Parallel Coupling of CFD-DEM simulations

MUG'2018

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Outline

Background

- What is XDEM?
- CFD-DEM Coupling

CFD-DEM Parallel Coupling

- Co-located Partitioning Strategy
- Dual-grid Multiscale Approach

Results

- Results Validation
- Performance Evaluation

Conclusion

- Future Work

What is XDEM?

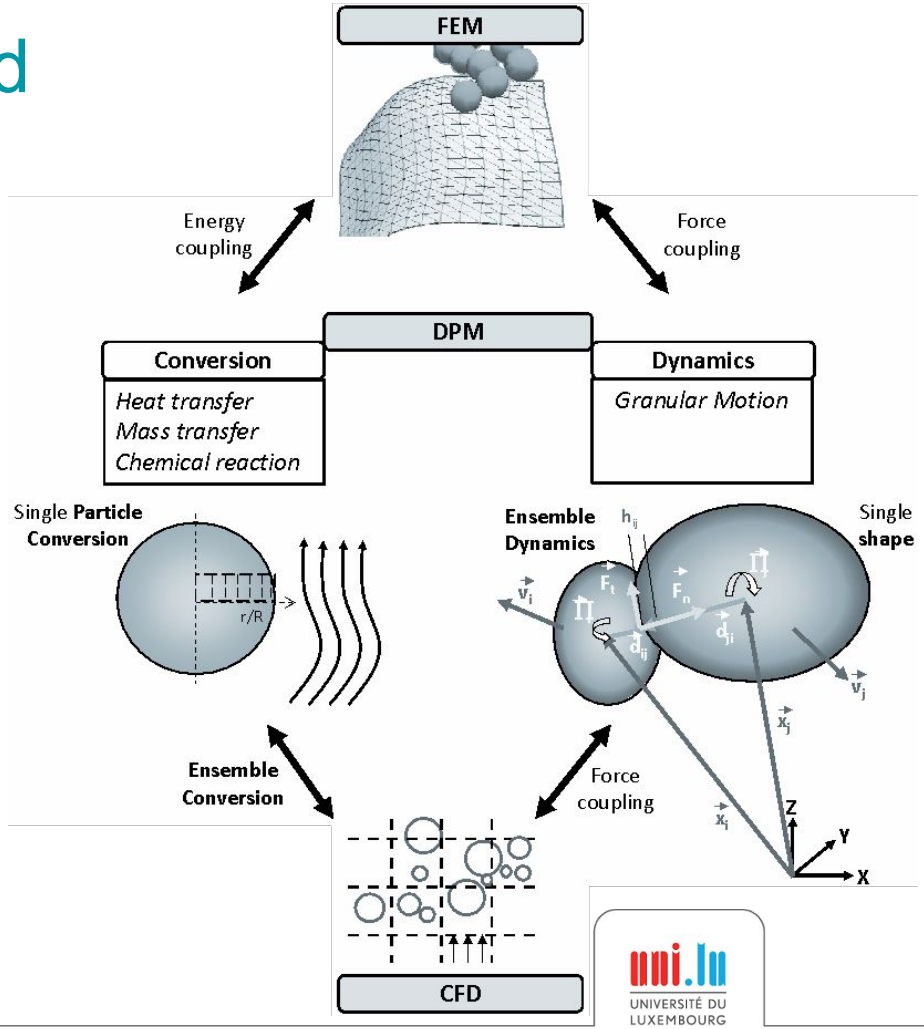
What is XDEM?

eXtended Discrete Element Method

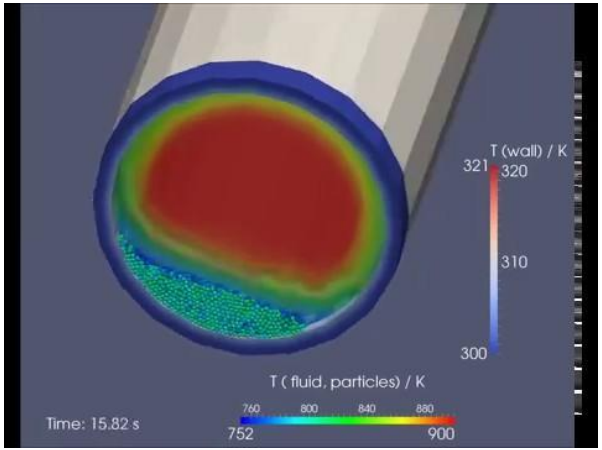
Dynamics
- Force and torques
- Particle motion

Conversion
- Heat and mass transfer
- Chemical reactions

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



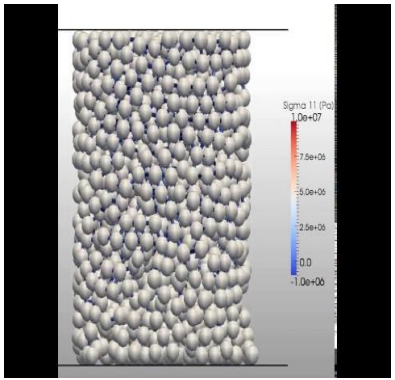
Examples



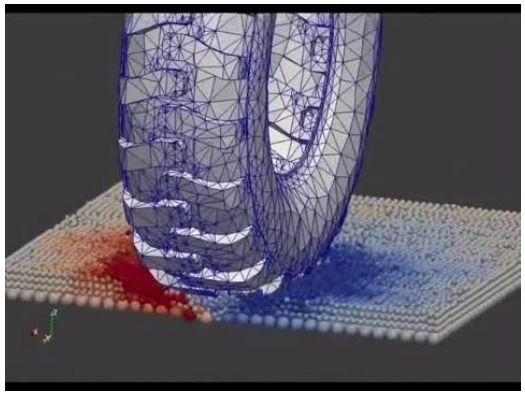
Heat transfer to the walls of a rotary furnace

Impacts on an elastic membrane

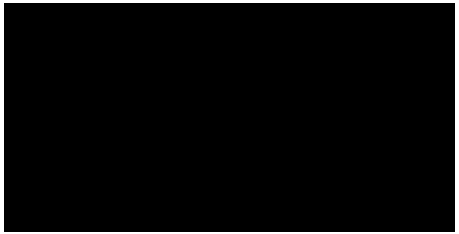
Charge/discharge of hoppers



Brittle failure



Tire rolling on snow



Fluidisation

(X)DEM needs HPC!

