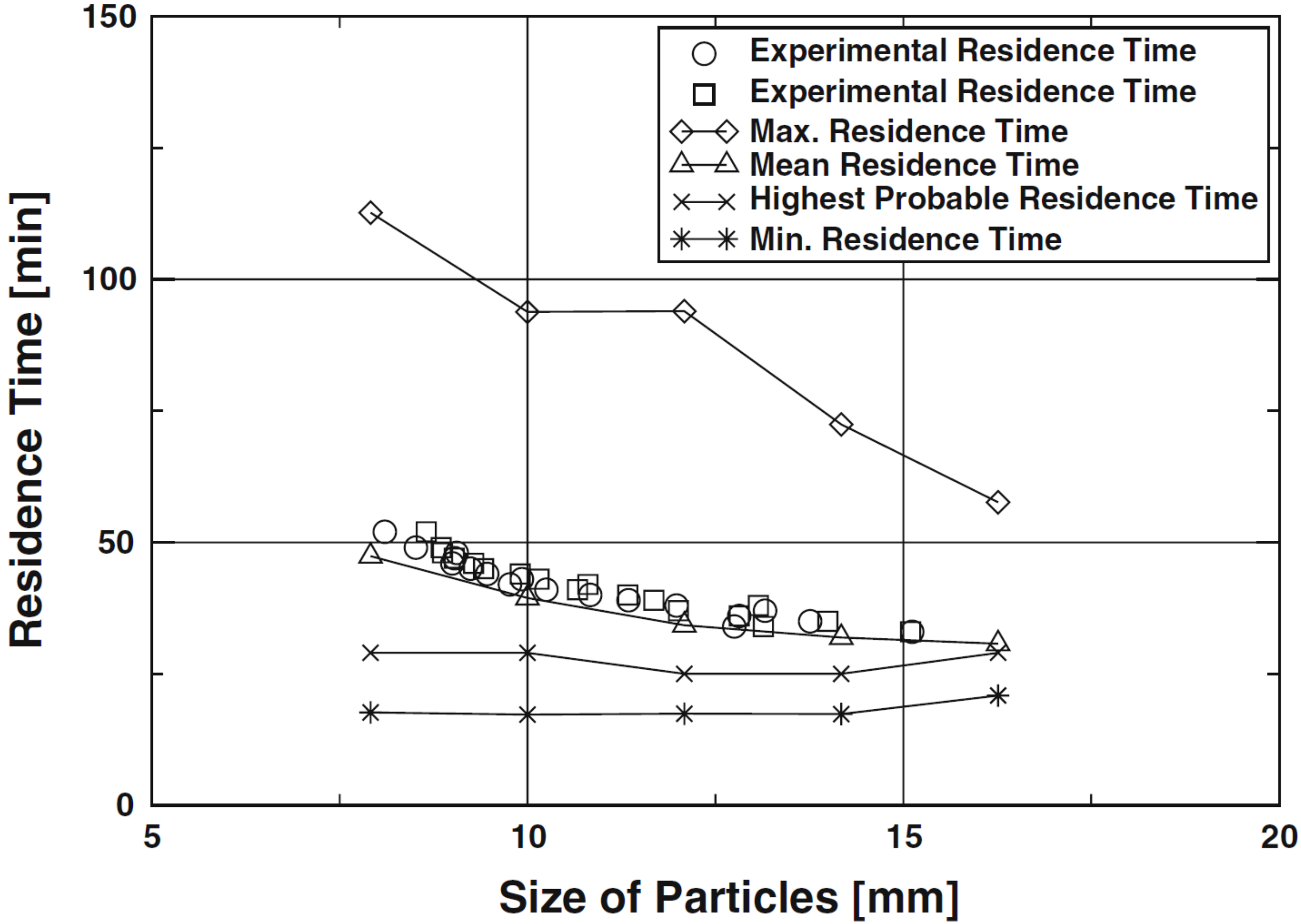




Vibrating Grate



Residence Time on a Forward Acting Grate

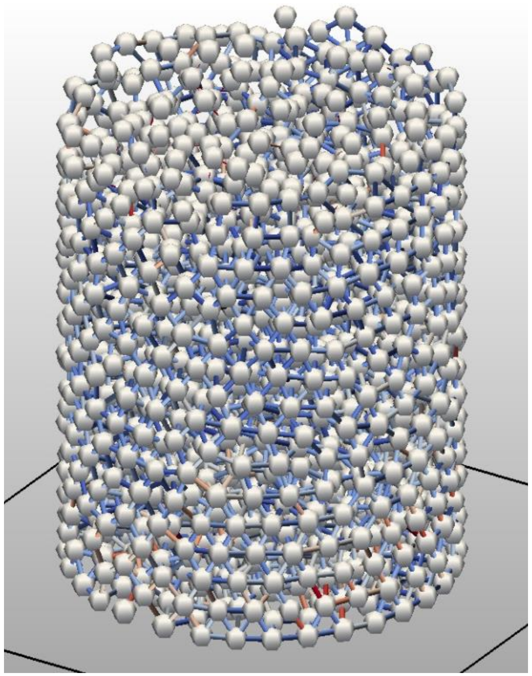


Transport of Debris

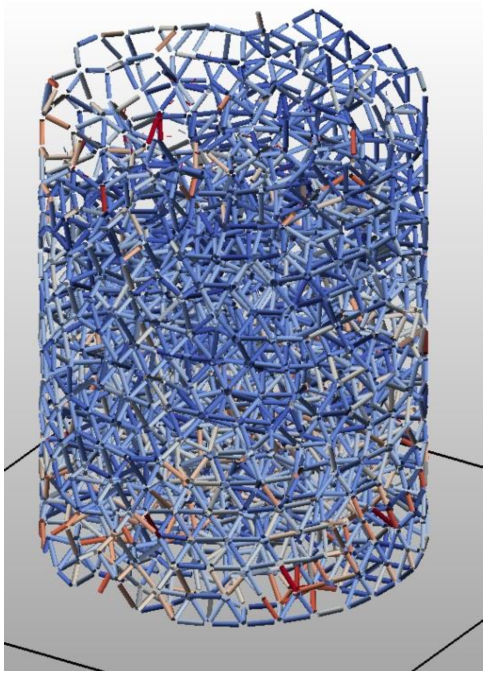
XDEM

Computational Material Science

