

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

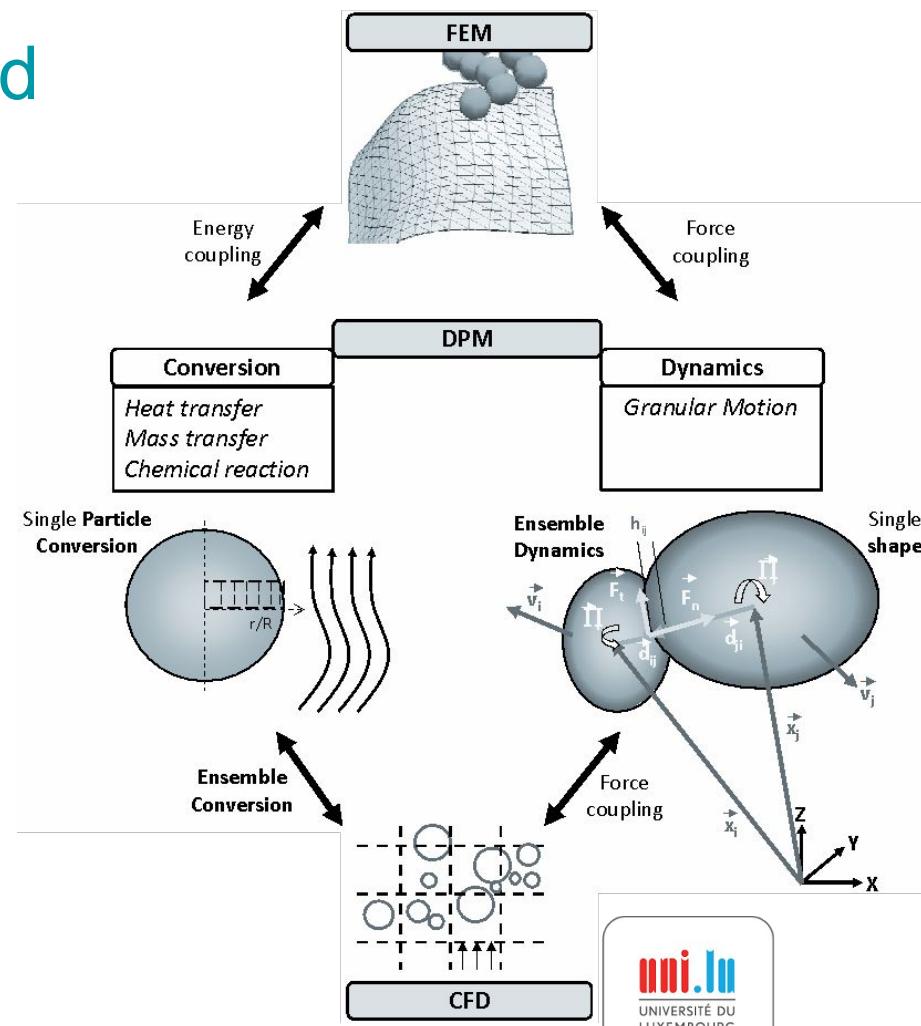
- Force and torques
- Particle motion

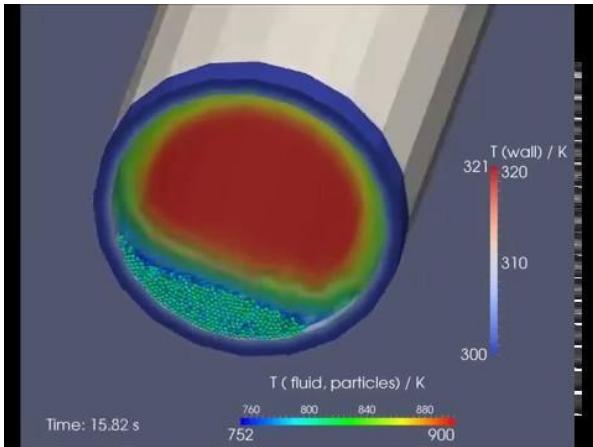
Particles Conversion

- Heat and mass transfer
- Chemical reactions

Coupled with

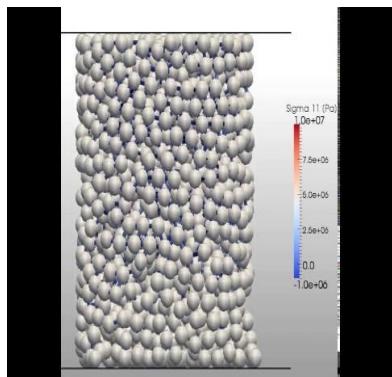
- Computational Fluid Dynamics (CFD)
- Finite Element Method (FEM)



