

High Performance Parallel Coupling of OpenFOAM+XDEM

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UL HPC School - User Session
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What is XDEM?

What is XDEM?

eXtended Discrete Element Method

Particles Dynamics

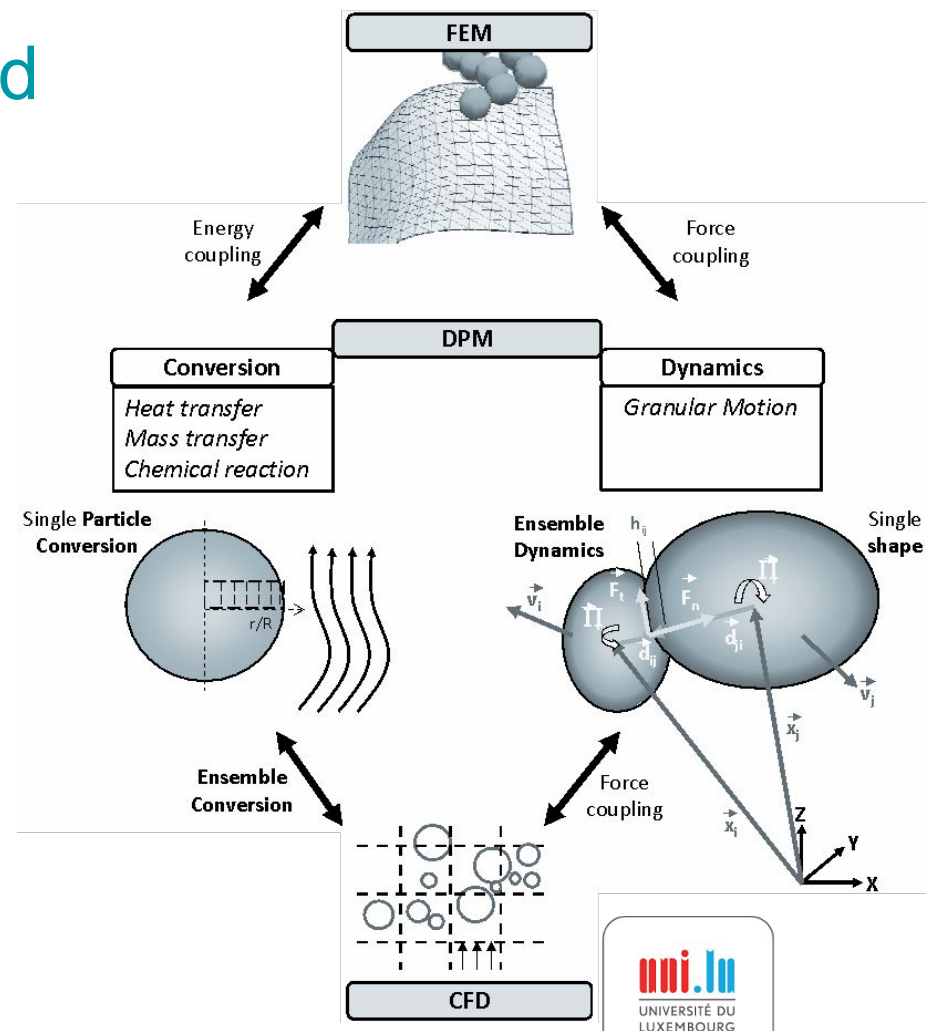
- Force and torques
- Particle motion

Particles Conversion

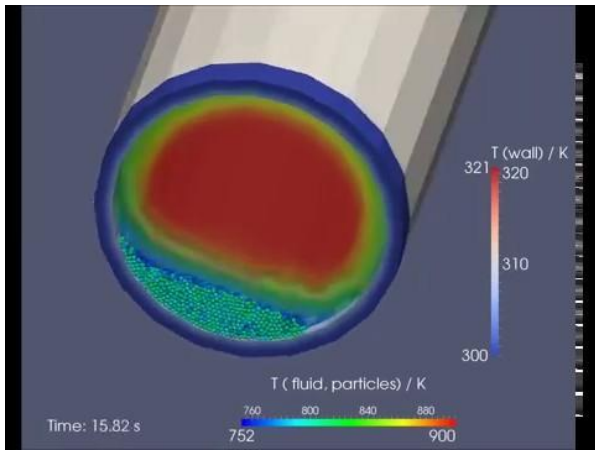
- Heat and mass transfer
- Chemical reactions