Computational Material Science



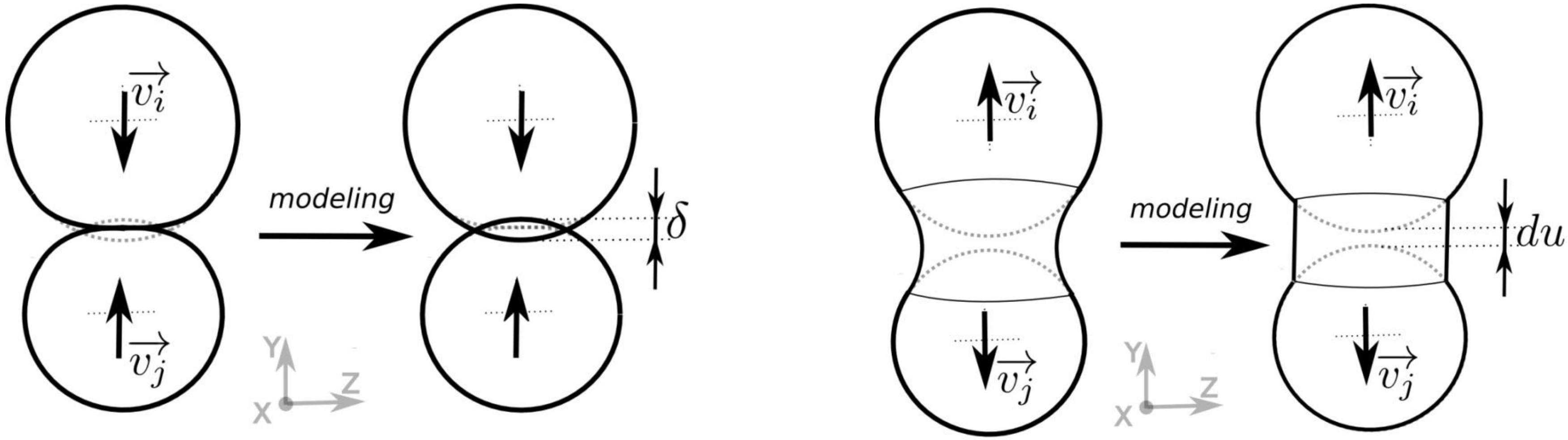
- Inclusion of arbitrary adhesive/bonding forces
- isotropic/anisotropic material behaviour
- crack development and propagation
- fracture mechanics due to mechanical impact or gas forces