Hopper charge

- 15 s of simulation
- 92 hours with 120 cores
- Est. seq. time > 4 months

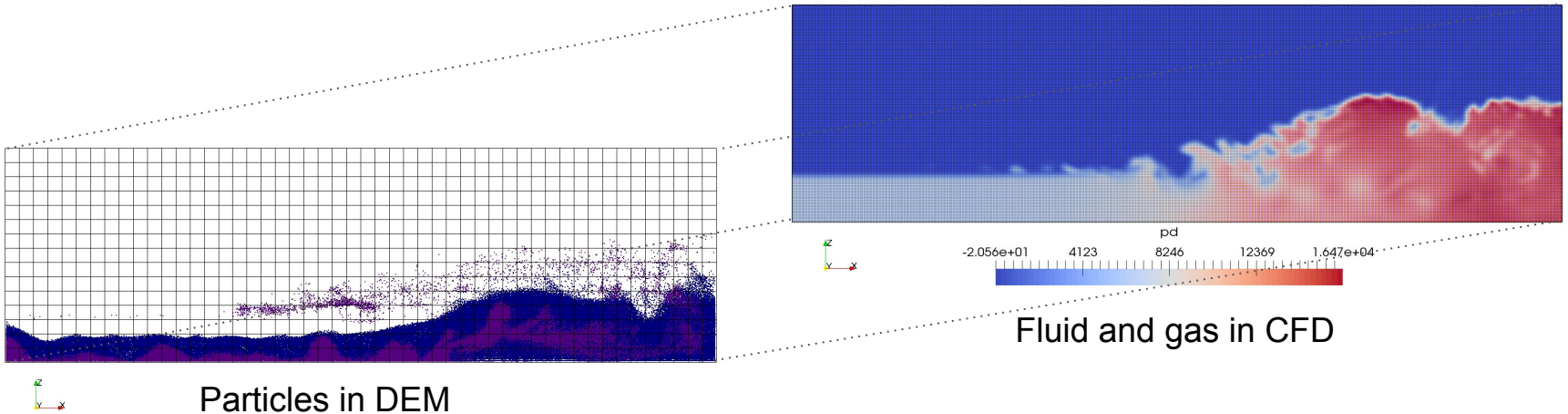
Hopper discharge

- 18 s of simulation
- 120 hours with 144 cores
- Est. seq. time > 6 months

CFD-DEM Coupling

CFD-(X)DEM Coupling

Moving particles interacting with fluid and gas



From CFD to DEM

- Lift force (buoyancy)
- Drag force

From DEM to CFD

- Porosity
- Particle source of momentum

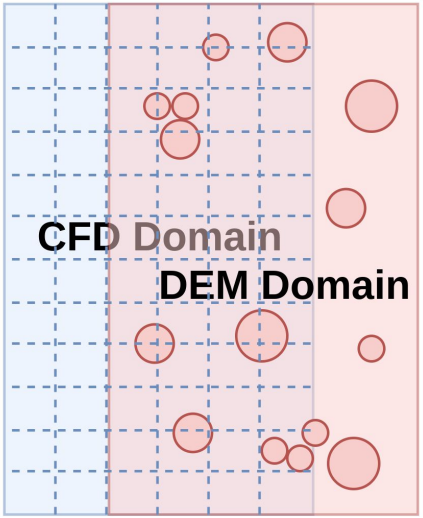
CFD ↔ XDEM

- Heat transfer
- Mass transfer

CFD-DEM Parallel Coupling: Challenges

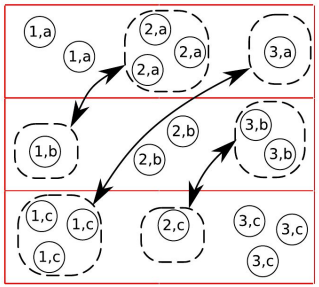
Challenges in CFD-XDEM parallel coupling

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



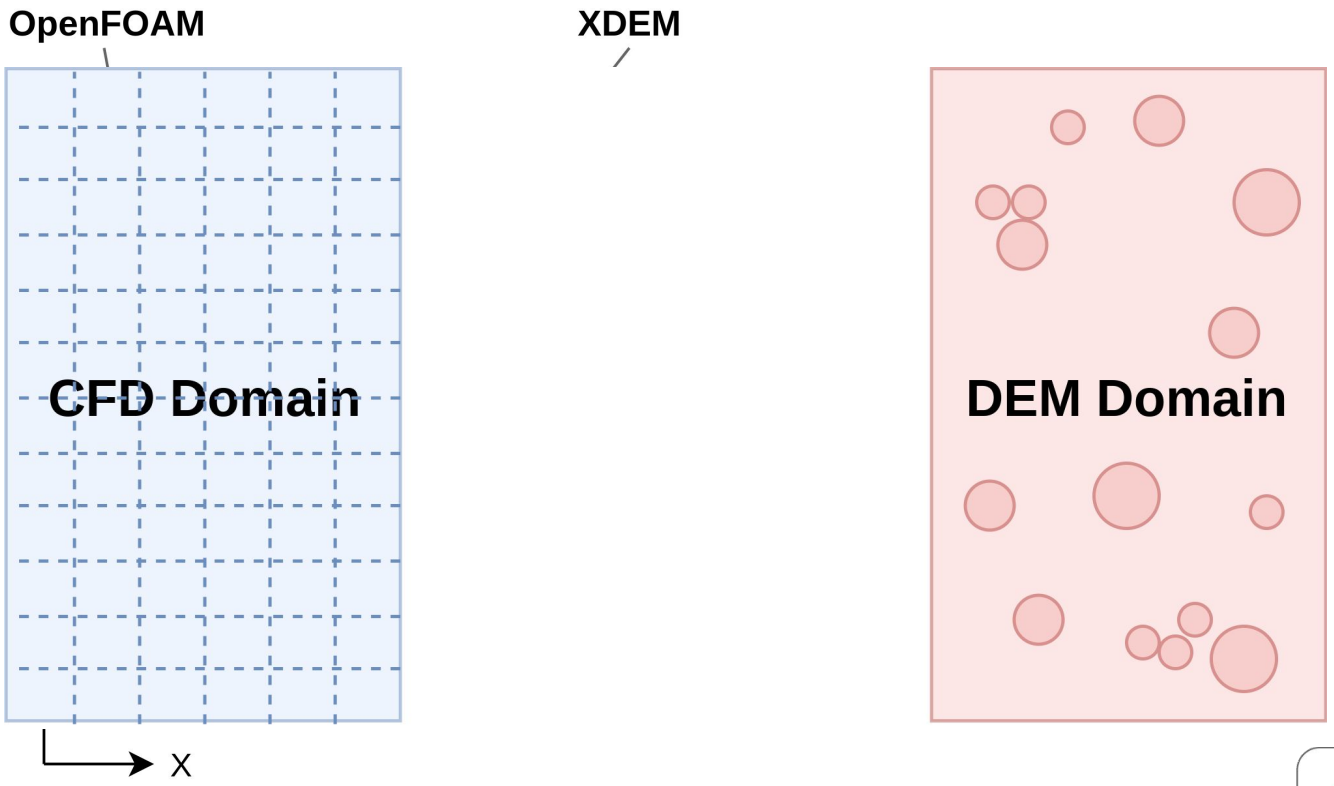
Classical Approaches

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



SediFoam [Sun2016]

