Parallel coupling strategy for multi-physics applications in eXtended Discrete Element Method

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http://luxdem.uni.lu/

HPC Knowledge Meeting '20
18 - 19 June 2020

Outline

Background

- What is XDEM?
- Multi-physics Coupling

CFD-DEM Parallel Coupling

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

Results

- Results Validation
- Performance Evaluation

Conclusion

- Future Work
- Open Issues

What is XDEM?

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eXtended Discrete Element Method

Particles Dynamics

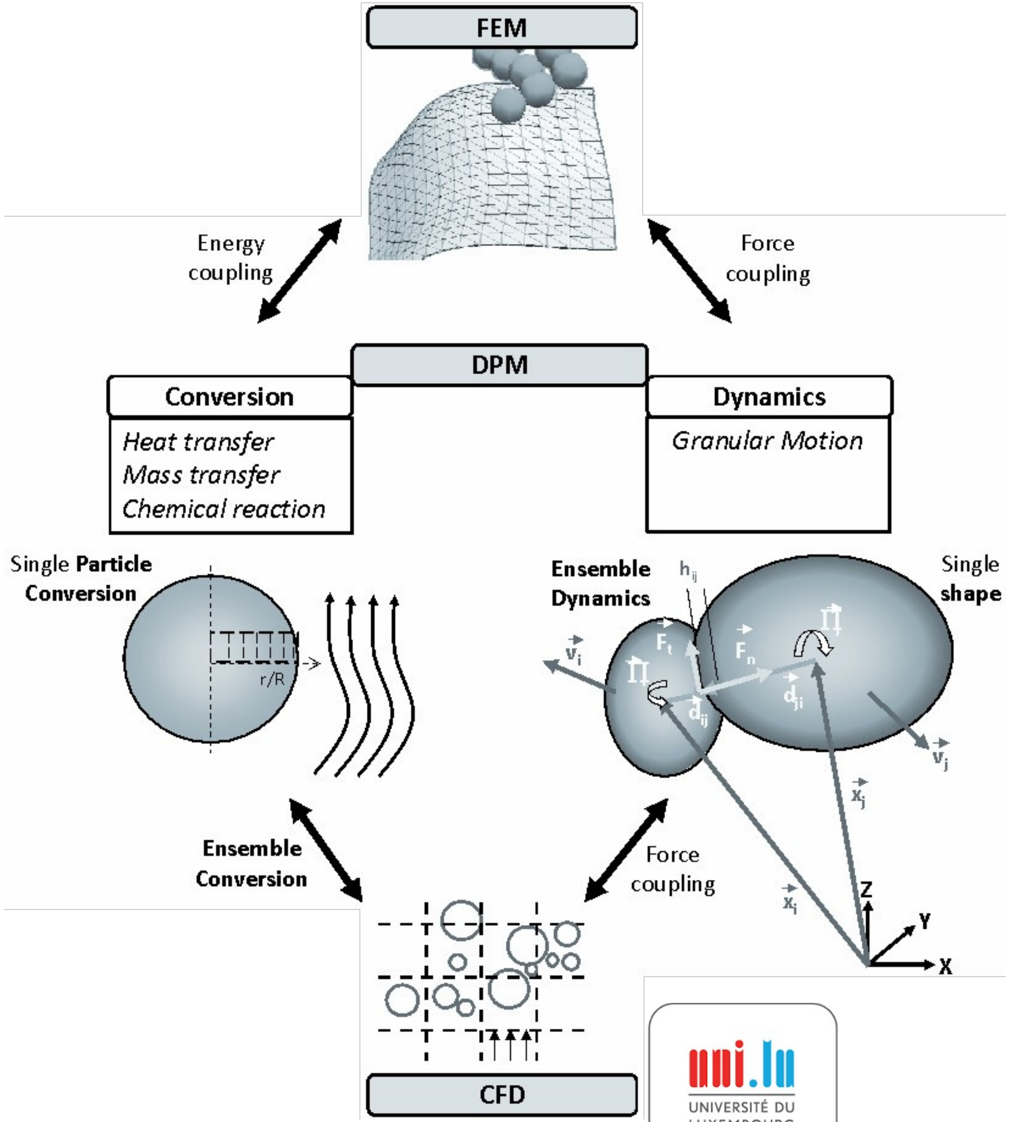
- Force and torques
- Particle motion

Particles Conversion

- Heat and mass transfer
- Chemical reactions

Coupled with

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



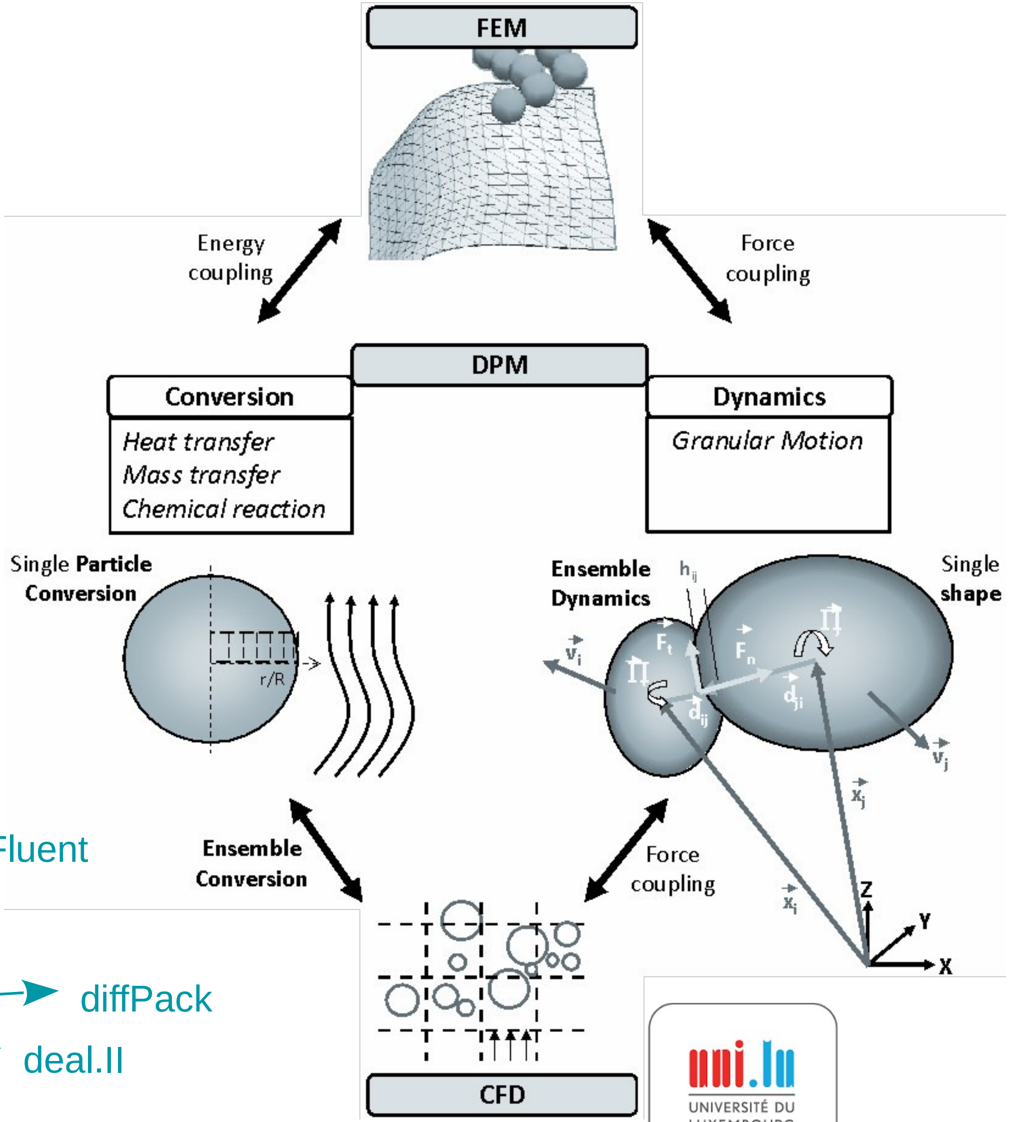
What is XDEM?