Collision and Bonding

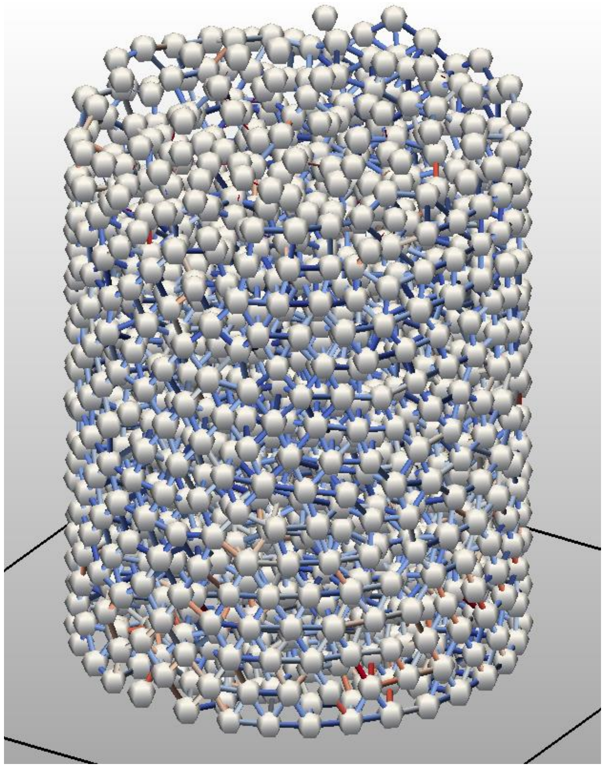
Collision

Bonding

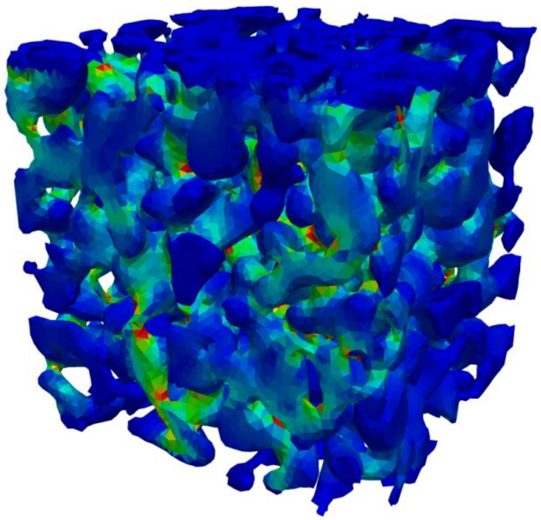


Complex Structures of Materials

Discrete Description

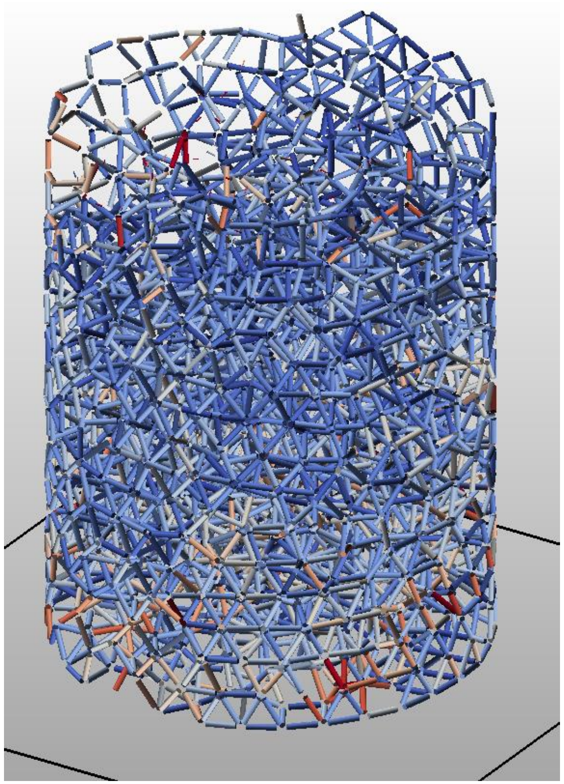


Material matrix



FEM by P. Hagenmuller (IRSTEA Grenoble)

