eXtended Discrete Element Method (XDEM) Research on UL HPC platform

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XDEM = Extended Discrete Element Method

XDEM software is multi-physics simulation toolbox modeling granular materials and processes.

Particle Motion
Snow, Sand, ...

Chemical Reactions
Coke, Iron ore, Biomass, ...

+ coupling external libraries:

CFD with OpenFoam, FEM with Diffpack
Domains of 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
- Additive manufacturing
XDEM Research Examples

Blast furnace

Rolling tire on snow
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Why using UL HPC facilities?

Granular dynamics applications

- Computation intensive = Time consuming
- Require the use of UL HPC facilities
Usage of UL HPC platform

XDEM model studies
- model validation (using parameter studies)
- execution of full simulations

Parallel/distributed code development
- Debugging, validation
- Scalability studies
### Domain Decomposition

- **Domain** = whole simulation space
- **Cell** = regular subdivision with a fixed size
- **Partition** = subset of cells assigned to a given process

### Partitioner and Load-Balancer

- Responsible for assigning a cell to a process
- Balance the workload
- Based on Orthogonal Recursive Bisection (ORB), Zoltan, PHG, etc...

### MPI Parallel Simulation Driver

- Schedule the modules on all the processes
- Exchange the data between processes (*Ghost particles in ghost cells*)
- Independent of the module implementation
- Based on **Message Passing Interface (MPI)**
Testcase - Tire

Sinkage of a Tire

- Simulate the vertical motion of the tire tread
- The tire is a rigid surface of 18,707 triangles
- Soil layer is made of 43,624 sand grains
- Sand grains are described as spherical particles of different radii
Testcase - Tire: Scalability

Parallel execution from 1 process to 64 processes (8 processes/node)

- 2 processes → 1.3X speedup
- 8 processes → 4.6X speedup
- 64 processes → 17.6X speedup
Testcase - Hopper

Hopper discharge

• Simulate hopper discharge
• The hopper is a rigid surface of 31,500 triangles
• Spherical particles of different radii
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Testcase - Hopper: Scalability

Parallel execution from 1 process to 48 processes (24 processes/node)

Xdem parallel results

Simulation time [s]

Number of processes
Testcase - Hopper discharge: Scalability

Xdem parallel results

48 processes → 21X speedup
## Conclusion

### Discrete Particle Method (DPM) software
- Multi-physics simulation toolbox
- Flexible and extensible design
- Parallel execution using MPI: 21x speedup with 48 processes

### Future work
- Hybrid approach: MPI + (OpenMP or GPU)
  - OpenMP or GPU: collision detection
Thank you for your attention