Coupled with

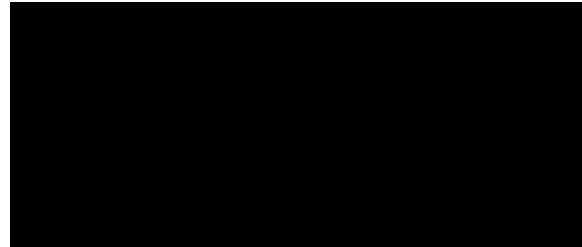
- Computational Fluid Dynamics (CFD)
- Finite Element Method (FEM)



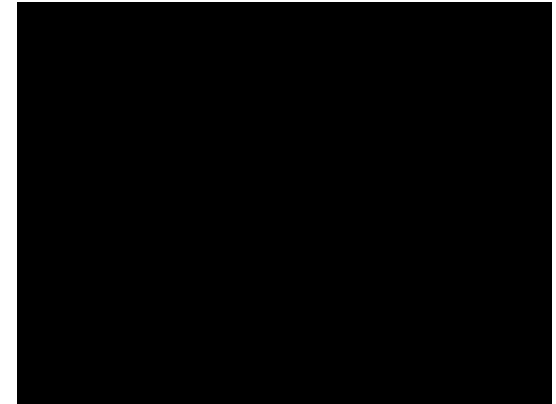
XDEM examples



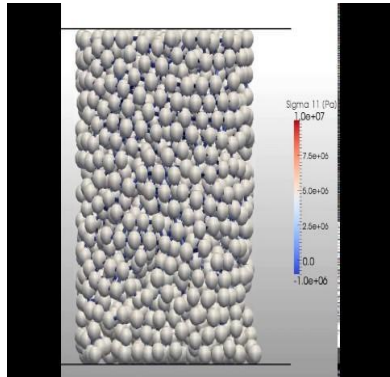
Heat transfer to the walls of a rotary furnace