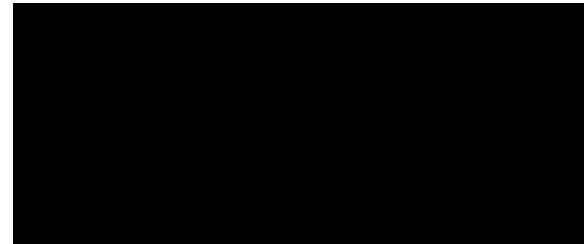


XDEM examples

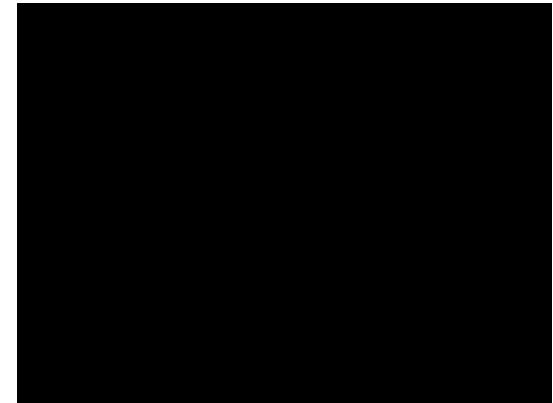
Heat transfer to the walls of a rotary furnace



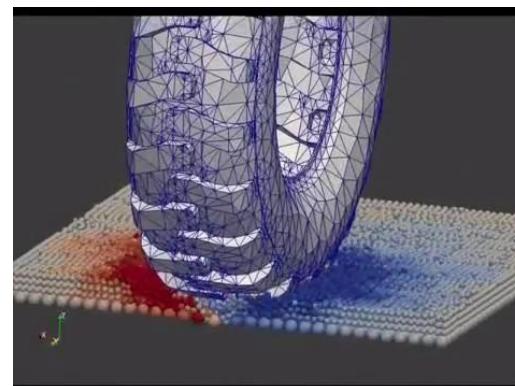
Brittle failure



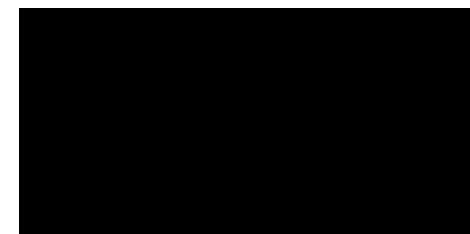
Impacts on an elastic membrane



Charge/discharge of hoppers



Tire rolling on snow

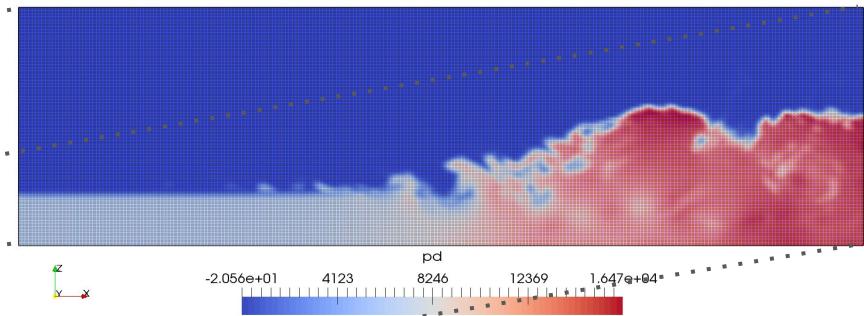
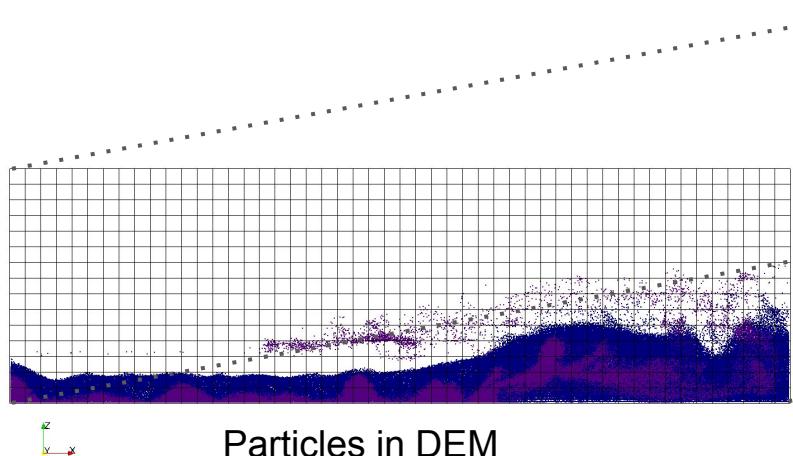


