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
Use case: 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 $\Rightarrow$ 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
Use case: Parameter study of snow compression

**Wrapper Launcher script**

- Based on the one provided on UL HPC website
- 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

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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

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