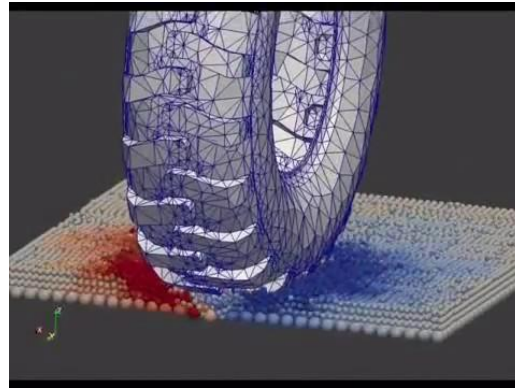
Impacts on an elastic membrane



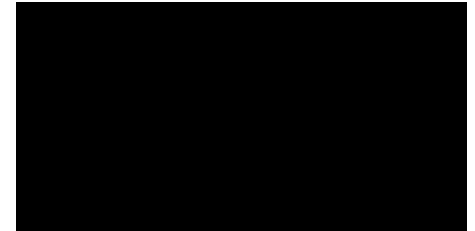
Charge/discharge of hoppers



Brittle failure



Tire rolling on snow



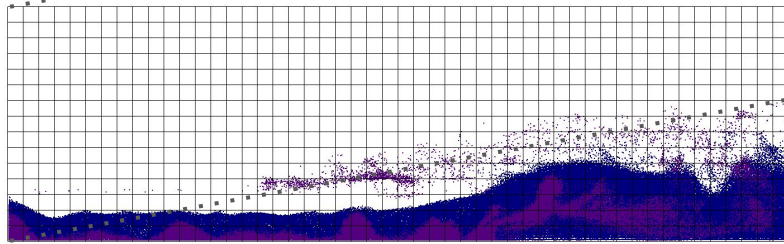
Fluidisation



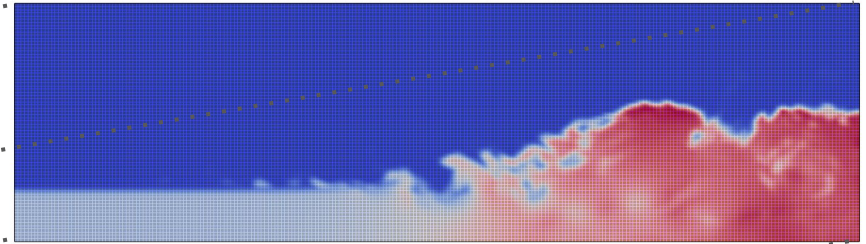
CFD-DEM Coupling

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

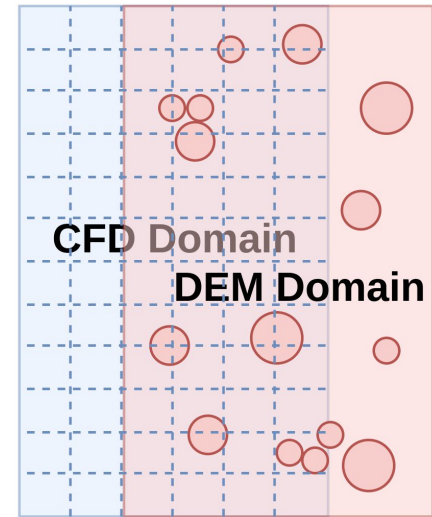
CFD ↔ XDEM

- Heat transfer
- Mass transfer

CFD-DEM Parallel Coupling: Challenges

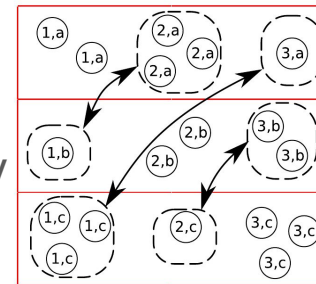
Challenges in CFD-XDEM parallel coupling

- 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

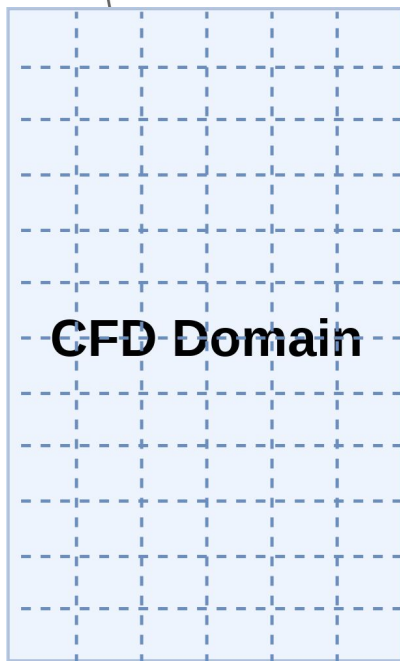


SediFoam [Sun2016]

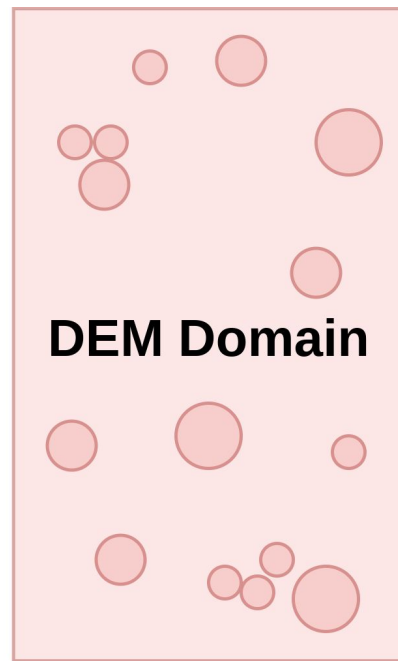


CFD-DEM Parallel Coupling: Challenges

OpenFOAM



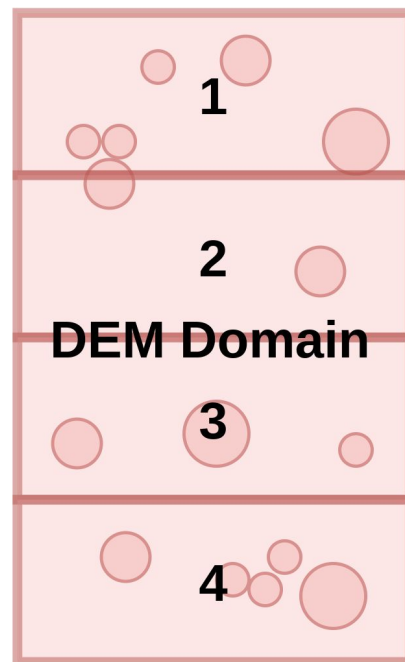
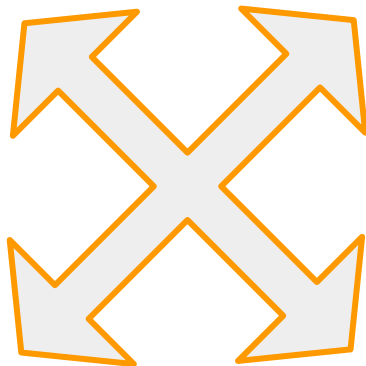
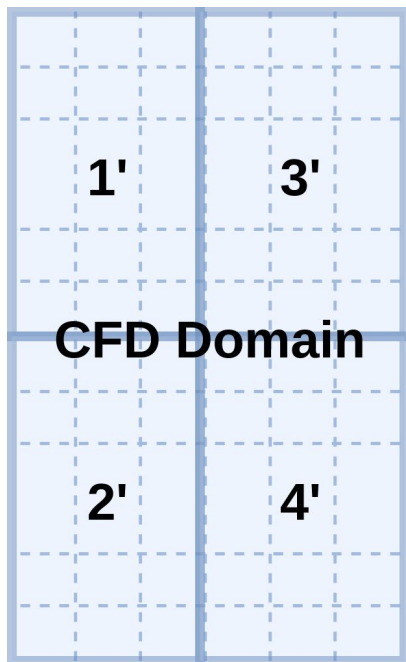
XDEM