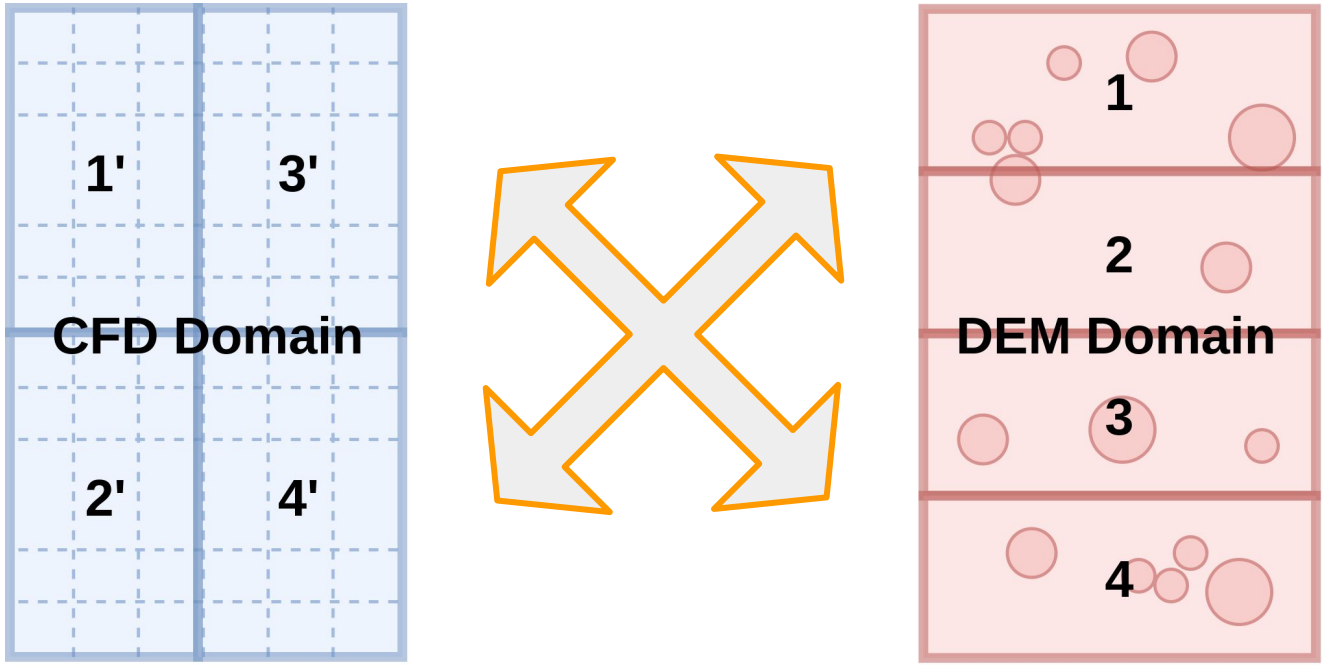
CFD-DEM Parallel Coupling: Challenges



The domains overlap in space

CFD-DEM Parallel Coupling: Challenges

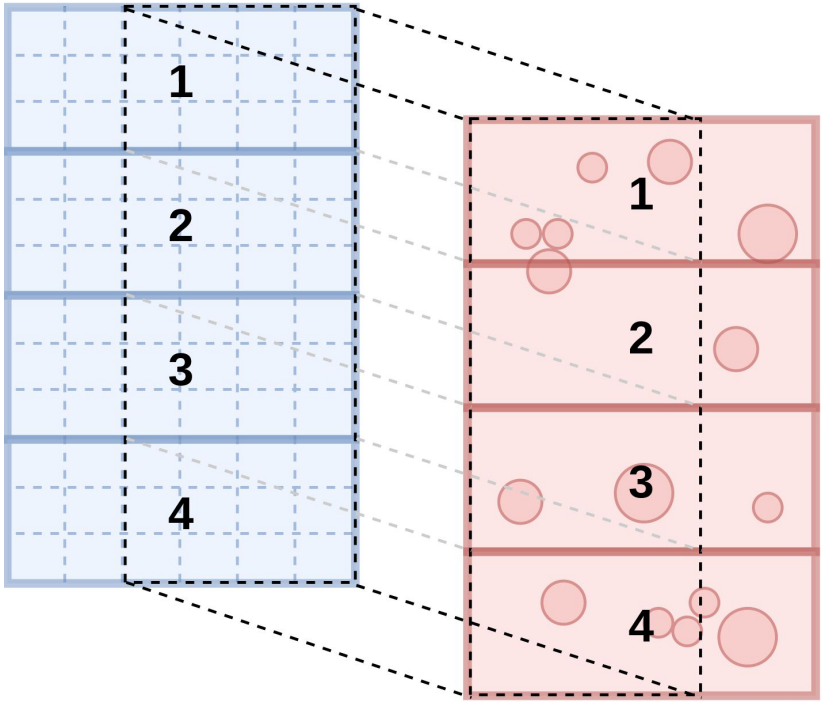
Classical Approach: the domains are partitioned independently



Unpredictable pattern and large volume of communication

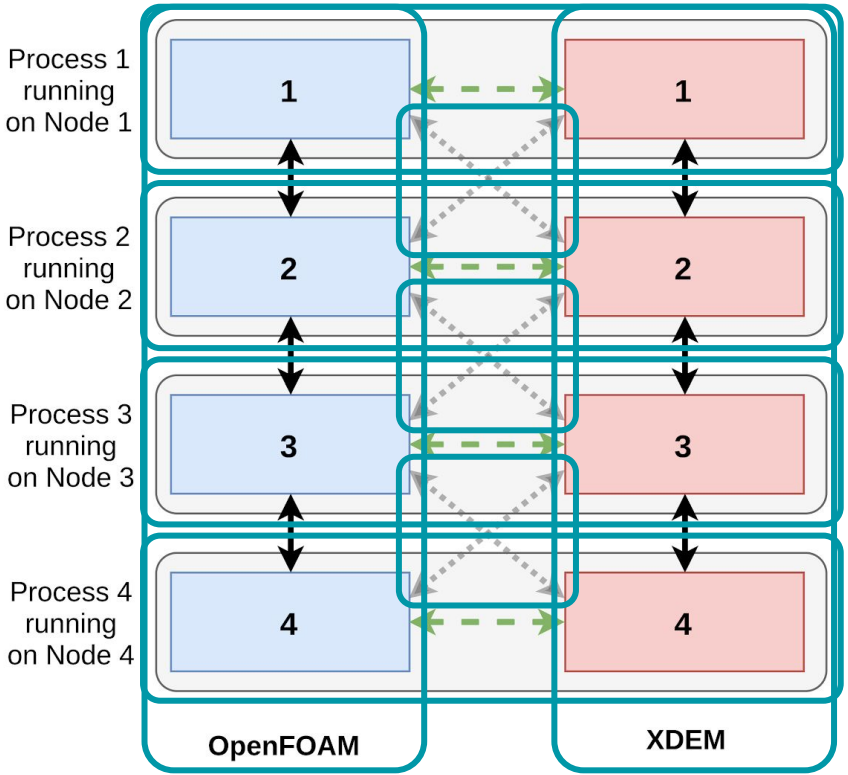
Co-located Partitioning Strategy

Co-located Partitioning Strategy



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

Co-located Partitioning Strategy



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

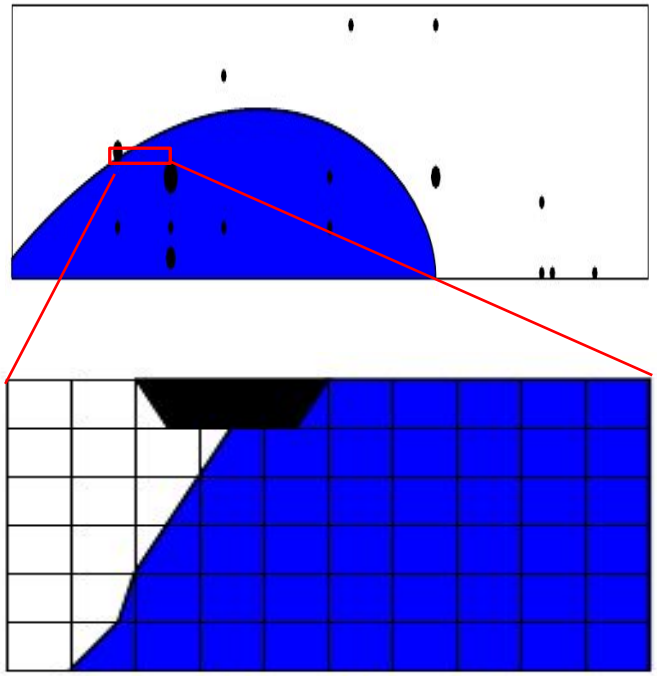
Intra-partition inter-physics Data Exchange using direct library function calls
fast because it is a direct intra-process memory access