Fluidisation

CFD-DEM Coupling

CFD-(X)DEM Coupling

Moving particles interacting with liquid and gas



From CFD to DEM

- Lift force (buoyancy)
- Drag force

From DEM to CFD

- Porosity
- Particle source of momentum

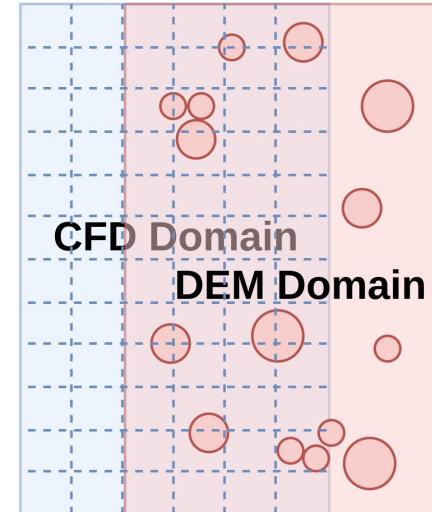
CFD ↔ XDEM

- Heat transfer
- Mass transfer

CFD-DEM Parallel Coupling: Challenges

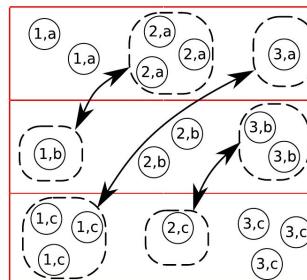
Challenges in CFD-XDEM parallel coupling

- 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

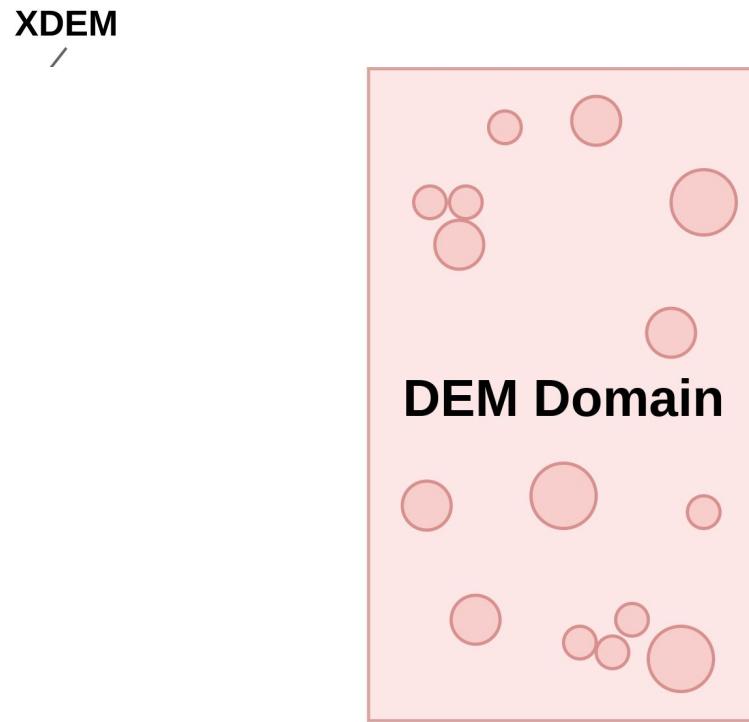
- Each software partitions its domain independently
- Data exchange in a peer-to-peer model



SediFoam [Sun2016]