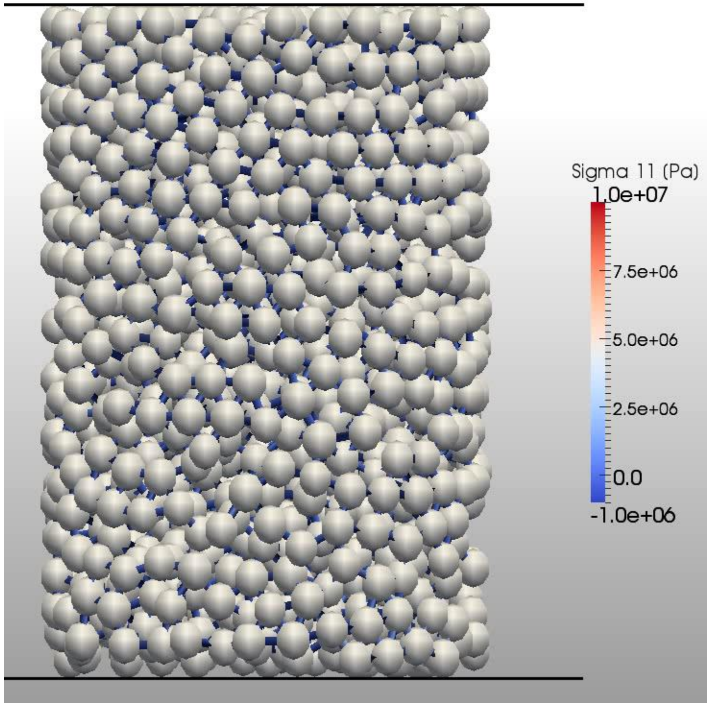
Stength of Bonds



Ductile – Brittle Behaviour

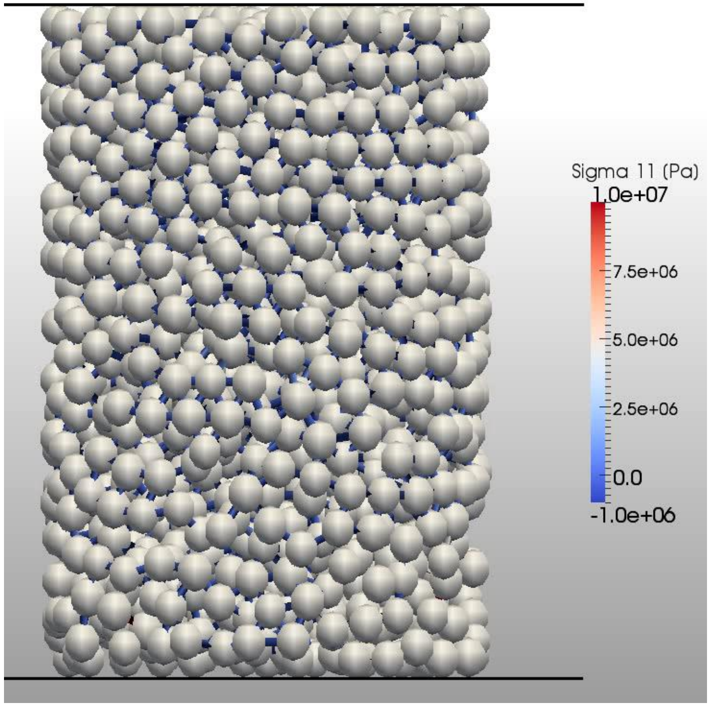
Duktile Failure

$10^{-6}s^{-1}$



Brittle Failure

$10^{-2}s^{-1}$



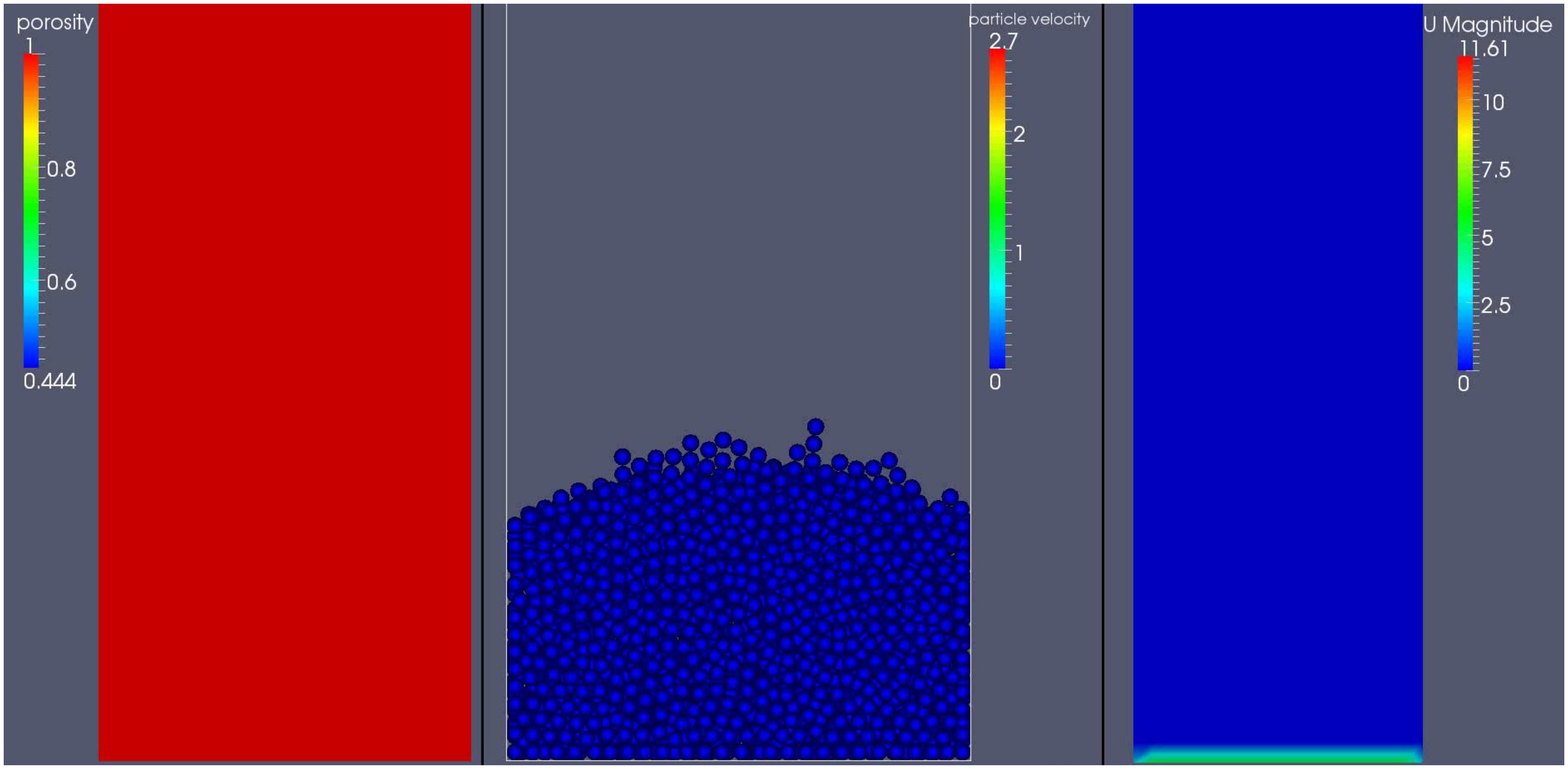
XDEM

Computational Fluid Dynamics & Finite Element Analysis

Stress/strain analysis of a Membrane

Tire-Ground Interaction

Fluidisation



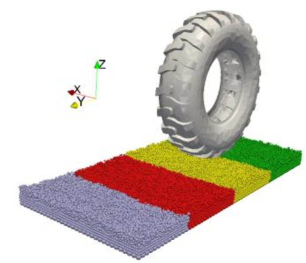
XDEM
&
High Performance Computing

