# High Performance Parallel Coupling of OpenFOAM+XDEM

X. Besseron, G. Pozzetti, A. Rousset, A. W. Mainassara Checkaraou and B. Peters

Research Unit in Engineering Science (RUES), University of Luxembourg
Luxembourg XDEM Research Centre, http://luxdem.uni.lu/

UL HPC School - User Session
June 2019

# What is XDEM?

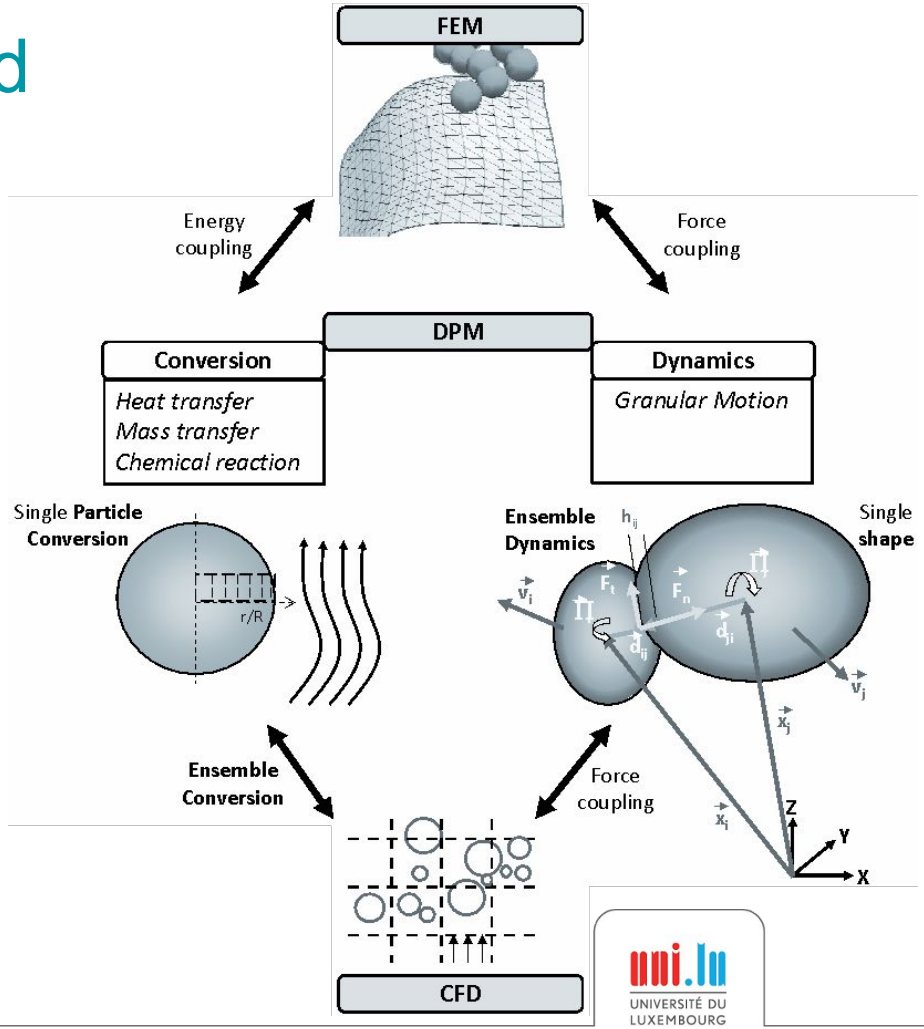
# What is XDEM?

**eXtended Discrete Element Method**

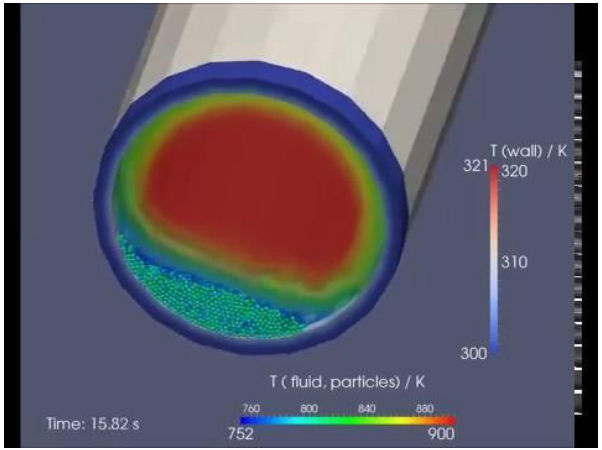
**Particles Dynamics**
- Force and torques
- Particle motion