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

Dual-Grid Multiscale Approach

Advantages of the dual-grid multiscale

Bulk coupling scale



Fluid fine scale

Coarse Mesh

Averaging Fluid-Particle interaction

Particle Fields

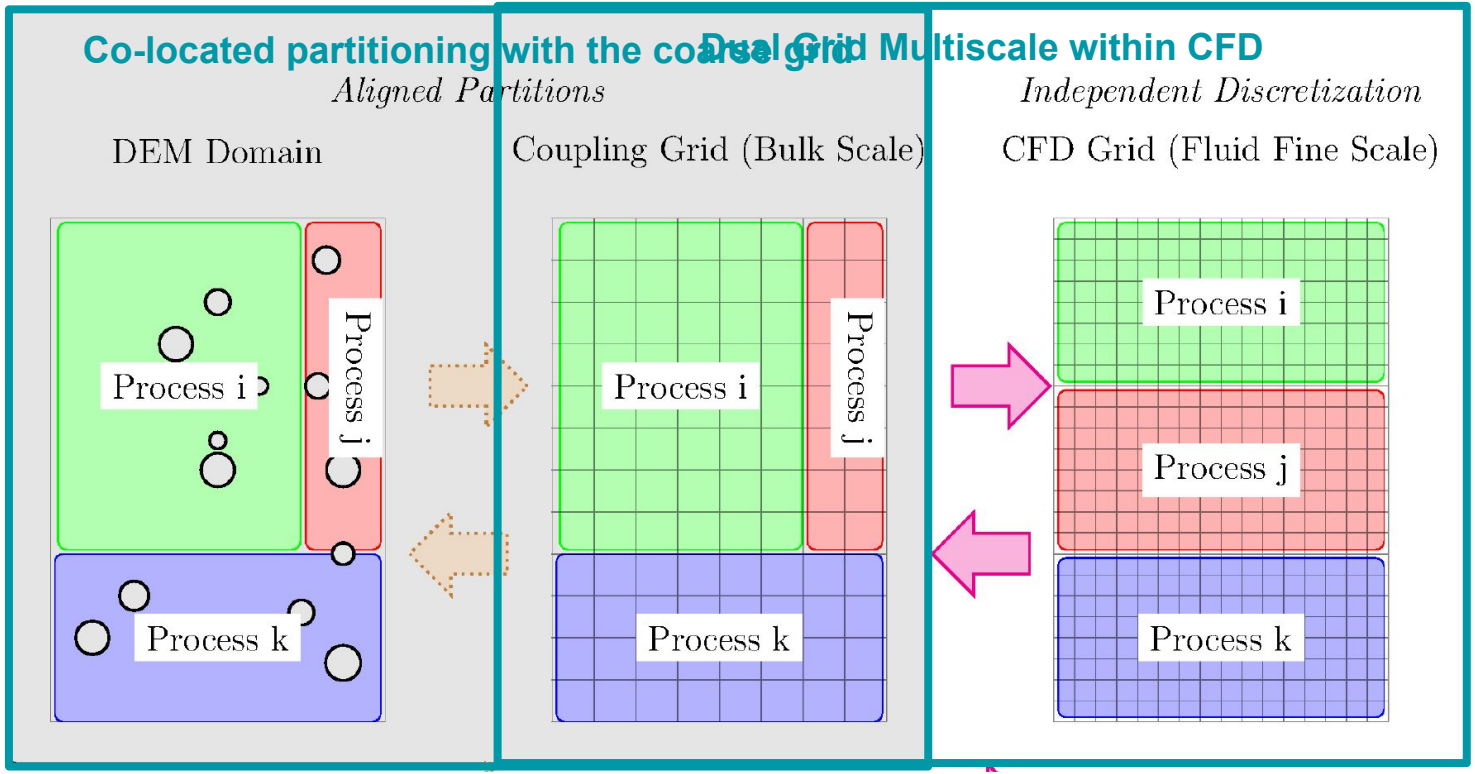
Fluid Solution

Fine Mesh

Solving fluid fine-scale

- **Keeping advantages of volume-averaged CFD-DEM**
- **Restoring grid-convergence of the CFD solution**

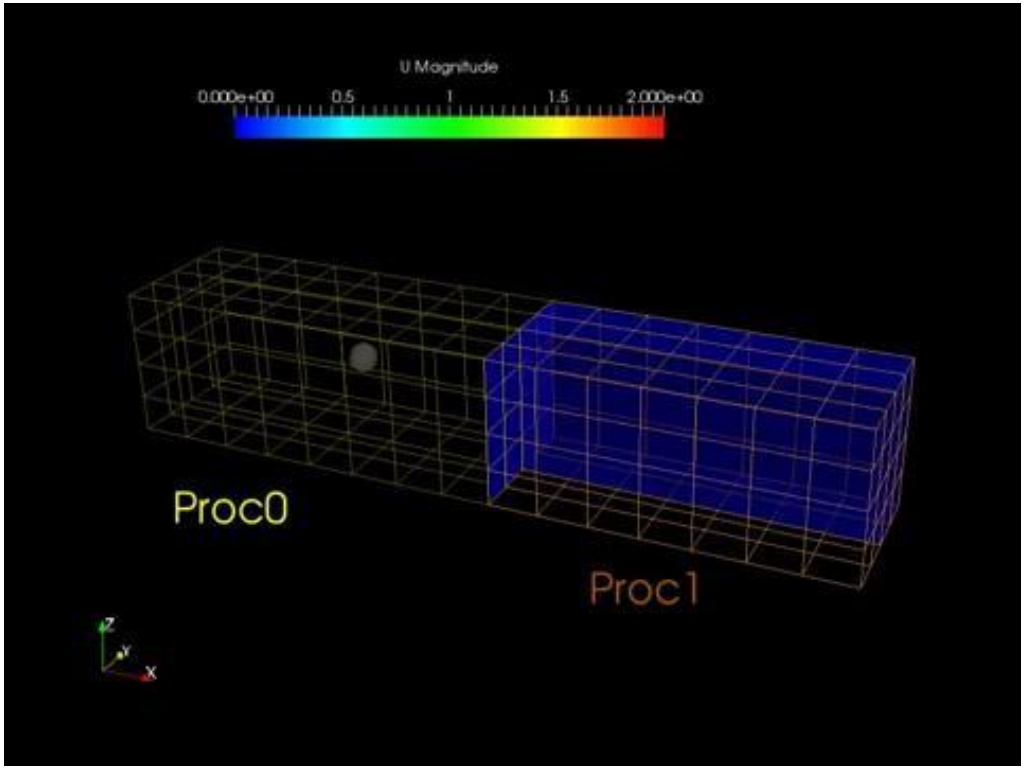
Dual grid and co-located partitioning



- No constraint on the partitioning of the fine mesh ⇒ better load-balancing for CFD
- Coarse mesh can be perfectly aligned with XDEM ⇒ no inter-partition inter-physics communication

Validation of the Results

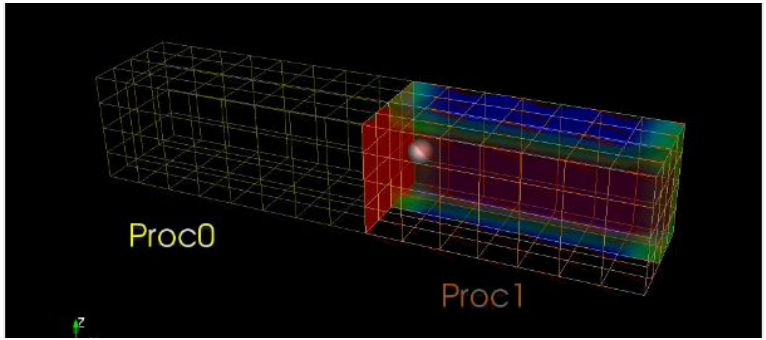
One particle crossing process boundaries