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

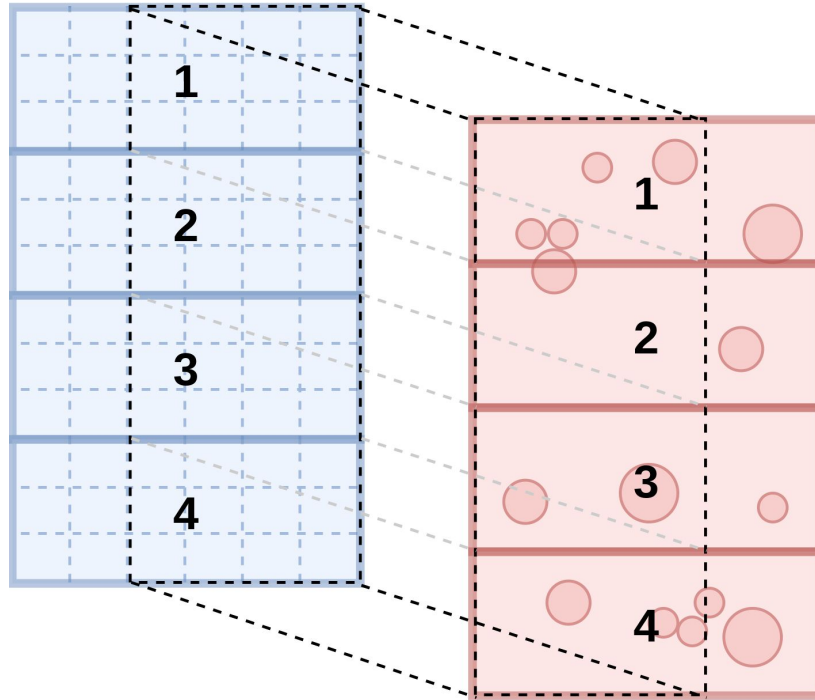
G. Pozzetti, X. Besseron, A. Rousset and B. Peters