**Particles Conversion**
- Heat and mass transfer
- Chemical reactions

**Coupled with**
- Computational Fluid Dynamics (CFD)
- Finite Element Method (FEM)



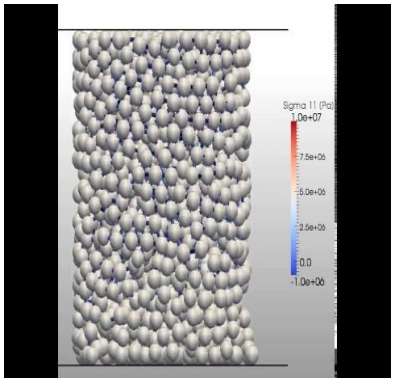
# XDEM examples



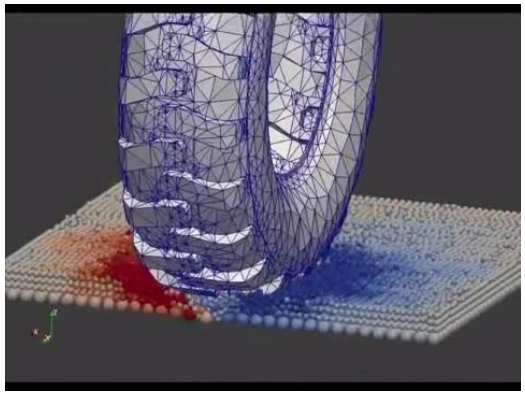

Heat transfer to the walls of a rotary furnace

Impacts on an elastic membrane

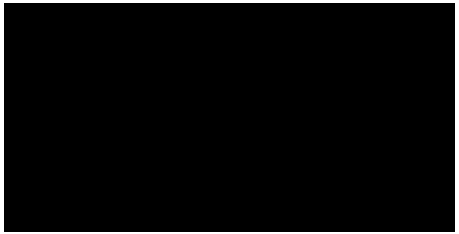
Charge/discharge of hoppers



Brittle failure



Tire rolling on snow

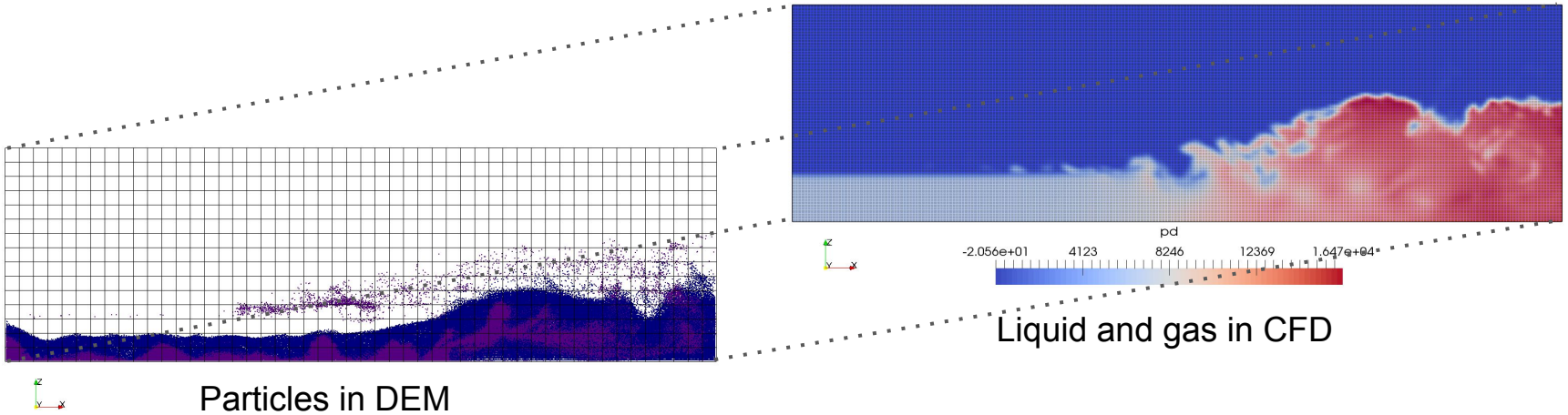


Fluidisation

# CFD-DEM Coupling

# CFD-(X)DEM Coupling

## Moving particles interacting with liquid and gas




Particles in DEM

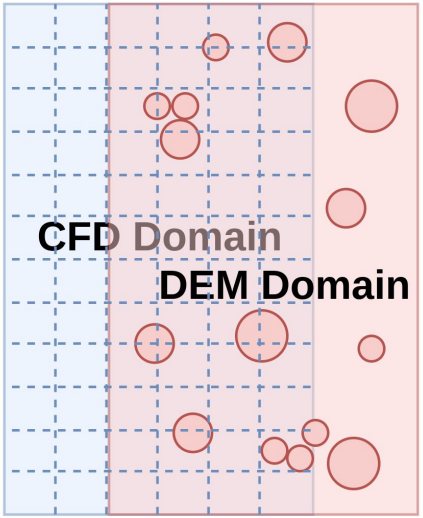
Liquid and gas in CFD

**From CFD to DEM**
- Lift force (buoyancy)
- Drag force

**From DEM to CFD**
- Porosity
- Particle source of momentum

**CFD ↔ XDEM**
- Heat transfer
- Mass transfer

# CFD-DEM Parallel Coupling: Challenges

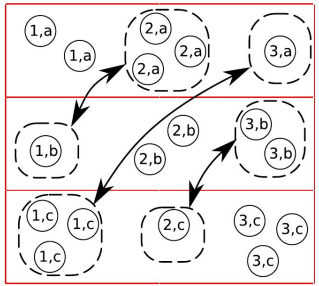



## Challenges in CFD-XDEM parallel coupling

- Combine different independent software
- Large volume of data to exchange
- Different distribution of the computation and of the data
- DEM data distribution is dynamic