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)** → OpenFOAM, ANSYS Fluent
- Finite Element Method (FEM) → diffPack, deal.II, CalculiX



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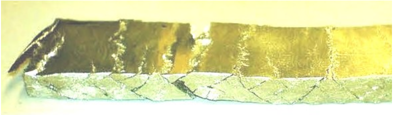
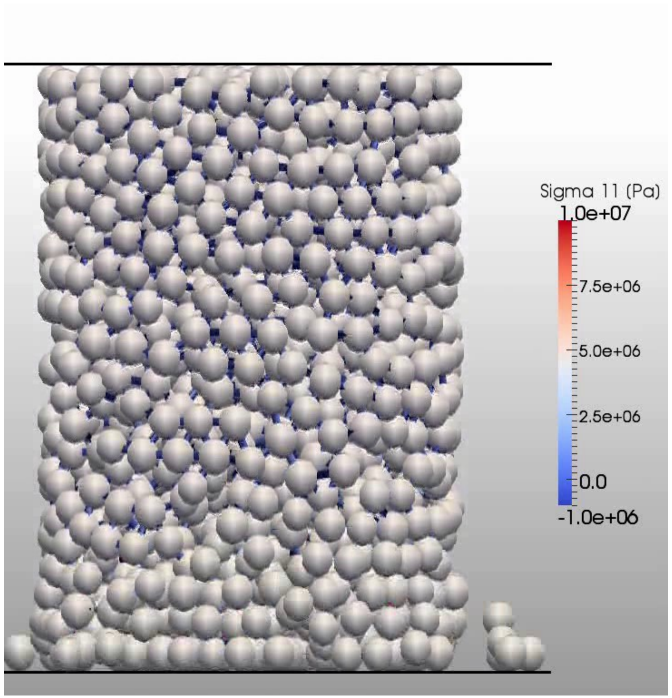
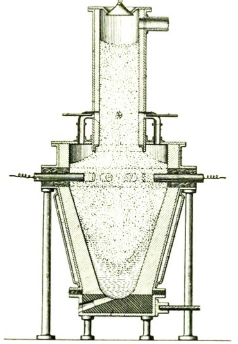
Application Examples: XDEM without coupling

