

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

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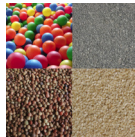


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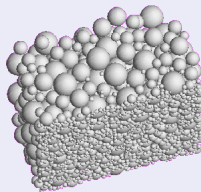
XDEM = Extended Discrete Element Method

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



Particle Motion

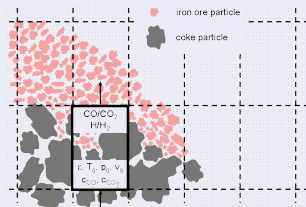
Snow, Sand, ...



+ coupling external libraries:

Chemical Reactions

Coke, Iron ore, Biomass, ...



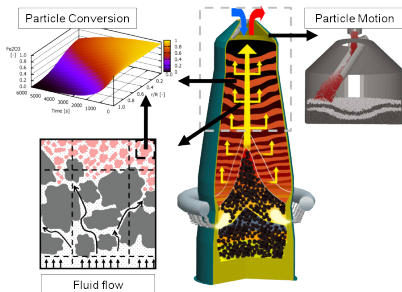
CFD with OpenFoam, FEM with Diffpack

Domains of Applications

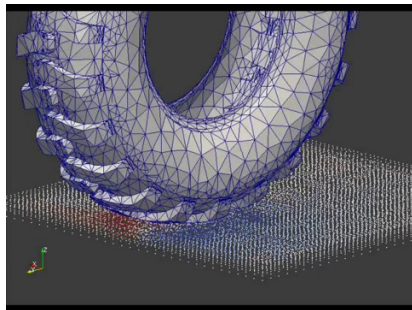
- Storage and transport of granular material
- Mining and its machinery
- Agriculture and its machinery
- Processing industry: Fluidised beds, fixed and moving bed reactors for
 - Drying
 - Thermal conversion (combustion, gasification)
 - Processing of raw materials
- Pharmaceutical industry e.g. coating,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

XDEM Research Examples

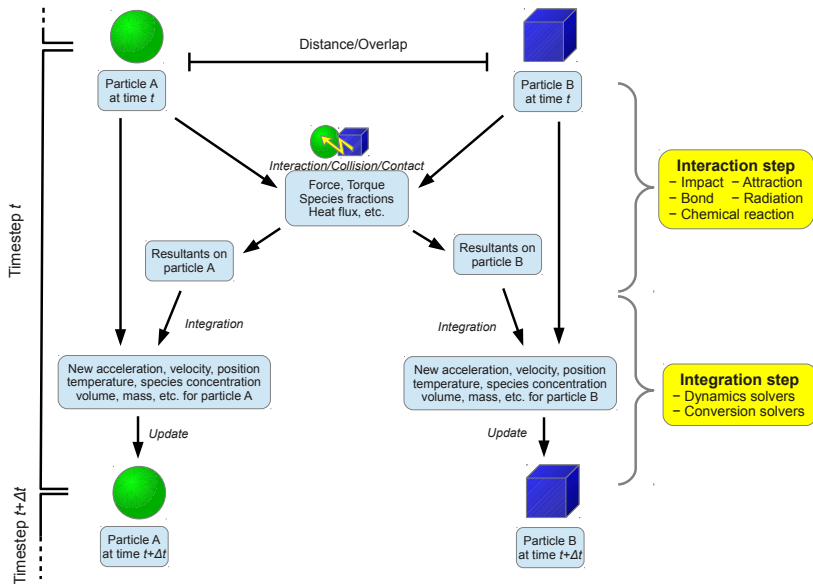
Blast furnace



Rolling tire on snow



XDEM Workflow (Dynamic phase)



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

XDEM - Parallel code design

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...

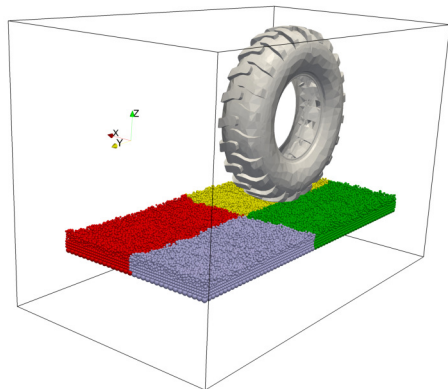
MPI Parallel Simulation Driver

- 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

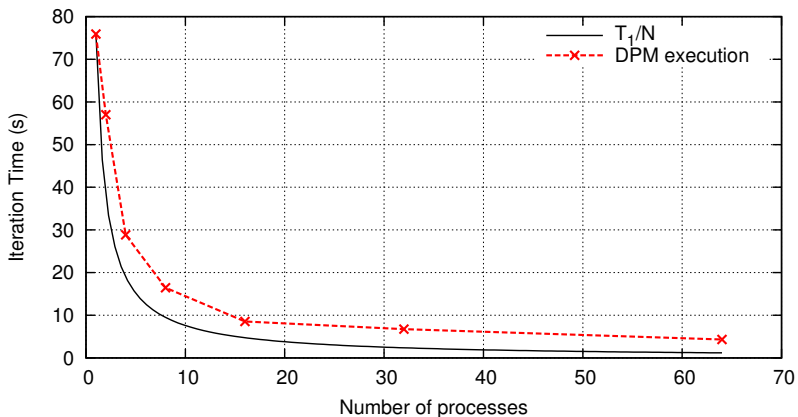
Sinkage of a Tire

- 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)