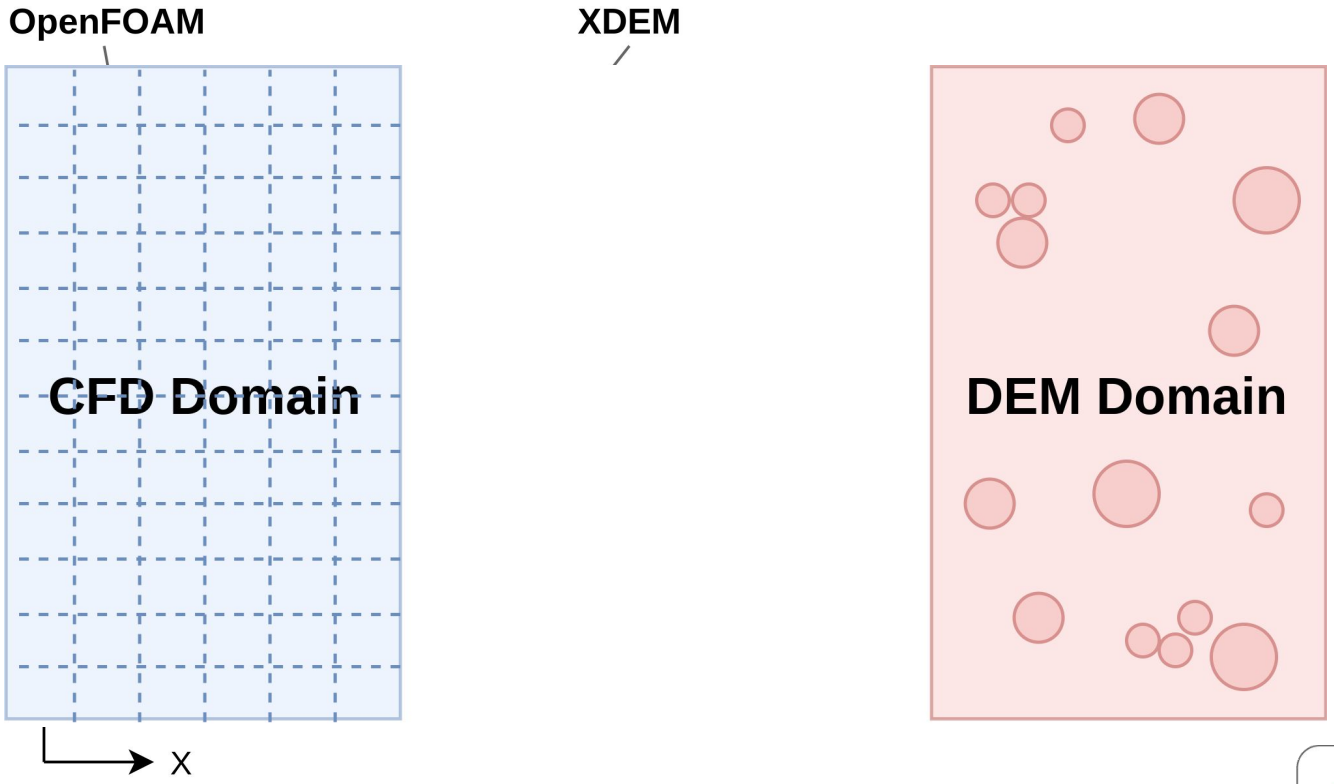
## Classical Approaches

- Each software partitions its domain independently
- Data exchange in a peer-to-peer model




SediFoam [Sun2016]