Journal of Advanced Powder Technology, December 2018

<https://doi.org/10.1016/j.appt.2018.08.025>

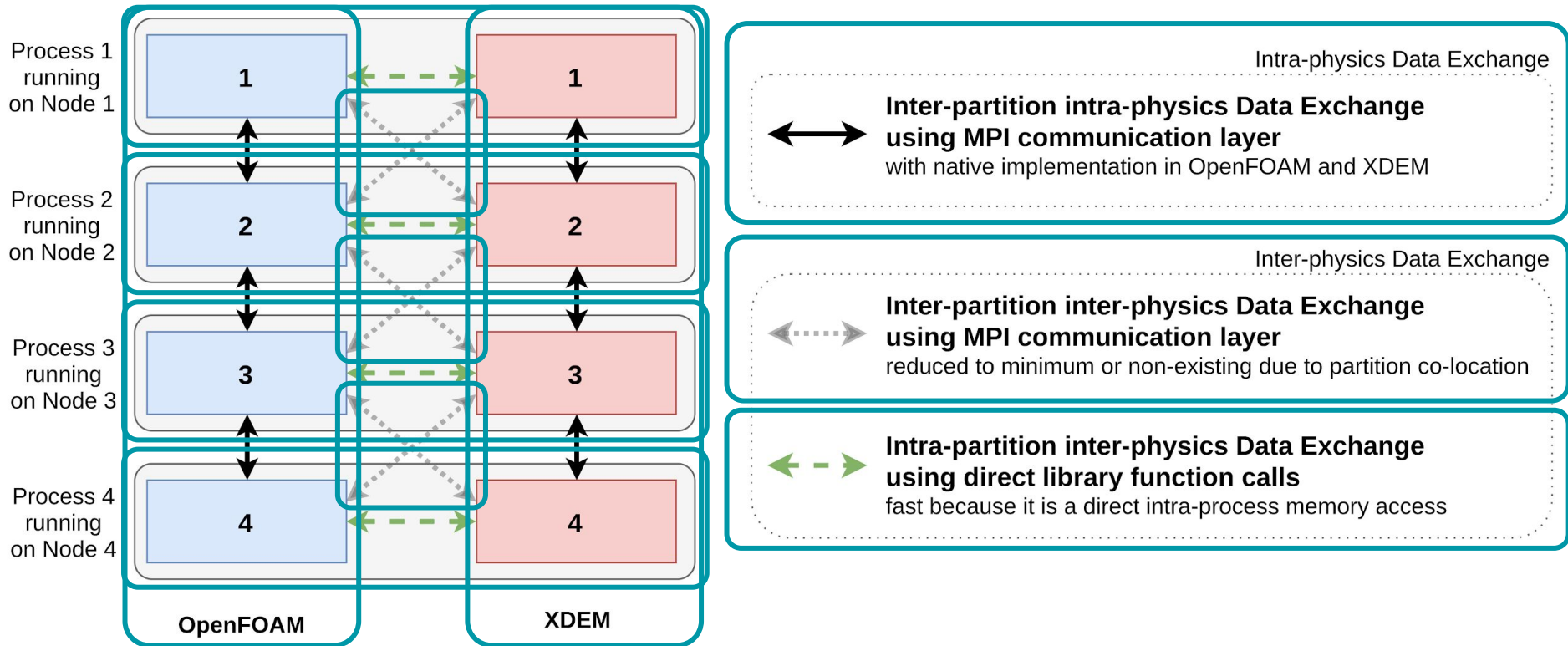


Co-located Partitioning Strategy



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

Co-located Partitioning Strategy: communication



Use direct library function calls if the two softwares are perfectly aligned

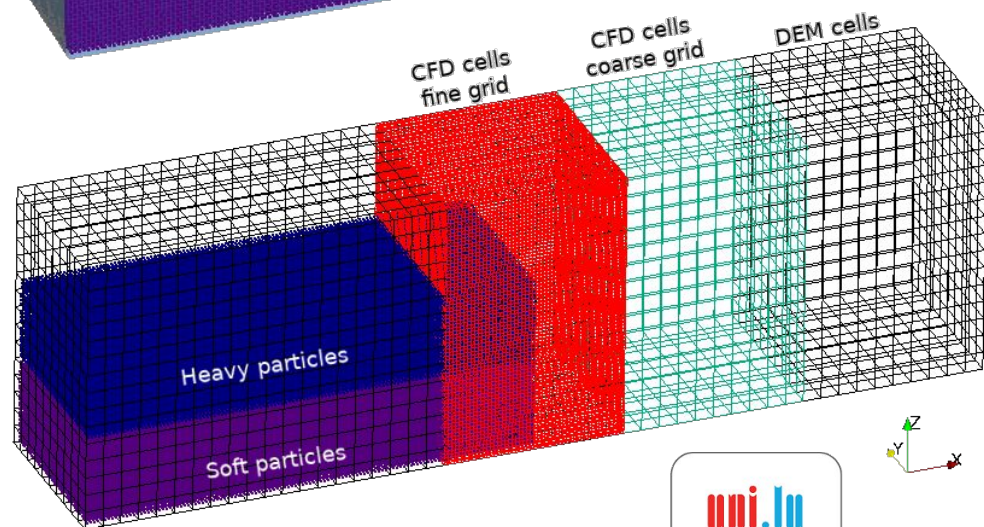
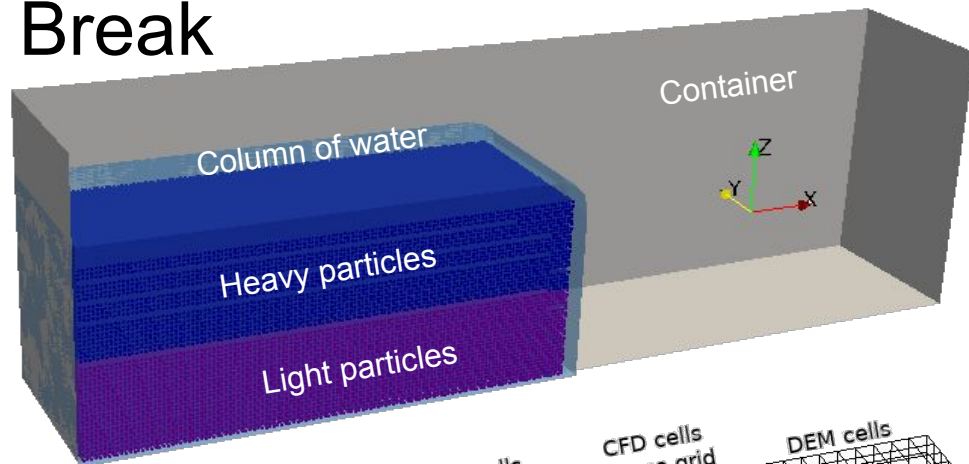