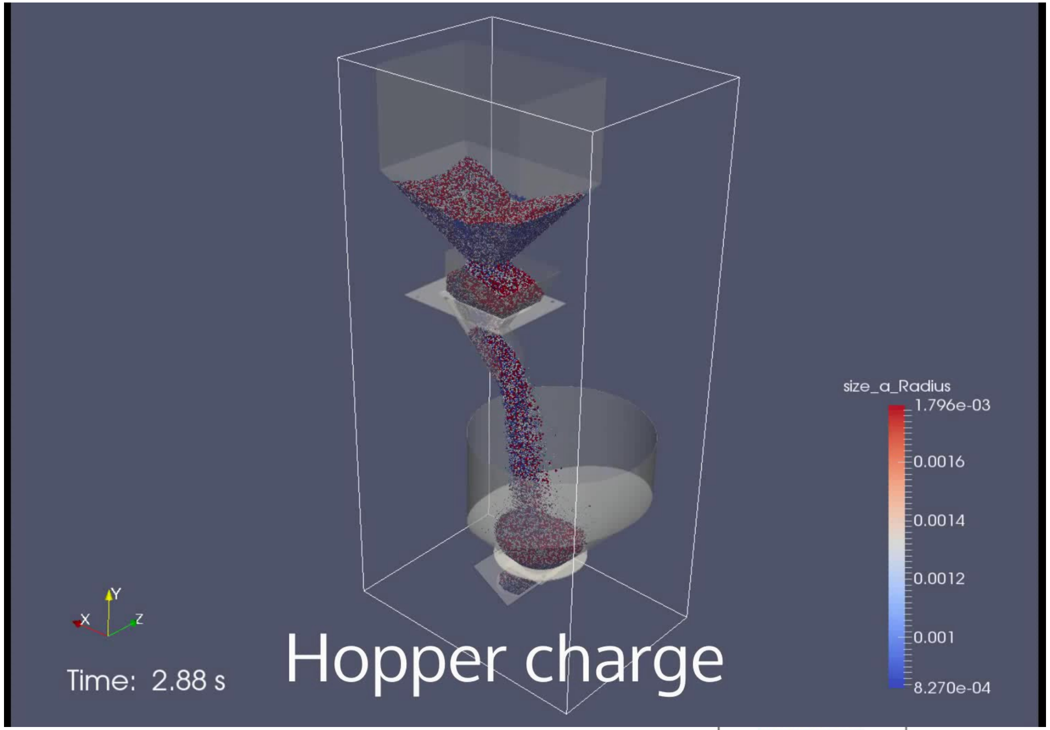


Brittle Failure



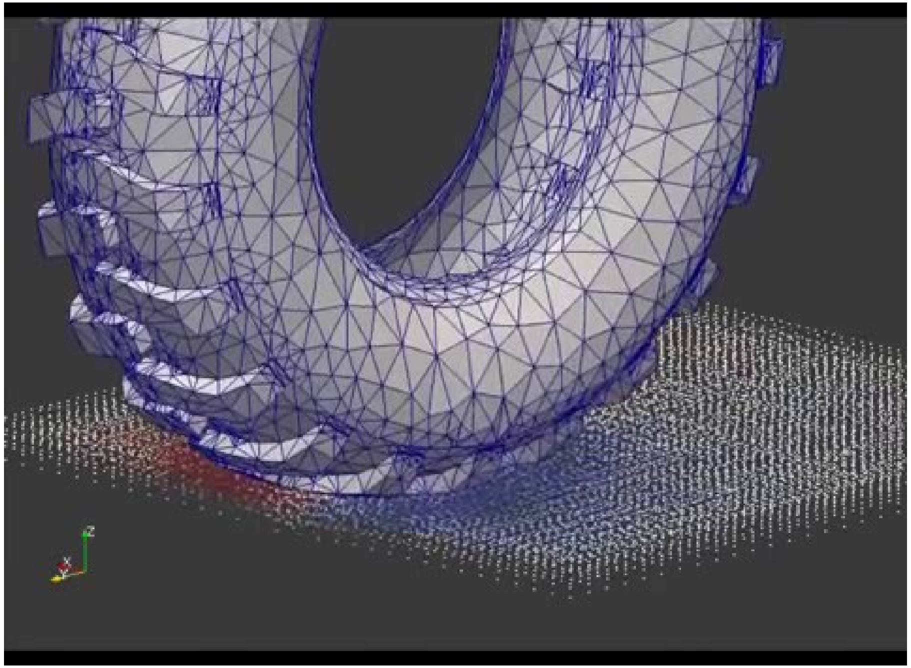
Hopper charge and discharge



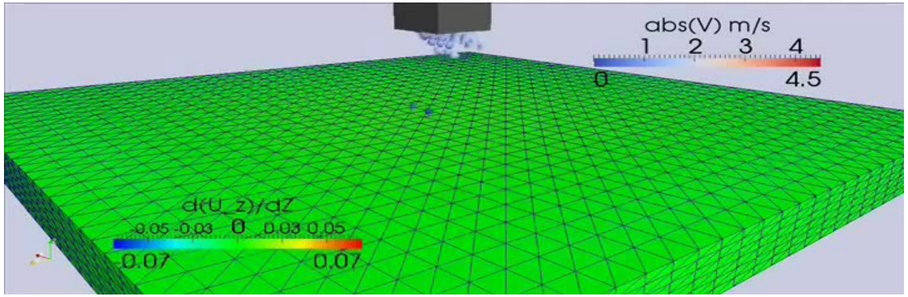


Application Examples: XDEM coupled with FEM

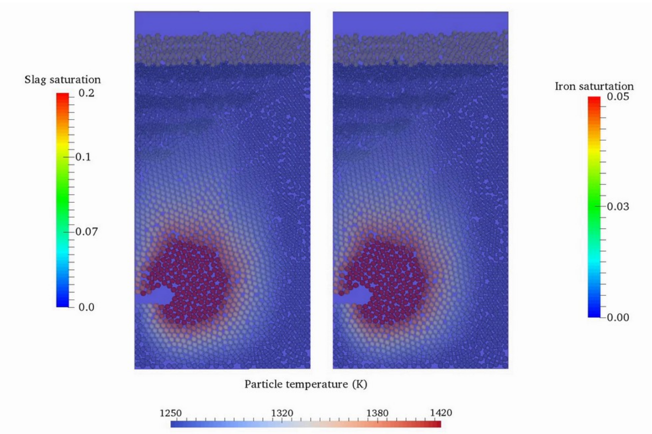
Deformation of a tire



Impact on an Elastic Membrane

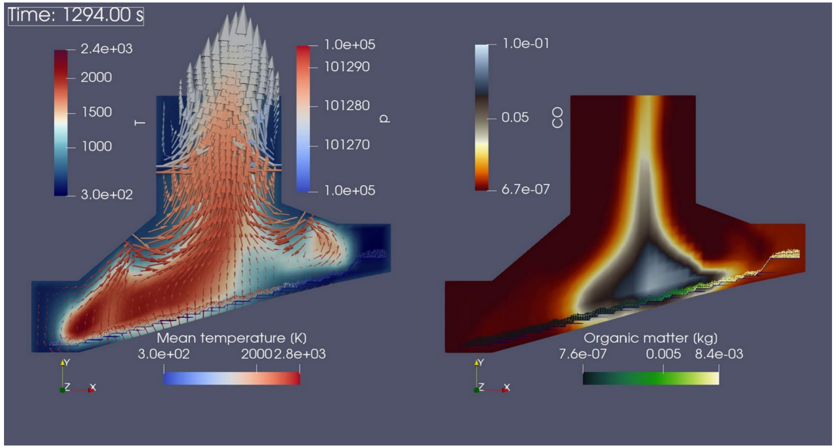


Application Examples: XDEM coupled with CFD

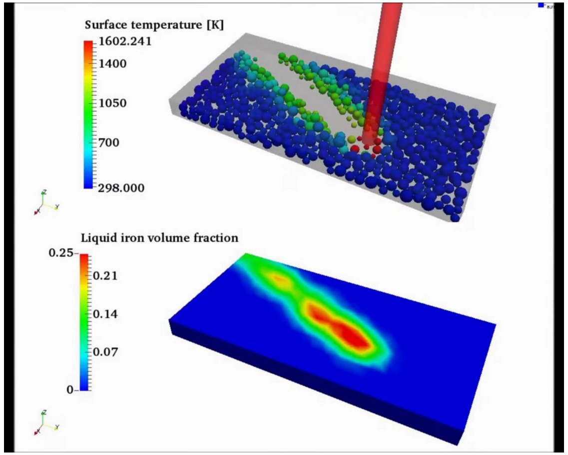


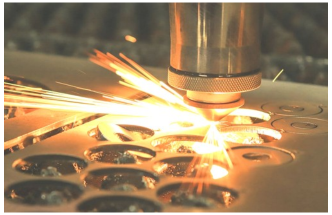
Iron & Slag production
in a Blast Furnace

Wood Conversion
in a Biomass Furnace