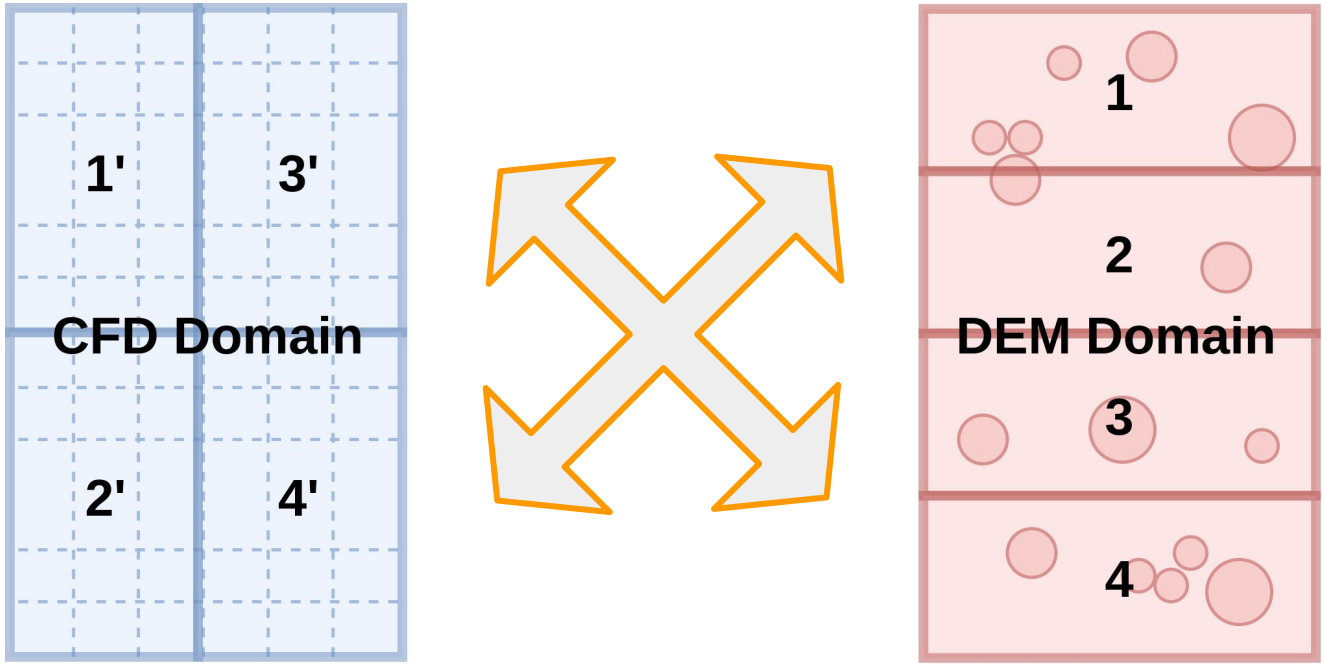
# CFD-DEM Parallel Coupling: Challenges




The domains overlap in space

# CFD-DEM Parallel Coupling: Challenges

**Classical Approach:** the domains are partitioned independently

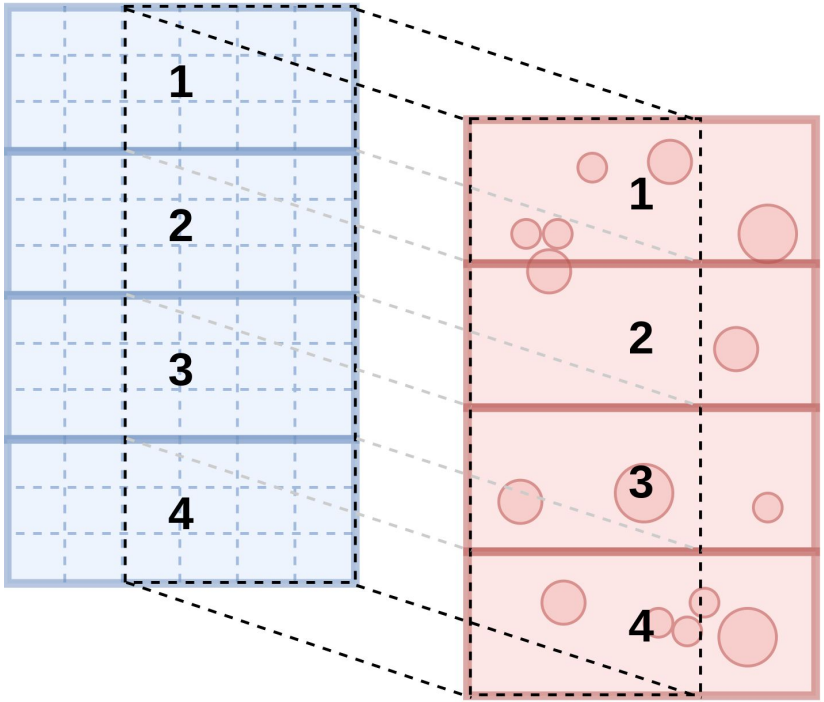



**Complex pattern and large volume of communication**

# Co-located Partitioning Strategy

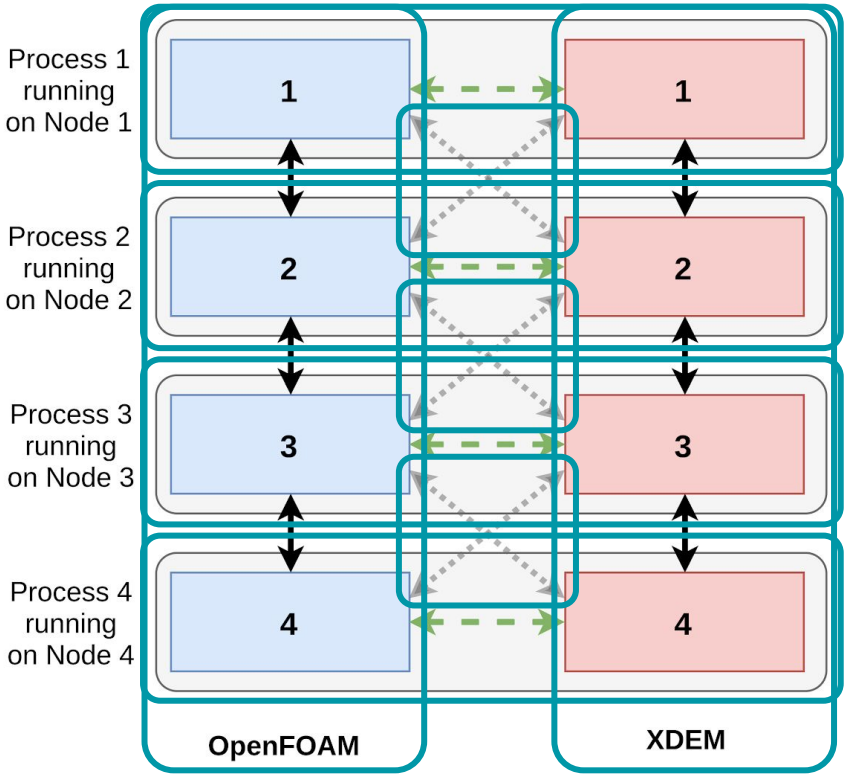
**A co-located partitions strategy for parallel CFD–DEM couplings**
G. Pozzetti, X. Besseron, A. Rousset and B. Peters
Journal of Advanced Powder Technology, December 2018
https://doi.org/10.1016/j.apt.2018.08.025