Parallel Implementation

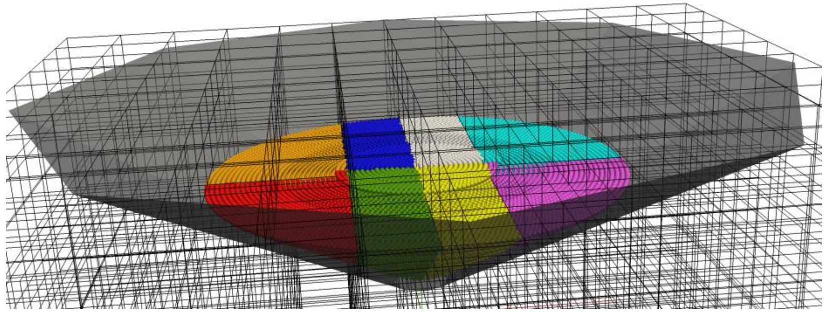
XDEM is computation intensive and uses a lot of memory

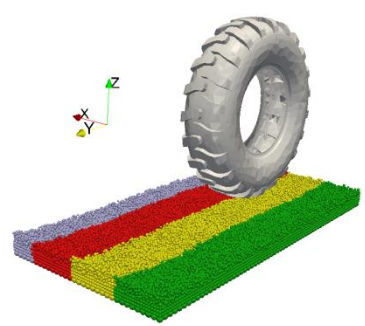
→ Parallel and distributed implementation

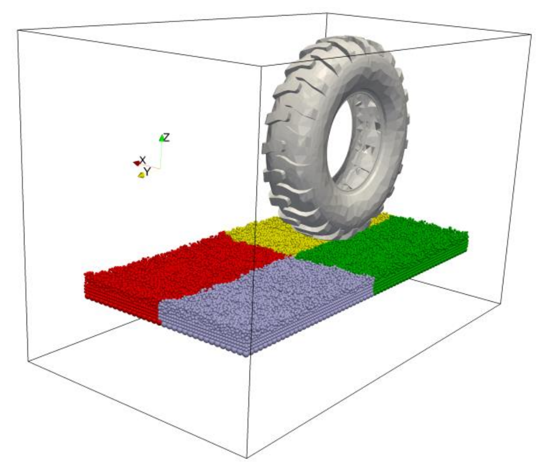
- Aggregates memory of many computing nodes
- Benefits from speedup of many computing cores



- Simulation Space Decomposition approach
- Load balancing based on
  - Orthogonal Recursive Bisection (ORB)
  - Metis partitioning library
- Communication using MPI







Future improvments for HPC

- OpenMP implementation
  → First trials showed promising results

- Accelerators: GPUs / Intel Xeon Phi
  → Probably the next big step for XDEM
  → Need to implement fast collision detection algorithms

- Post-processing / Visualization
  → Currently in 2 steps:
  Data reconstruction + Offline visualization
  → Need for real-time data processing and visualization