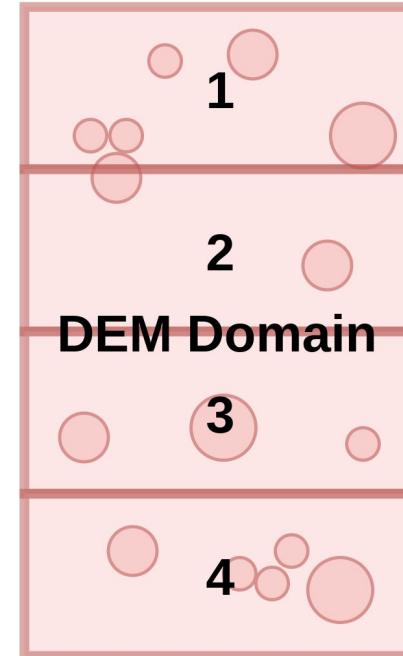
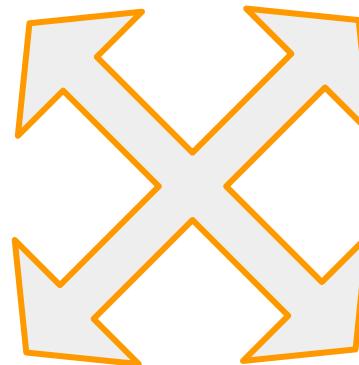
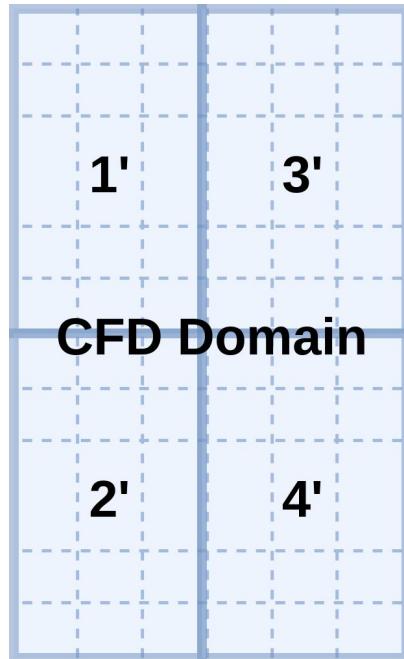
CFD-DEM Parallel Coupling: Challenges



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

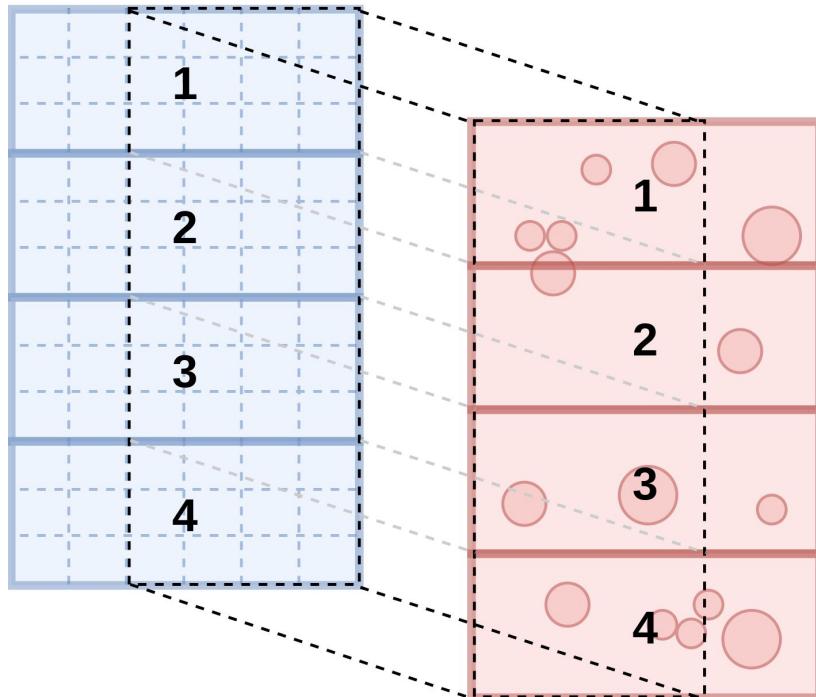
G. Pozzetti, X. Besson, A. Rousset and B. Peters