# Co-located Partitioning Strategy




Domain elements co-located in domain space are assigned to the same partition

# Co-located Partitioning Strategy: communication




Intra-physics Data Exchange

**Inter-partition intra-physics Data Exchange using MPI communication layer**
with native implementation in OpenFOAM and XDEM

Inter-physics Data Exchange

**Inter-partition inter-physics Data Exchange using MPI communication layer**
reduced to minimum or non-existing due to partition co-location

**Intra-partition inter-physics Data Exchange using direct library function calls**
fast because it is a direct intra-process memory access

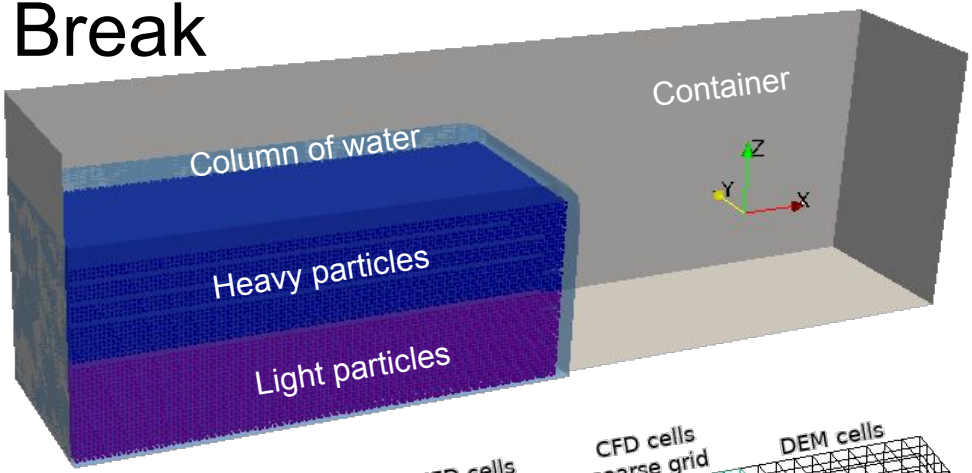
With a tight coupling of software
if the two software are perfectly aligned