Performance Evaluation

Realistic Testcase: Dam Break

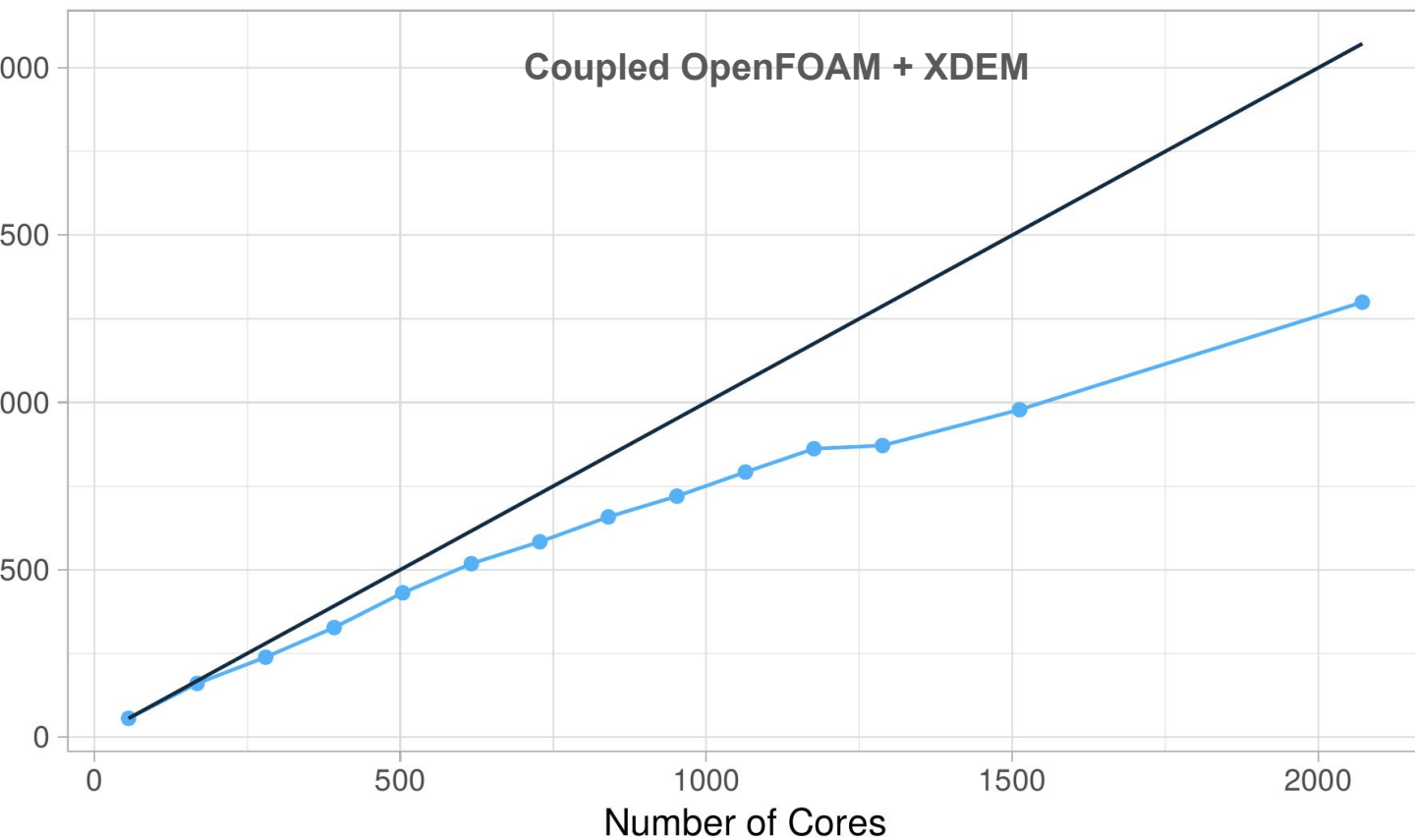
Setup

- 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