Journal of Advanced Powder Technology, December 2018

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

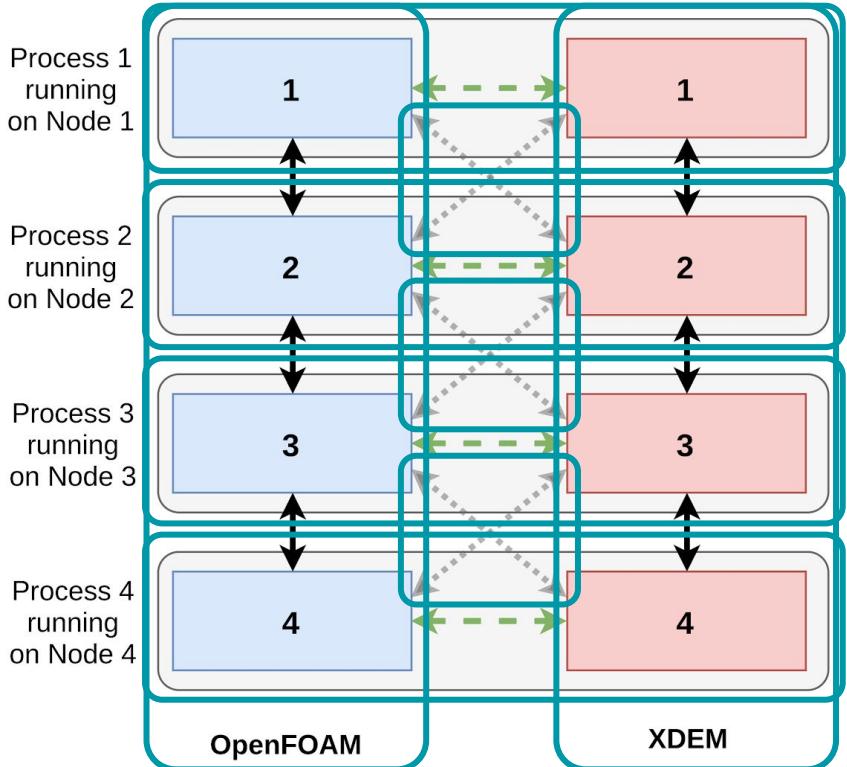


Co-located Partitioning Strategy



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

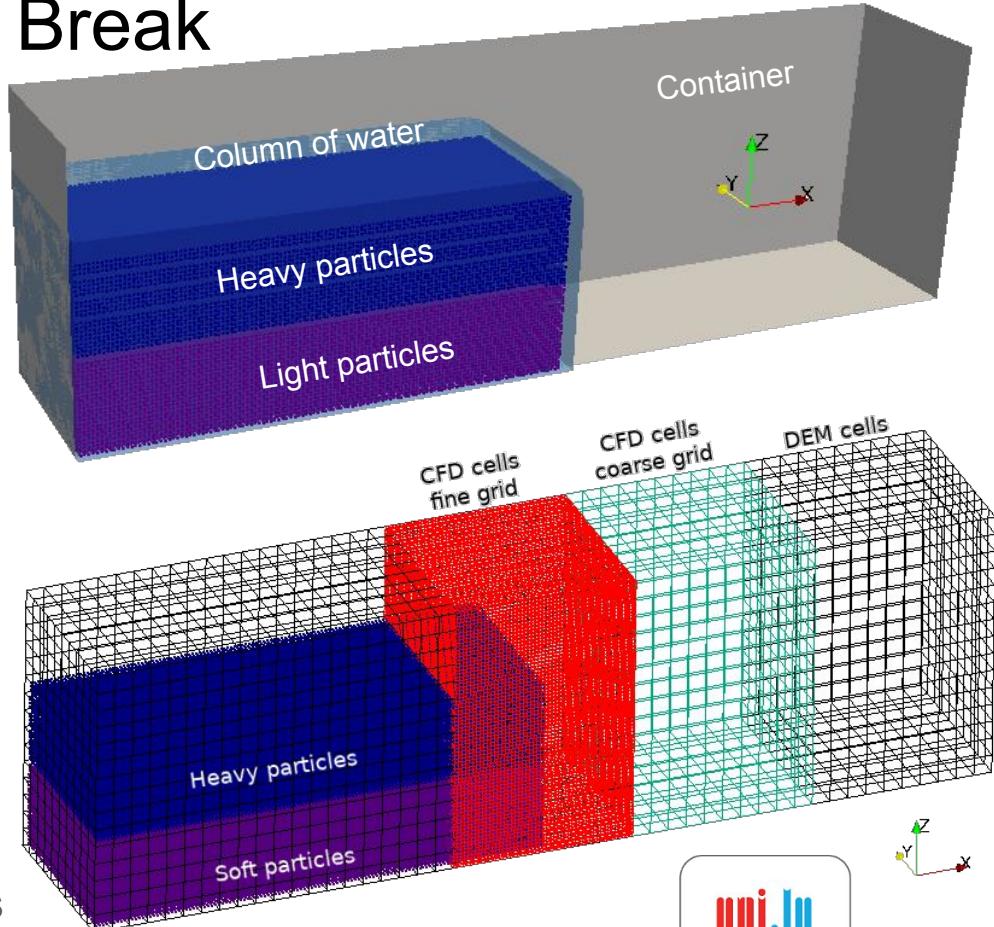
With a direct implementation strategy has software if the two softwares are perfectly aligned executable,