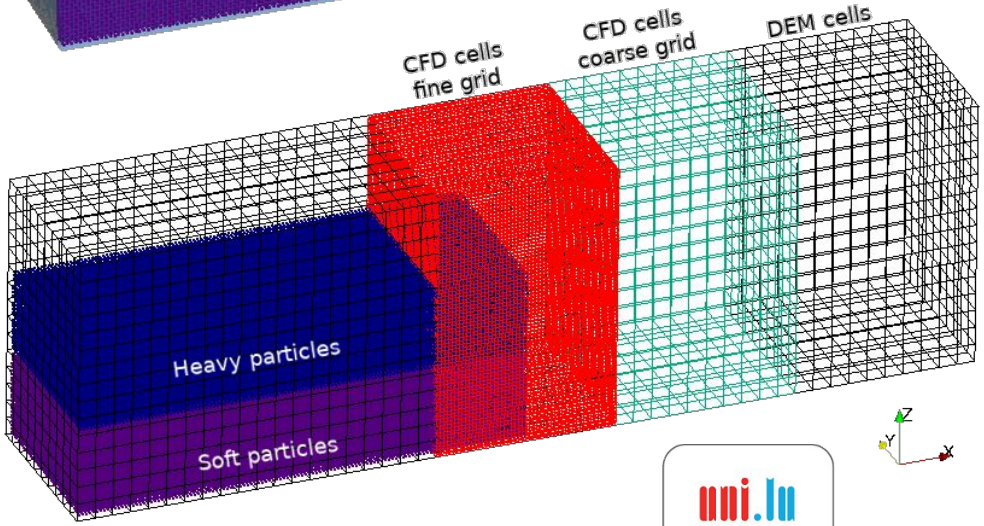
# Performance Evaluation

# Realistic Testcase: Dam Break

**Setup**

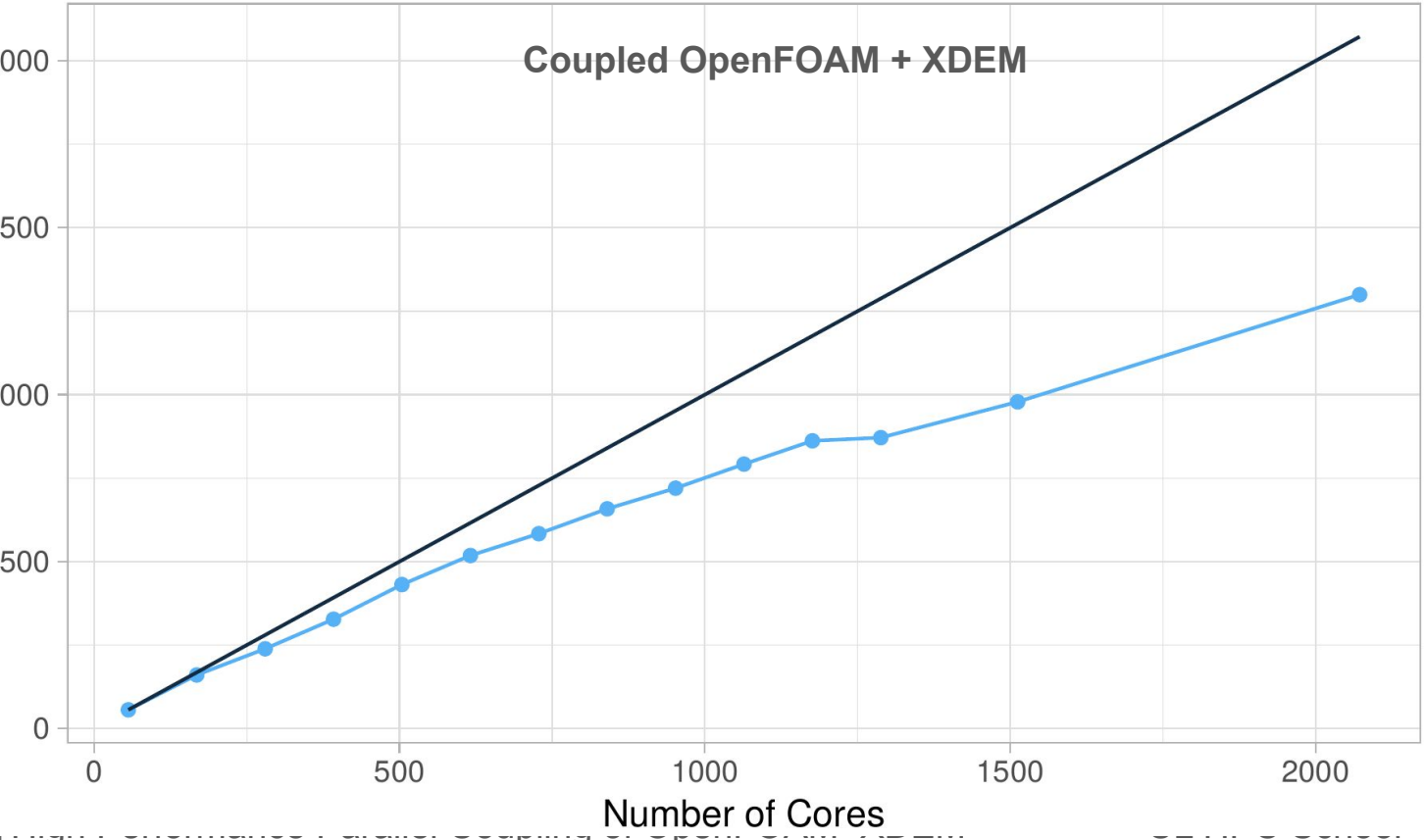
- 2.35M particles
- 10M CFD cells in the fine grid
- 500k CFD cells in the coarse grid
- Co-located partitions + Dual Grid
- Non-uniform distribution