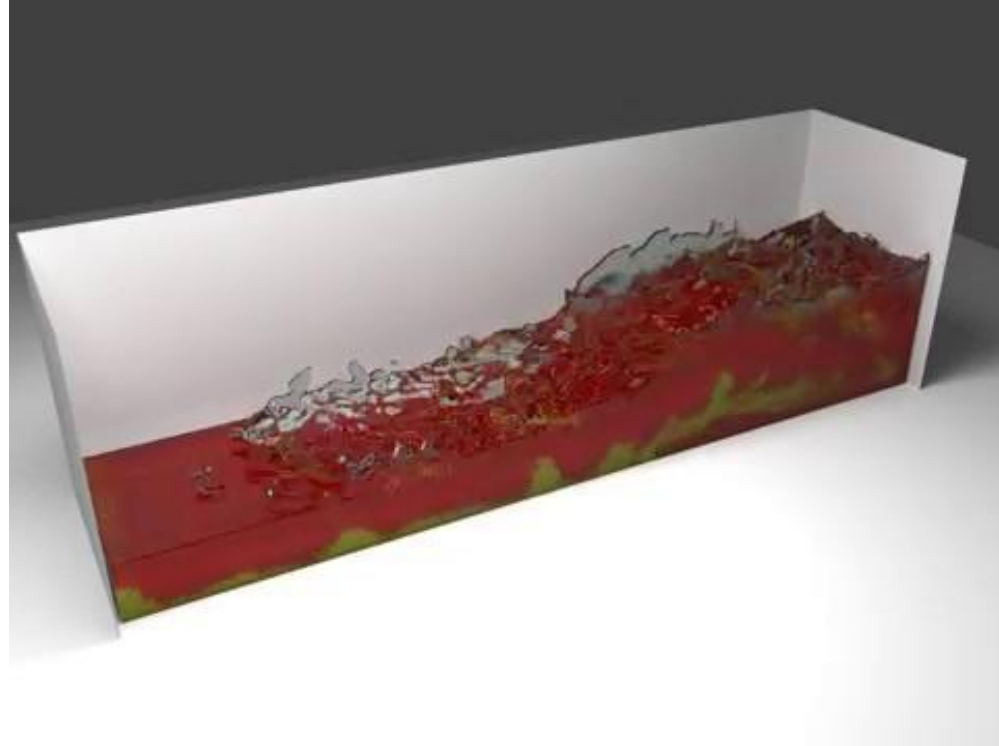
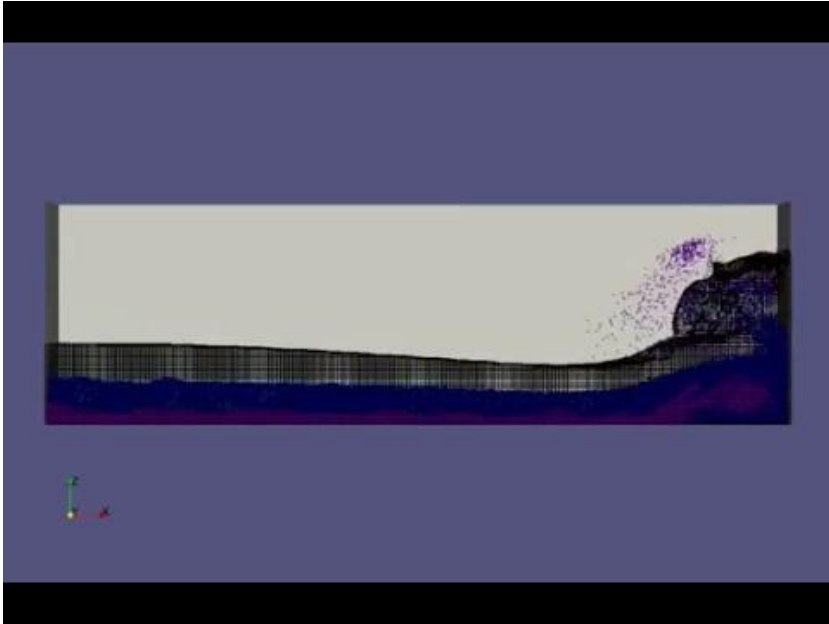
Dam Break scalability (preliminary results)



