XDEM:
Extended Discrete Element Method

Workshop on HPC Collaboration between Europe and Latin America
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Luxembourg XDEM Research Centre
http://luxdem.uni.lu/
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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

XDEM: Extended Discrete Element Method
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
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

XDEM: Extended Discrete Element Method
Void Space and Gas Velocity

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Drying

XDEM: Extended Discrete Element Method
Packed Bed Conversion

XDEM: Extended Discrete Element Method
Thermal Conversion: Reduction

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XDEM

Computational Dynamics
Predicted 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
Residence Time on a Forward Acting Grate

![Graph showing residence time vs. size of particles. The graph includes data points for experimental residence time, max. residence time, mean residence time, highest probable residence time, and min. residence time.]
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

\[ \vec{v}_i \]
\[ \vec{v}_j \]

\[ \text{modeling} \]
\[ \delta \]

Bonding

\[ \vec{v}_i \]
\[ \vec{v}_j \]

\[ \text{modeling} \]
\[ du \]
Complex Structures of Materials

Discrete Description  Material matrix  Stength of Bonds

FEM by P. Hagenmuller (IRSTEA Grenoble)

XDEM: Extended Discrete Element Method
Ductile – Brittle Behaviour

Ductile Failure

Brittle Failure

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

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

Sigma 11 (Pa) 

1.0e+07  

7.5e+06  

5.0e+06  

2.5e+06  

0.0  

-1.0e+06
XDEM

Computational Fluid Dynamics & Finite Element Analysis
Stress/strain analysis of a Membrane
Fluidisation

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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 improvements 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 your attention!

Question?

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