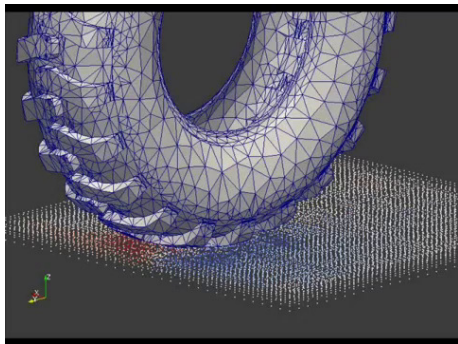


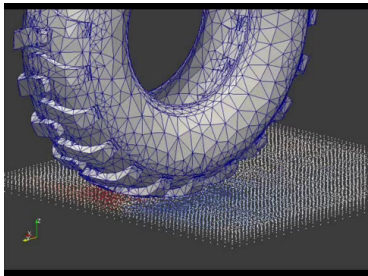
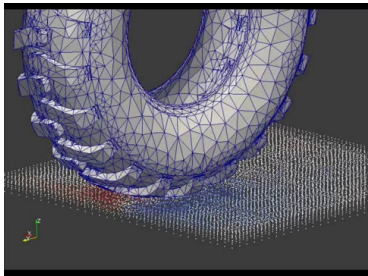
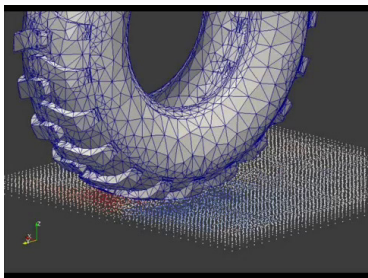
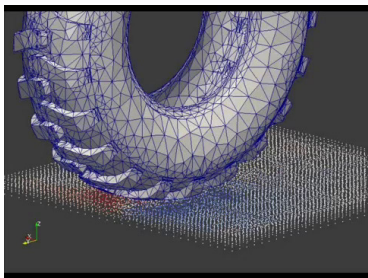
2 processes → 1.3X speedup
8 processes → 4.6X speedup
64 processes → 17.6X speedup

Testcase - Hopper

Hopper discharge

- Simulate hopper discharge
- The hopper is a rigid surface of 31,500 triangles
- Spherical particles of different radii

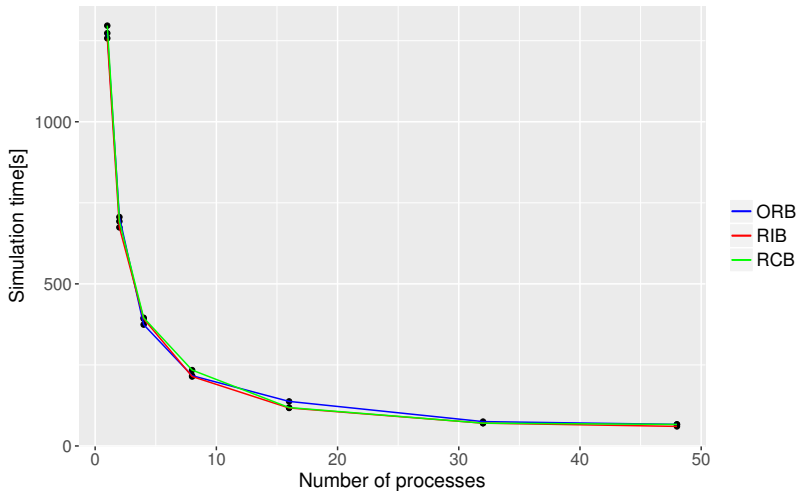




Testcase - Hopper: Scalability

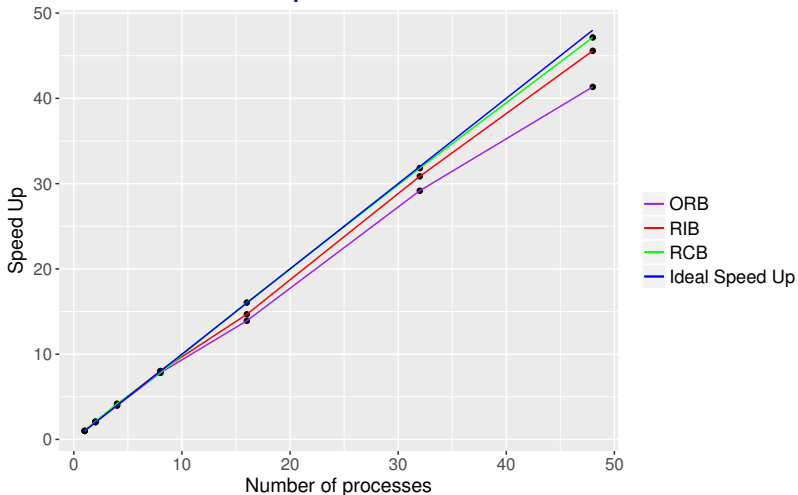
Parallel execution from 1 process to 48 processes (24 processes/node)

Xdem parallel results



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