**63%
efficiency**



Realistic Testcase: Dam Break



LuXDEM Research on UL HPC

LuXDEM Research on UL HPC 1/2

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

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

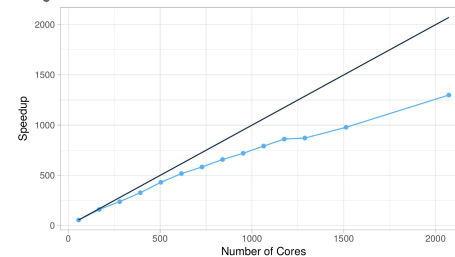
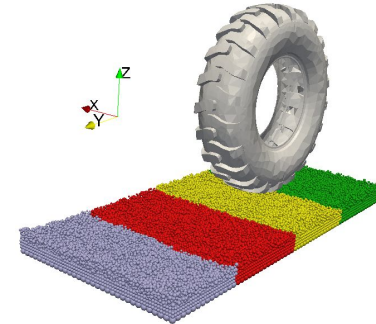
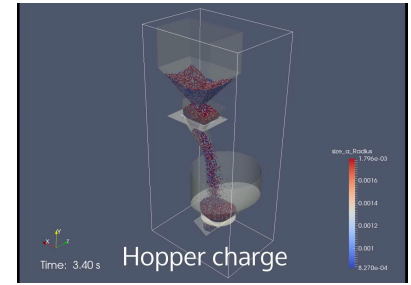
- XDEM requires more than 15 dependencies or tools
 - foam-Extend, SuperLU, METIS, SCOTCH, Zoltan, ParaView, etc.
- 3 toolchains supported
 - Intel Compiler + Intel MPI, GCC + OpenMPI, GCC + MVAPICH2
- Installed in our project directory and available for our team members



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



Questions?

Thank you for your attention!

Luxembourg XDEM Research Centre

<http://luxdem.uni.lu/>

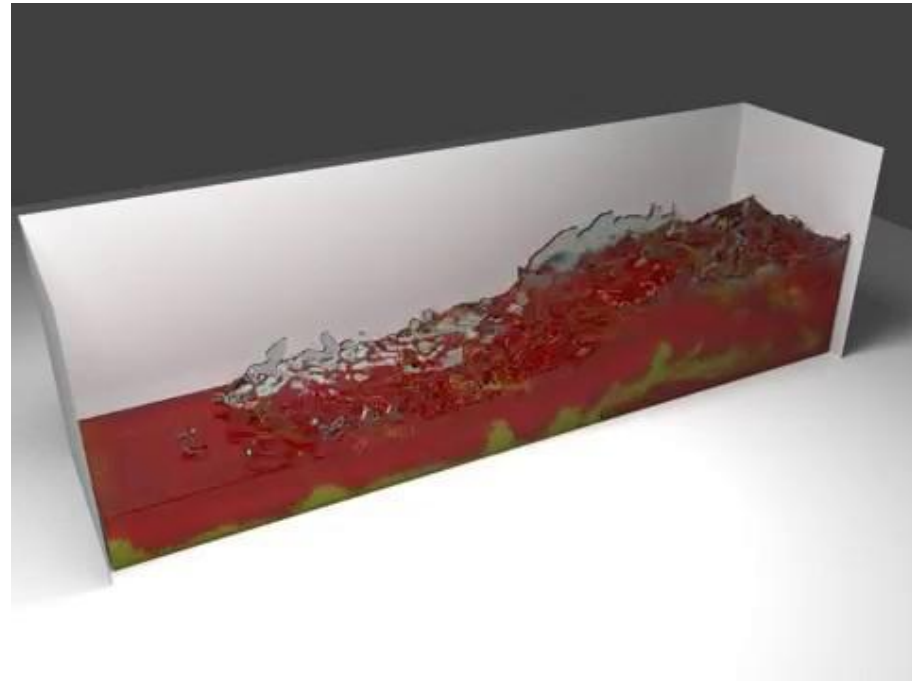
University of Luxembourg

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>



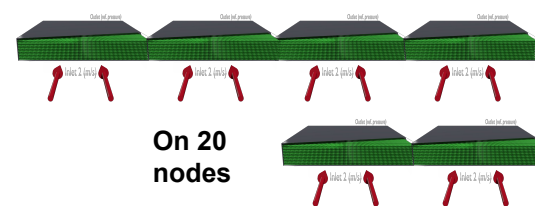
The experiments presented in this work were carried out using the HPC facilities of the University of Luxembourg. <https://hpc.uni.lu>

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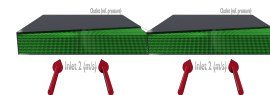


Weak Scalability Communication Overhead

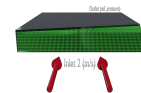
On 40
nodes



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