Performance Evaluation

Realistic Testcase: Dam Break

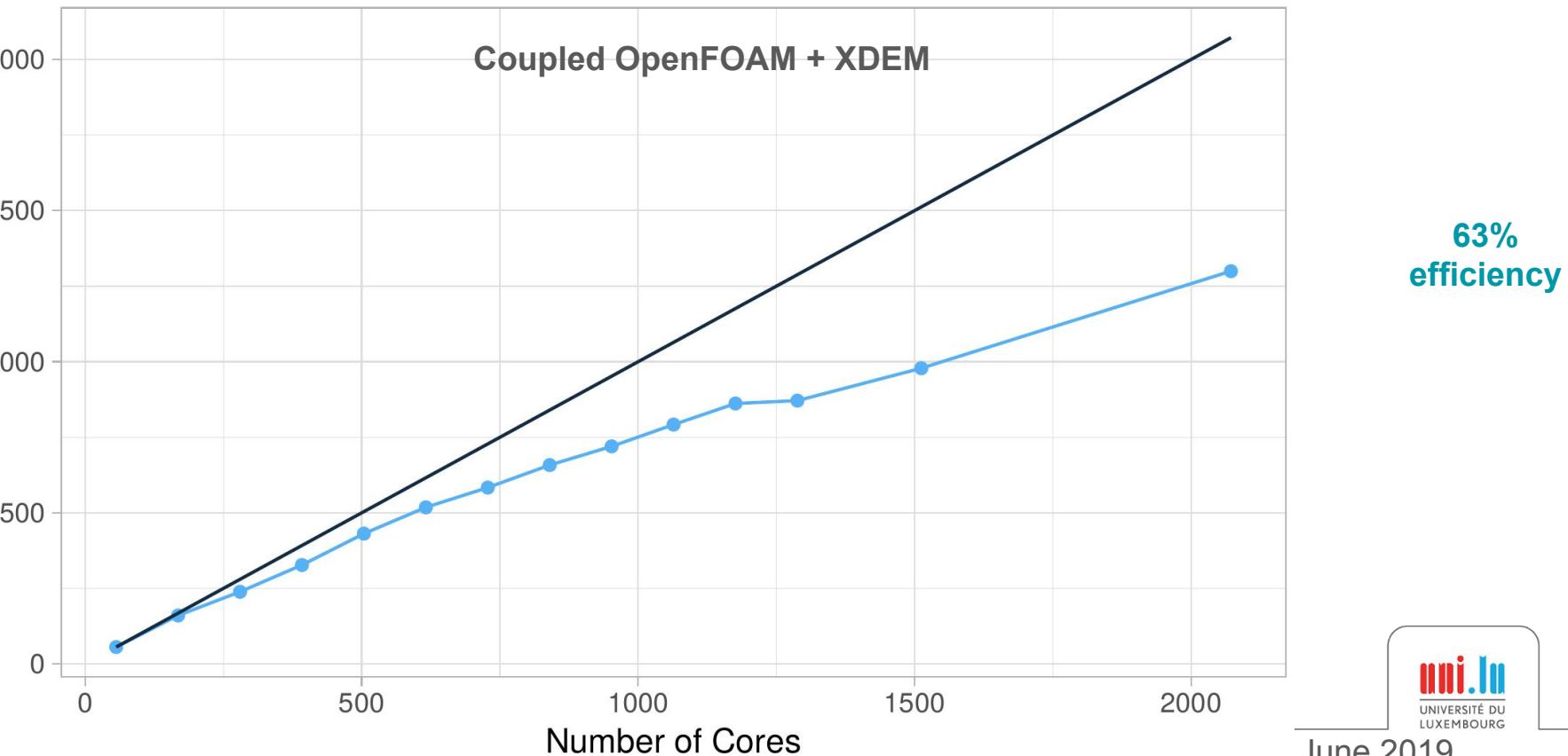
Setup

- 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