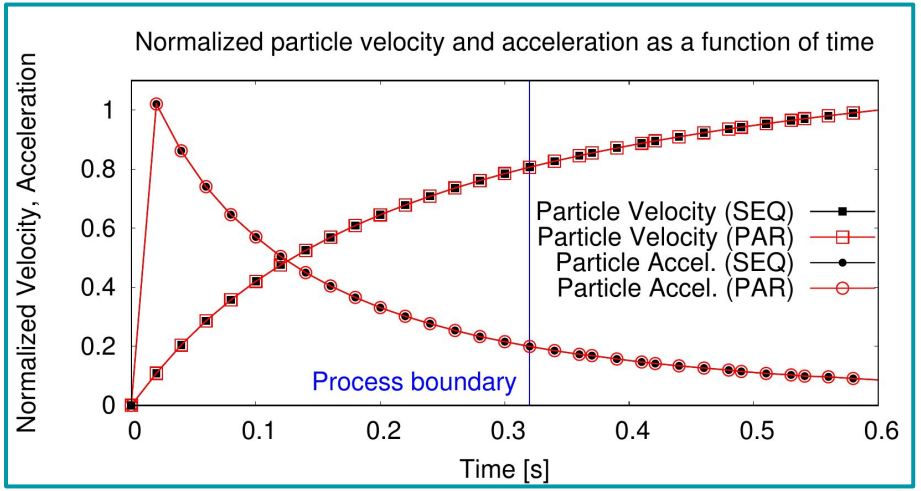


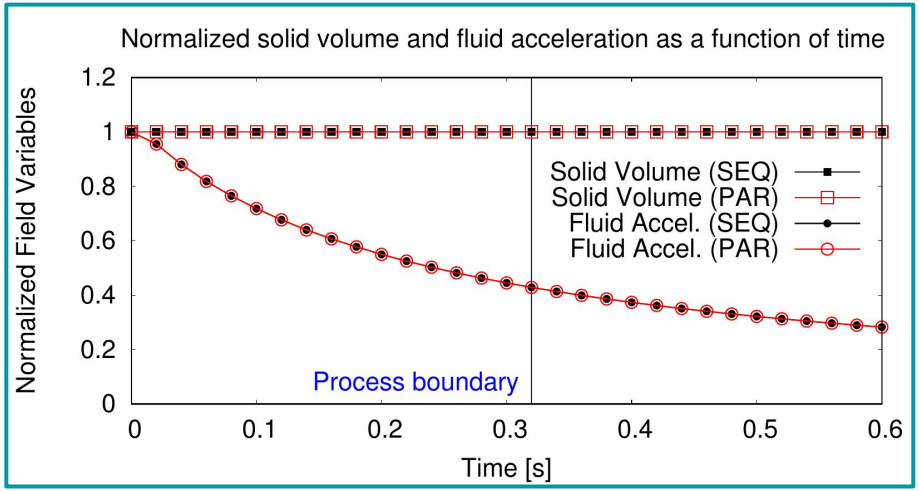
Setup

- one particle
- accelerated by the fluid
- moving from one process to another

One particle crossing process boundaries



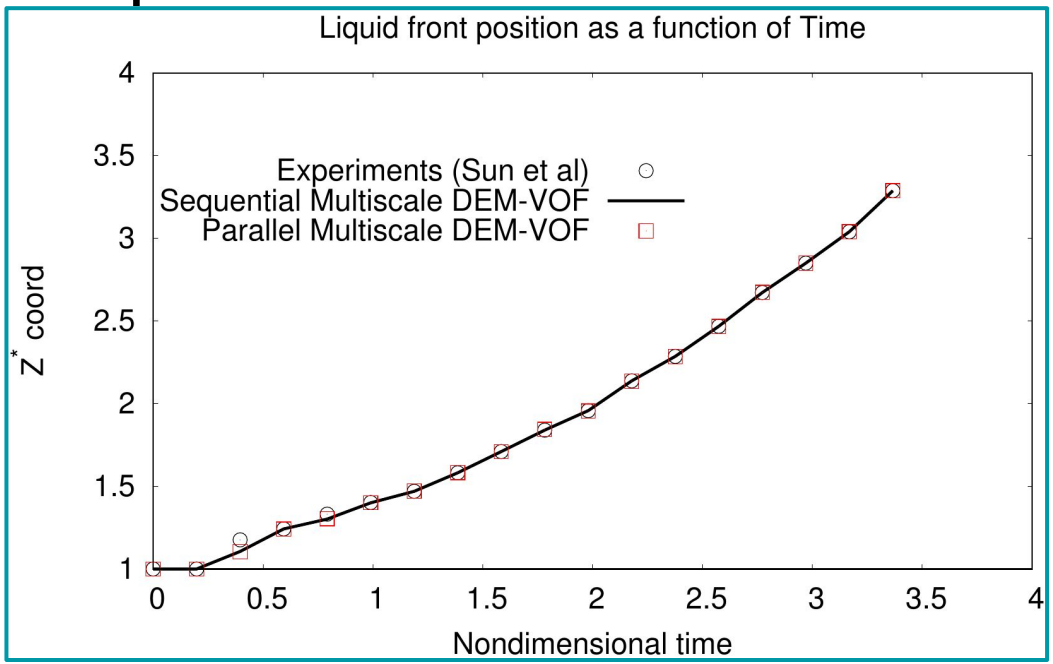


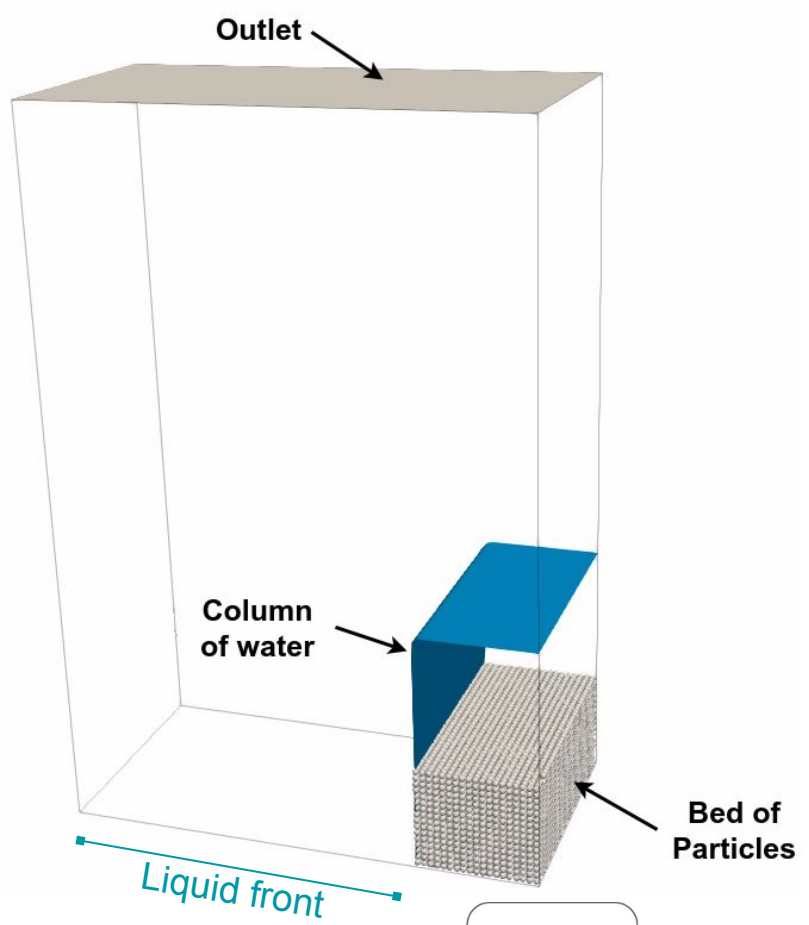


Results

- drag force & particle velocity are continuous
- Identical between sequential and parallel execution

