

XDEM Research on UL HPC platform

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XDEM = Extended Discrete Element Method

Discrete Element Method (DEM)

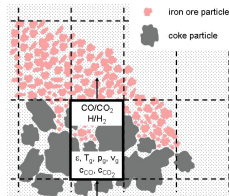
- models the motion of granular materials

eXtended by thermodynamics properties

- temperature
- chemical composition

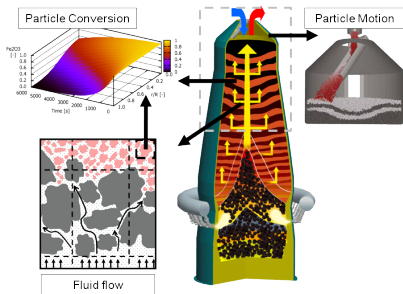
coupled with external software

- Computational Fluid Dynamics (CFD), e.g. OpenFoam
- Finite Element Analysis (FEA), e.g. DiffPack

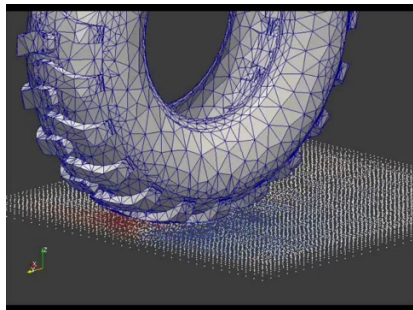


XDEM Research Examples

Blast furnace



Rolling tire on snow



Usage of UL HPC platform

XDEM model studies

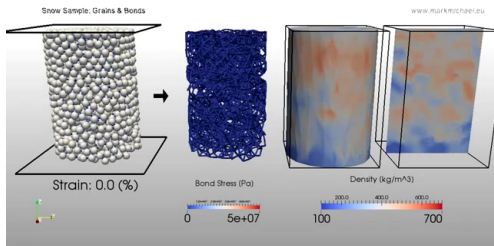
- model validation (using parameter studies)
- execution of full simulations

Parallel/distributed code development

- Debugging, validation
- Scalability studies

⇒ Equivalent to more than 21 years of sequential computing

Usecase: Parameter study of snow compression



Large number of sequential jobs

Different values for the physical quantities:

- 7 sample dimensions
- 6 compression velocities
- 3 grain sizes
- 8 bond structures
- 5 temperatures

Usecase: Parameter study of snow compression

Long execution time for each job

- from 5 days up to 2 months

Maximum walltime on the cluster is 5 days ⇒ **Checkpoint/Restart!**

Principle: Execution is split in many consecutive jobs

- Submit the job with a wrapper launcher script
- When the job reach the walltime, it is checkpointed
- The job is resubmitted (`idempotent` type in OAR)
- If the job ends normally, it is not resubmitted

Usecase: Parameter study of snow compression

Wrapper Launcher script

- Based on the one provided on UL HPC website ¹
- Handle checkpoint, restart and resubmission automatically
- Do NOT require application modification

Checkpoint/Restart

- Based on Berkeley Lab Checkpoint/Restart (BLCR)
- Do NOT require application modification ²

¹ See `launcher-scripts/bash/besteffort/launcher_checkpoint_restart.sh` on UL HPC Git Hub

² Some conditions may apply ;-)

Usecase: Parameter study of snow compression

Use walltime of 24 hours only

- Progress is checkpointed every day
- Do not block nodes for a long time

Automatic cleanup of old checkpoint files

- Checkpoint older than a day are deleted
- Limit disk space usage

Other usecases: Parallel development

Debugging of parallel application

- Requires interactive session
- Usually on a small amount of nodes
- During the work day

Scalability studies

- Requires a large number of nodes (ideally all the nodes!)
- Reasonable amount of time (a few hours usually)
- During nights or weekends

Conclusion

HPC clusters are shared resources

- Shared resources = CPU, memory, network, storage
- Take in account other users
- Do not waste resources, optimize your workflow!
- Read and follow the Acceptable Use Policy ³

Best practices

- Avoid long walltime, use checkpoint/restart instead
- Use besteffort job when possible
- Avoid using all the nodes during the workdays

³<https://hpc.uni.lu/users/AUP.html>