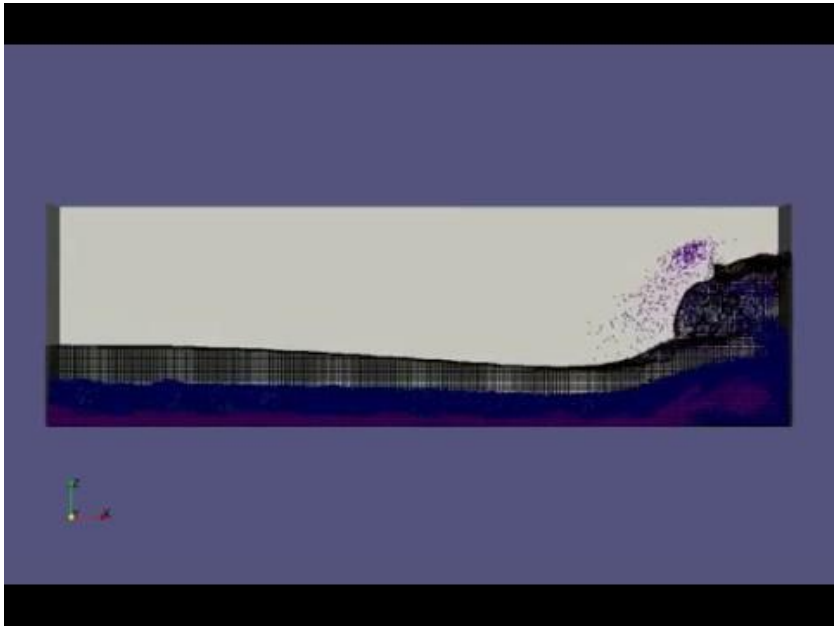

Running scalability test from 4 to 78 nodes

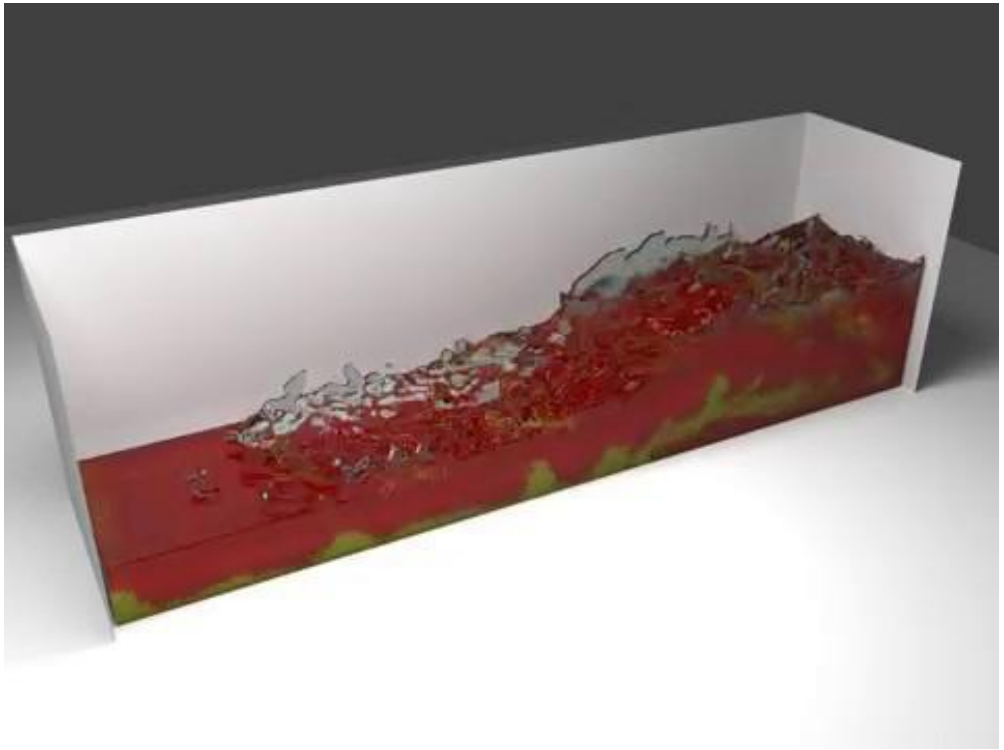
# Dam Break scalability (preliminary results)




**63% efficiency**

# Realistic Testcase: Dam Break





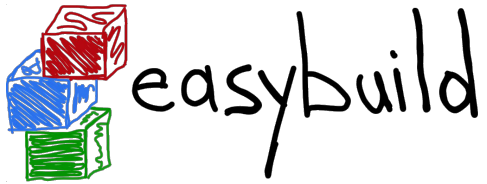
# LuXDEM Resarch on UL HPC

# LuXDEM Research on UL HPC 1/2

4,481,331 of core.hours used since the launch of Iris

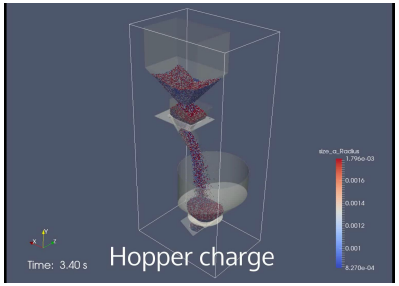
Developing, testing and running our own MPI+OpenMPI C++ code: XDEM

Dedicated set of modules build on top of the ones provided by UL HPC



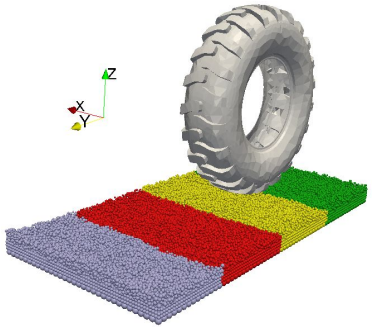

- XDEM requires more than 15 dependencies or tools
  - foam-Extend, SuperLU, METIS, SCOTCH, Zoltan, ParaView, etc.
- 3 toolchains supported
  - Intel Compiler + Intel MPI, GCC + OpenMPI, GCC + MVAPICH2
- Installed in our project directory and available for our team members