Liquid Front in a Dam Break





Results

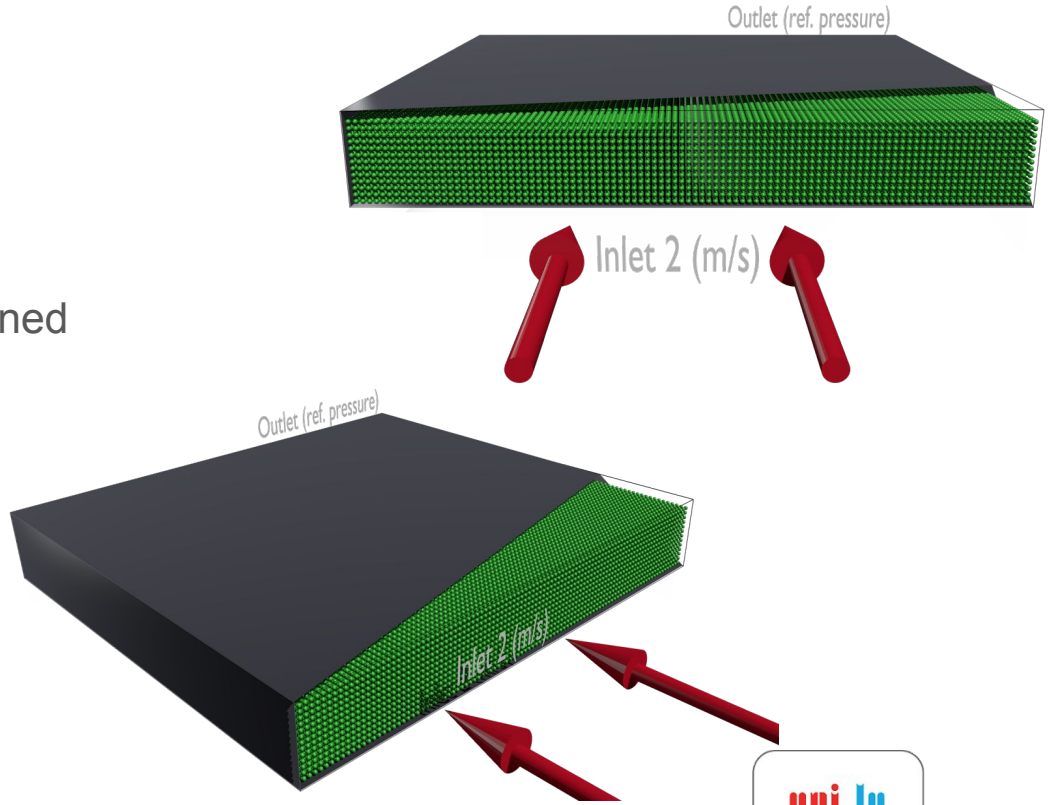
- position of the liquid front
- identical between sequential and parallel
- identical with experimental data

Performance Evaluation

Scalability results (co-located only)

Setup

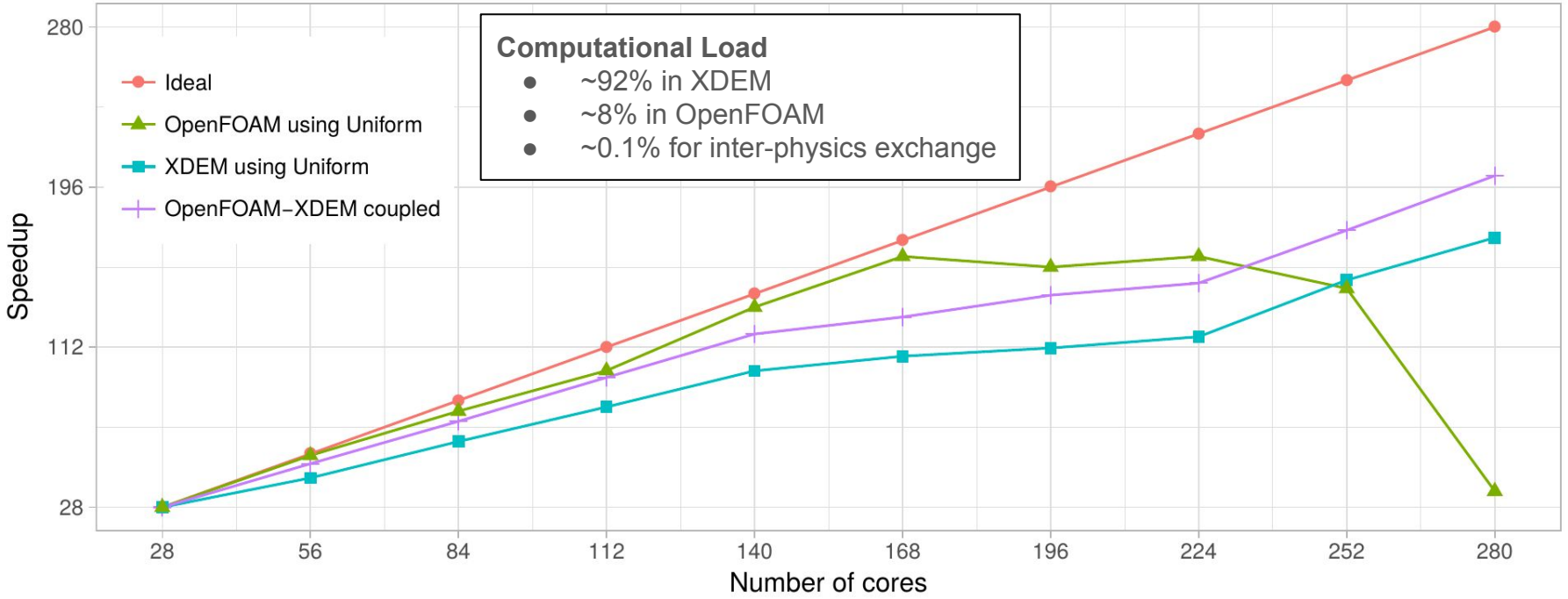
- 10 million particles
- 1 million CFD cells
- CFD mesh and DEM grid are aligned
- Uniform distribution
- From 1 to 10 nodes



Computation Load

- ~92% in XDEM
- ~8% in OpenFOAM
- ~0.1% for inter-physics exchange

Scalability results (co-located only)



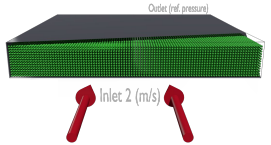
- OpenFOAM is underloaded (< 3600 CFD cells per process)
- Coupled execution follows the behavior of the dominant part

Weak Scalability / Communication Overhead

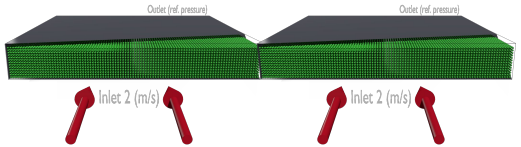
Setup

- ~4464 particles per process
- ~4464 CFD cells per process
- Co-located partitions + Dual Grid
- Uniform distribution
- 10, 20 and 40 nodes

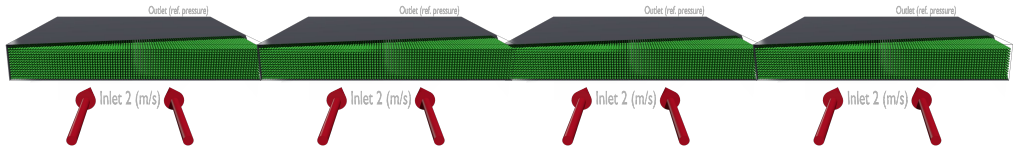
On 10 nodes



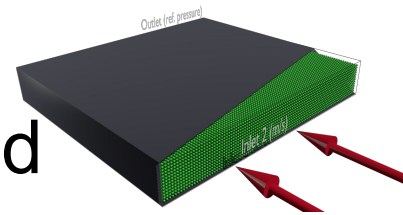
On 20 nodes



On 40 nodes



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)