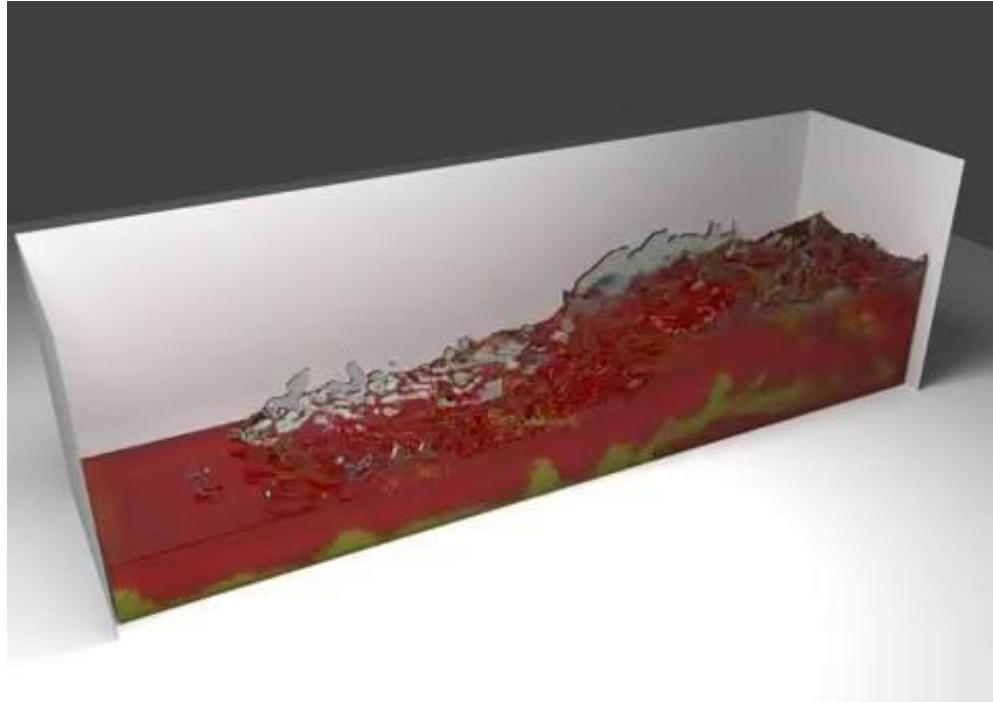
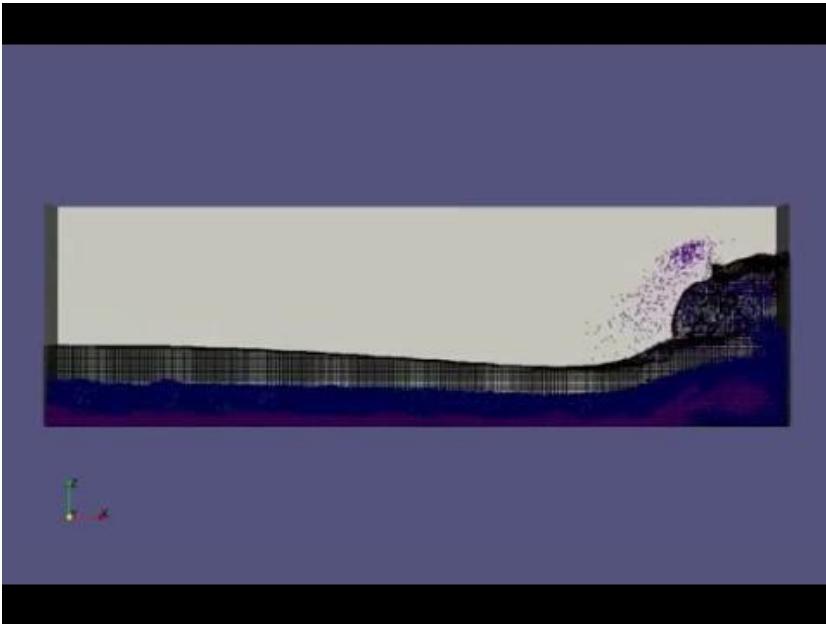


Running scalability test from 4 to 78 nodes

Dam Break scalability (preliminary results)