Summary

XDEM is a novel and advanced simulation framework for multi-physics applications

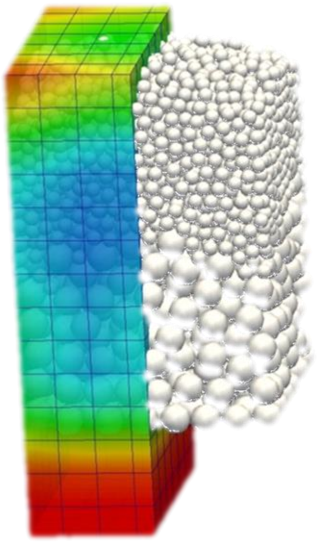
XDEM is versatile

- Multi-phases, particle-based simulations
- Motion, Thermo-dynamical and Chemical conversion
- Coupling with CFD and FEA libraries

→ Large range of industrial applications

XDEM is getting ready for HPC

- MPI-based parallel implementation
- Accelerator support coming?



Potential collaborations

XDEM team: 90% of mechanical/chemical engineers
→ Need additional expertise in Computer Science / HPC

Engineering aspect

- New industrial applications
- New “models” to include

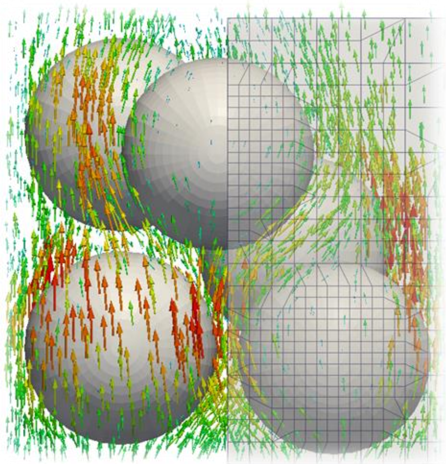
High Performance Computing aspect

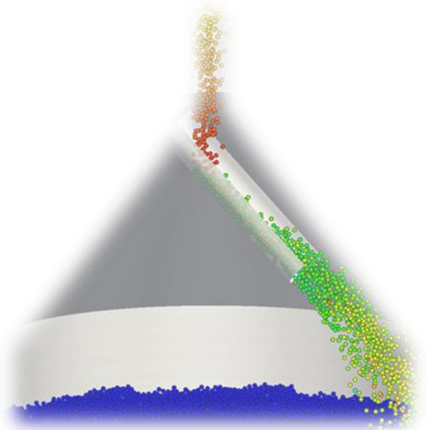
- OpenMP implementation
- Accelerators support: GPUs / Intel Xeon Phi

Post-processing / Visualization

- Real-time visualization tool

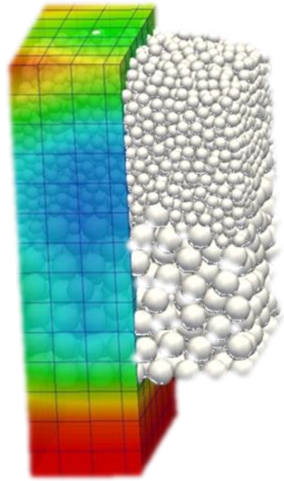
Thank you for you attention!

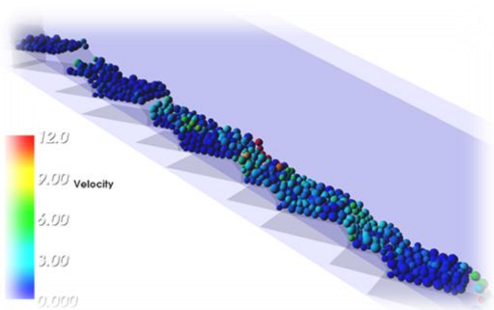




Question?

Luxembourg XDEM Research Centre
http://luxdem.uni.lu/





Bernhard Peters bernhard.peters@uni.lu
Xavier Besseron xavier.besseron@uni.lu