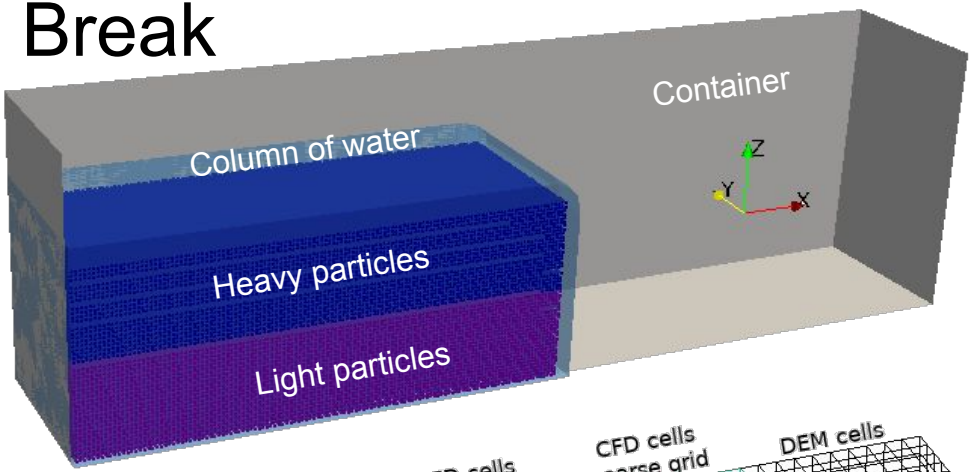
- **MFIX:** +160% overhead from 64 to 256 processes [Gopalakrishnan2013]
- **SediFoam:** +50% overhead from 128 to 512 processes [Sun2016]

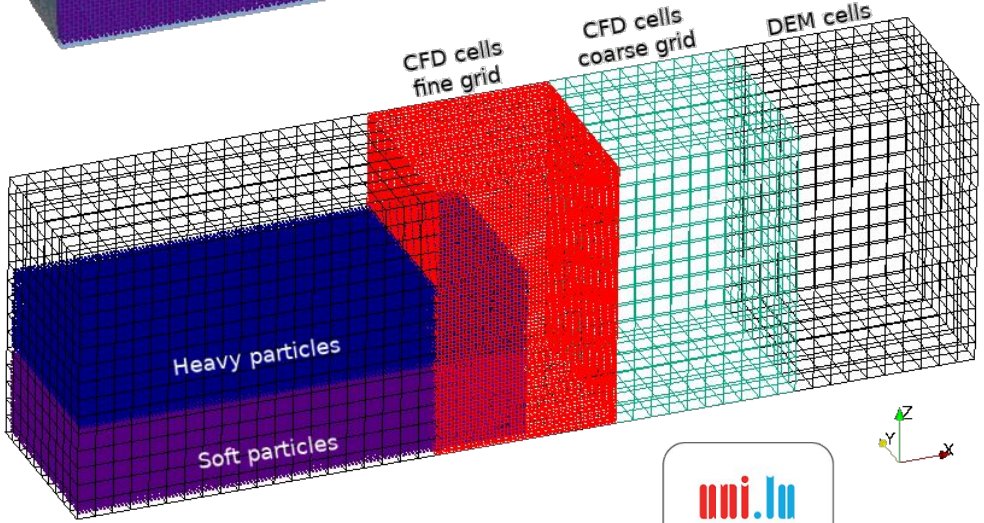
→ due to large increase of p2p communication

Realistic Testcase: Dam Break

Setup

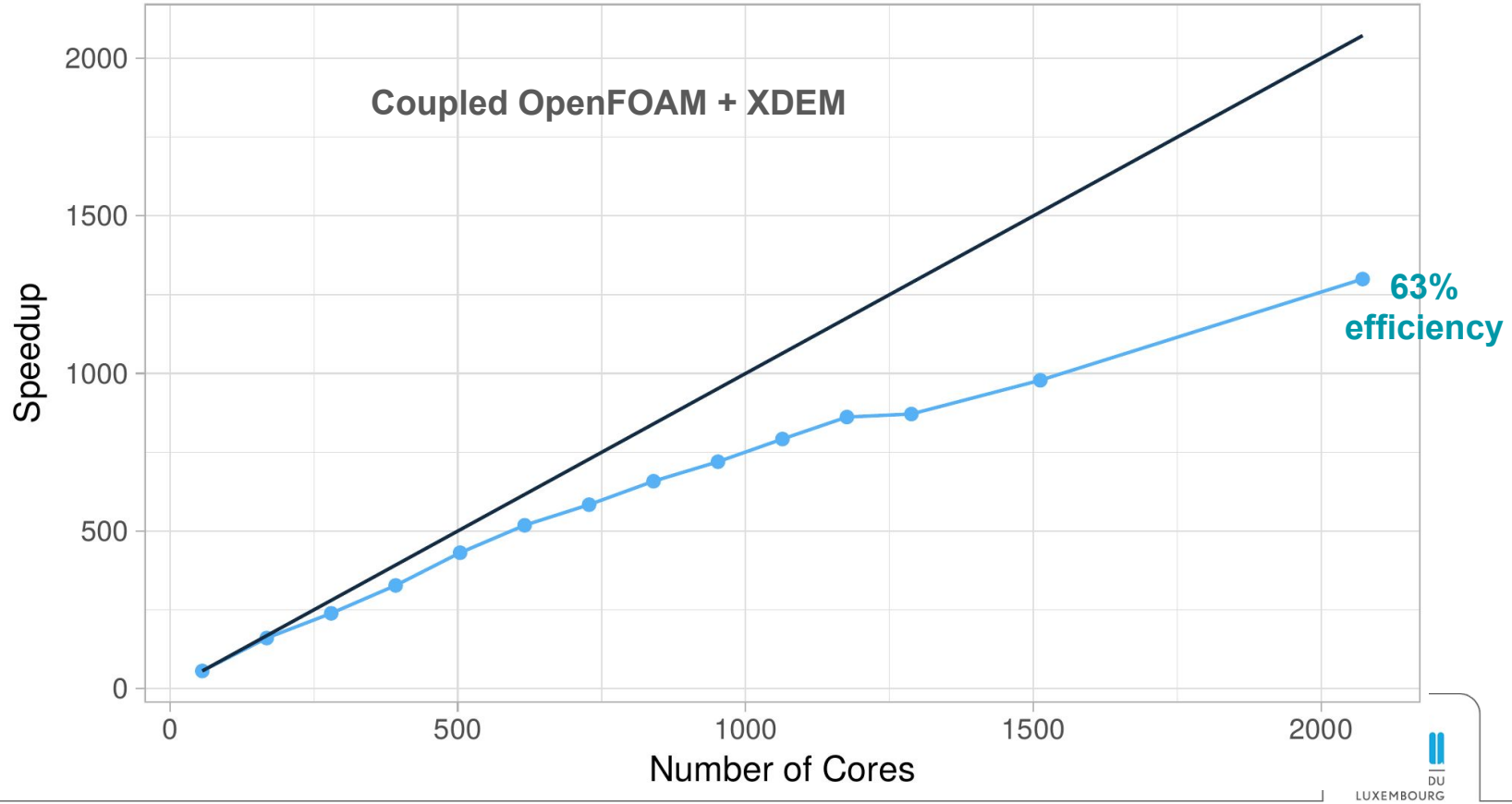
- 2.35M particles
- 10M CFD cells in the fine grid
- 500k CFD cells in the coarse grid
- Co-located partitions + Dual Grid
- Non-uniform distribution