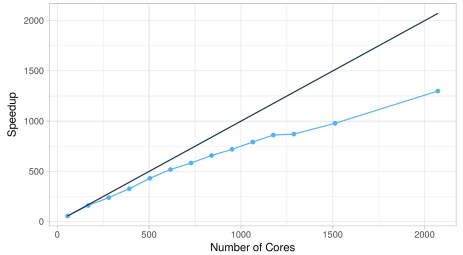
# LuXDEM Research on UL HPC 2/2



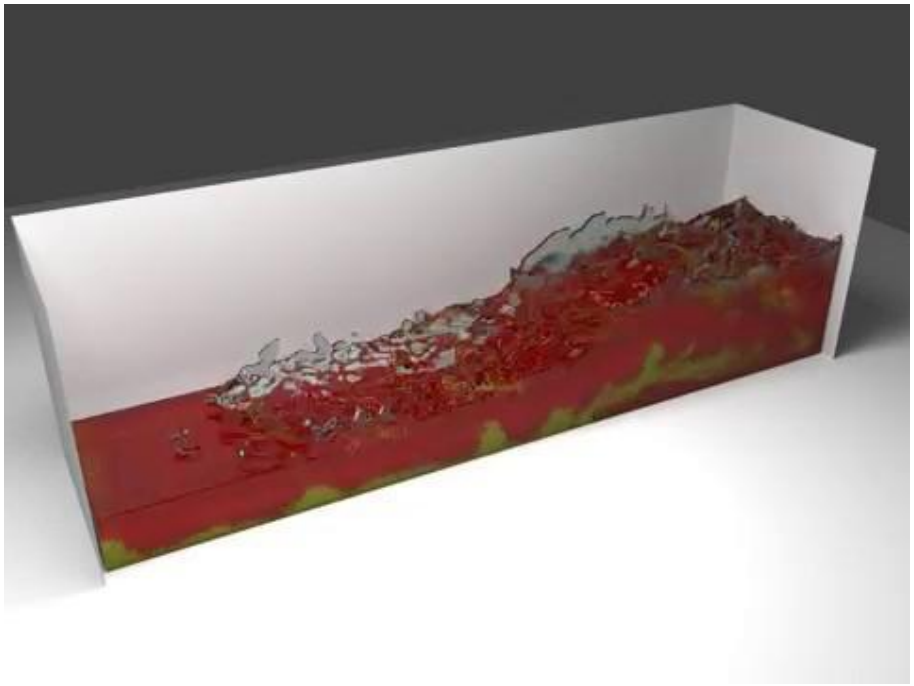

Main types of jobs

- XDEM simulations in ‘production’ mode,
  - Small number of cores (< 100) for a long time, in batch mode
  - Sometime with checkpoint/restart
- Post-processing of the XDEM (e.g. visualization)
  - Few cores (<6) for a short time in interactive mode
- Development & performance evaluation of XDEM
  - Large number of cores (> 700) for a short time (< 6 hours)
  - Mainly scalability studies
  - Complex launchers: varying number of cores, many toolchains, ...



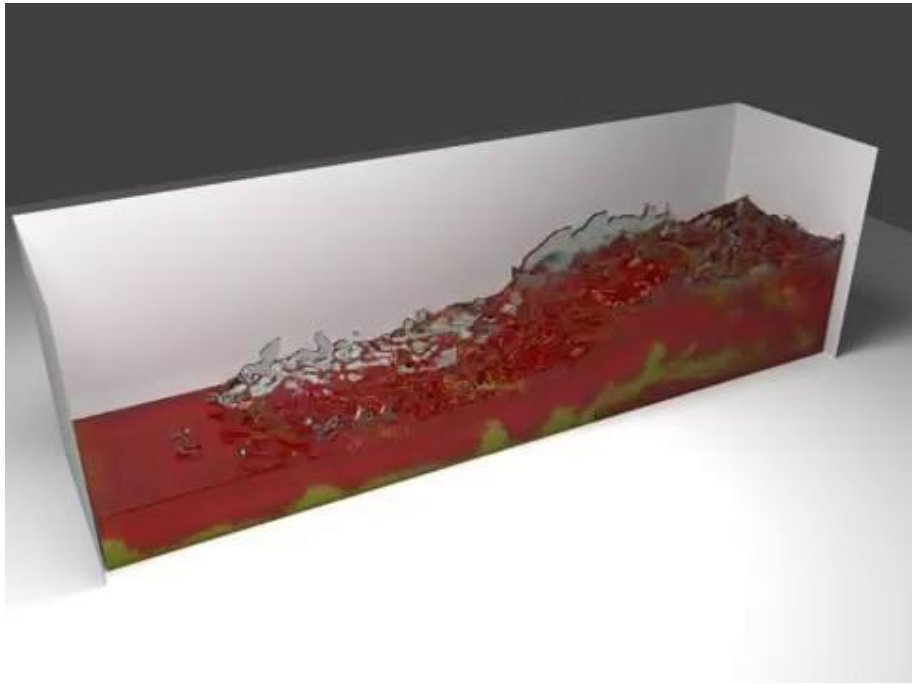



# Questions?



# Thank you for your attention!

Luxembourg XDEM Research Centre
http://luxdem.uni.lu/
University of Luxembourg



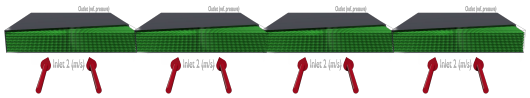
**A parallel dual-grid multiscale approach to CFD–DEM couplings**
G. Pozzetti, H. Jasak, X. Besseron, A. Rousset and B. Peters
Journal of Computational Physics, February 2019
https://doi.org/10.1016/j.jcp.2018.11.030

The experiments presented in this work were carried out using the HPC facilities of the University of Luxembourg. https://hpc.uni.lu

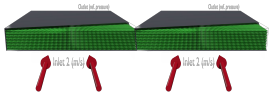
This research is in the framework of the project DigitalTwin, supported by the programme Investissement pour la compétitivité et emploi - European Regional Development Fund under grant agreement 2016-01-002-06.

# Weak Scalability
# Communication Overhead

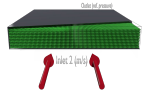
On 40 nodes



On 20 nodes



On 10 nodes



| #nodes | #cores #processes | Total #particles | Total #CFD cells | Average Timestep | Overhead | Inter-Physics Exchange |
|---|---|---|---|---|---|---|
| 10 | 280 | 2.5M | 2.5M | 1.612 s | - | 0.7 ms |
| 20 | 560 | 5M | 5M | 1.618 s | 1% | 0.6 ms |
| 40 | 1120 | 10M | 10M | 1.650 s | 2.3% | 0.6 ms |

**Other CFD-DEM solutions from literature** (on similar configurations)

- **MFIX: +160%** overhead from 64 to 256 processes [Gopalakrishnan2013]
- **SediFoam: +50%** overhead from 128 to 512 processes [Sun2016]

→ due to large increase of process-to-process communication