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

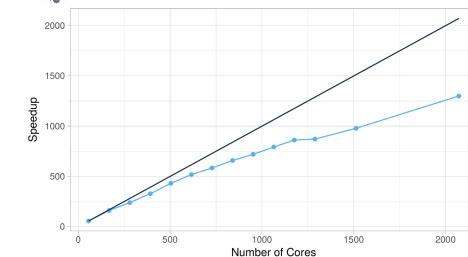
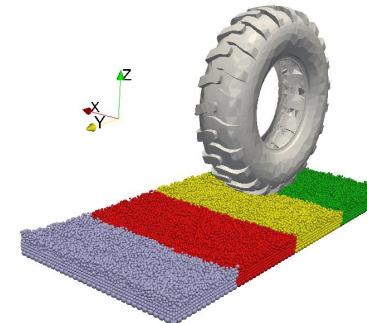
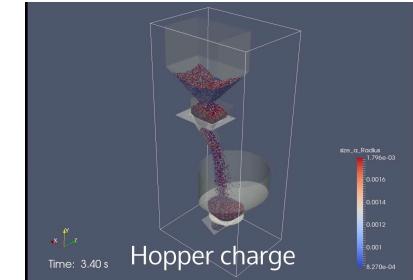
- XDEM requires more than 15 dependencies or tools
 - foam-Extend, SuperLU, METIS, SCOTCH, Zoltan, ParaView, etc.
- 3 toolchains supported
 - Intel Compiler + Intel MPI, GCC + OpenMPI, GCC + MVAPICH2
- Installed in our project directory and available for our team members



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/>

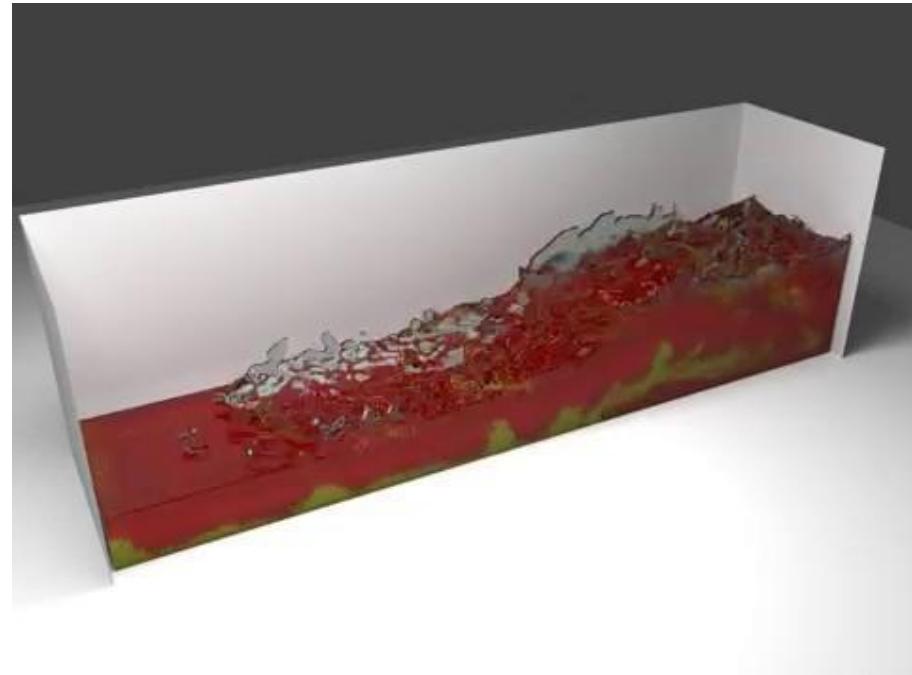
University of Luxembourg

A parallel dual-grid multiscale approach to CFD–DEM couplings

G. Pozzetti, H. Jasak, X. Besson, A. Rousset and B. Peters

Journal of Computational Physics, February 2019

<https://doi.org/10.1016/j.jcp.2018.11.030>



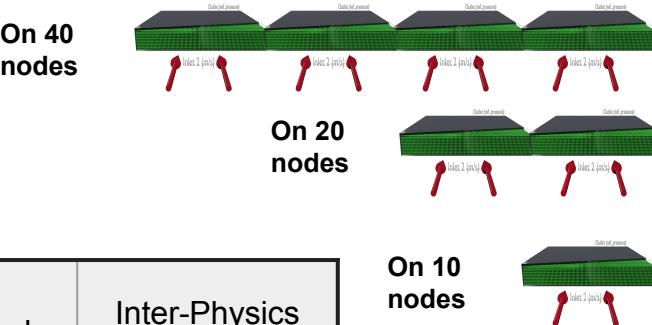
The experiments presented in this work were carried out using the HPC facilities of the University of Luxembourg. <https://hpc.uni.lu>



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



#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