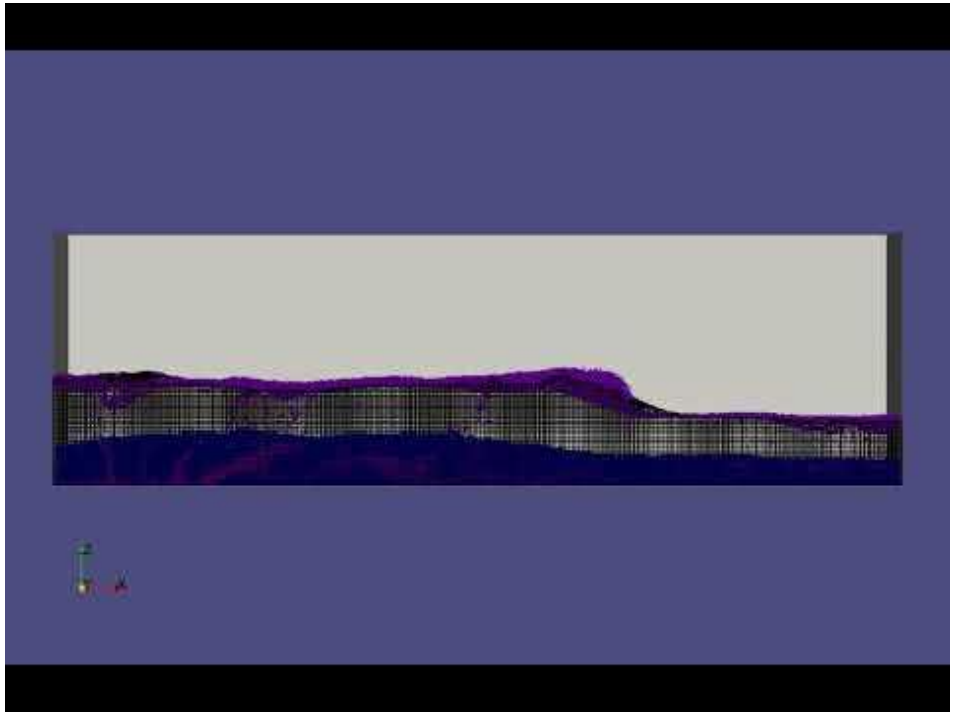


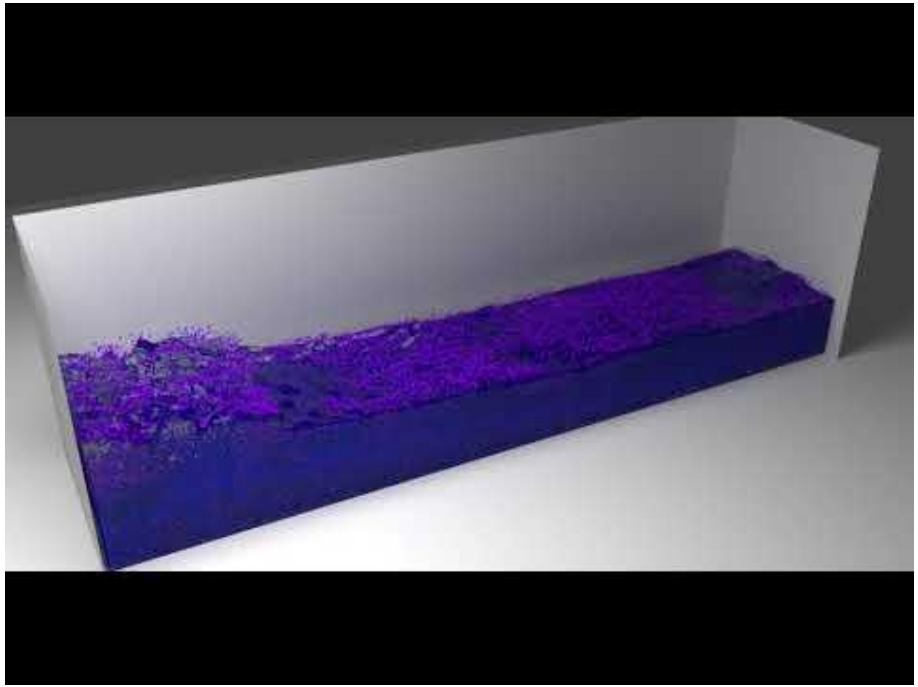
Running scalability test from 4 to 78 nodes

Dam Break scalability (preliminary results)



Realistic Testcase: Dam Break





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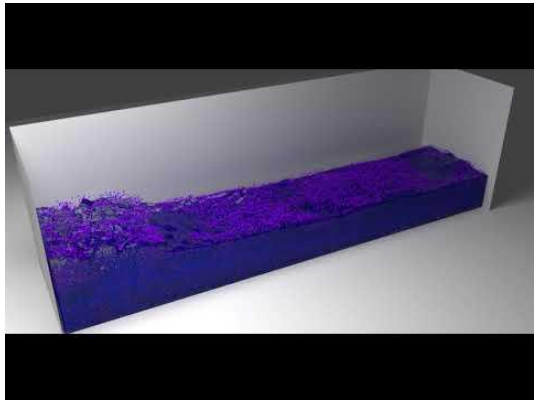
Conclusion

Parallel Coupling of CFD-DEM simulations

Leveraging 2 ideas

- Co-located partitioning
  - Reduce the volume of communication
  - Impose constraint on the partitioning
- Dual grid multiscale
  - Better convergence of the solution & simplify averaging of the CFD-DEM coupling
  - Relax the constraint on the partitioning



Future work / Other issues

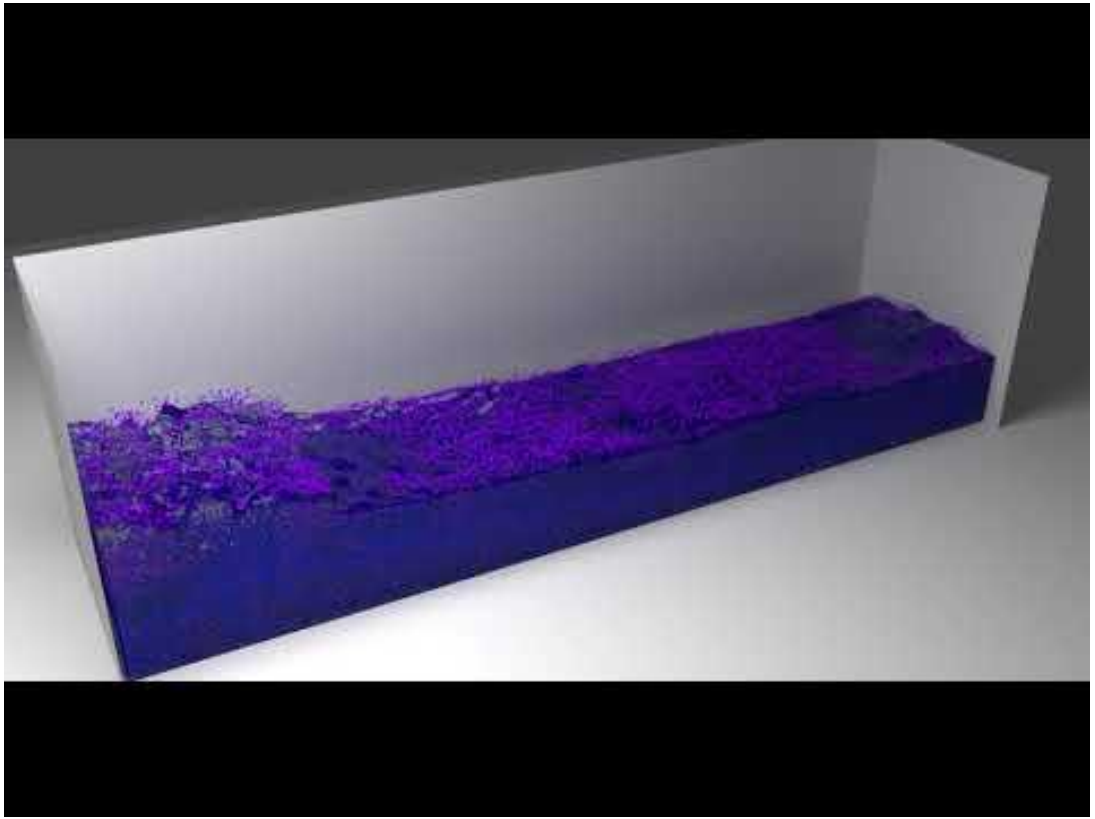
- Multiphysics-aware partitioner
- Dynamics load-balancing

Co-located partitioning

Dual grid multiscale

CFD-DEM Parallel Coupling

Thank you for your attention!



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