Selective Laser Melting
in Additive Manufacturing





Multi-Physics Coupling

surface vs. volume coupling

Multi-Physics Coupling

Numerical Methods

- Computation Fluid Dynamics (CFD)
- Finite Element Method (FEM)
- Discrete Element Method (DEM)
- ...

Different Software

- Instead of a monolithic software

Different Mesh Topology

Numerical Method Constraints

- Time step size
- Convergence
- ...

Technical Constraints

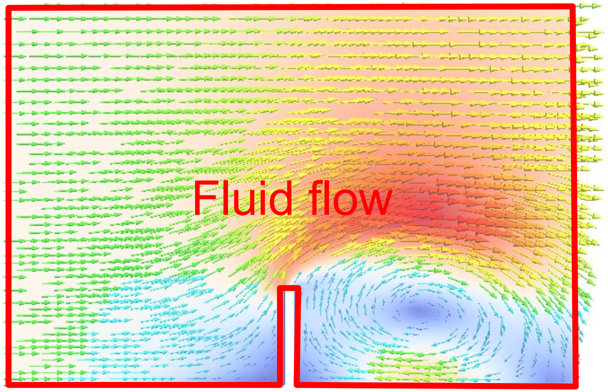
- Coupling API
- Communication / Data exchange
- Scalability
- ...

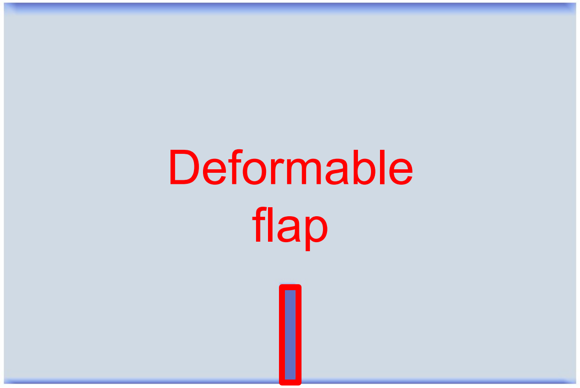
Physics Constraints

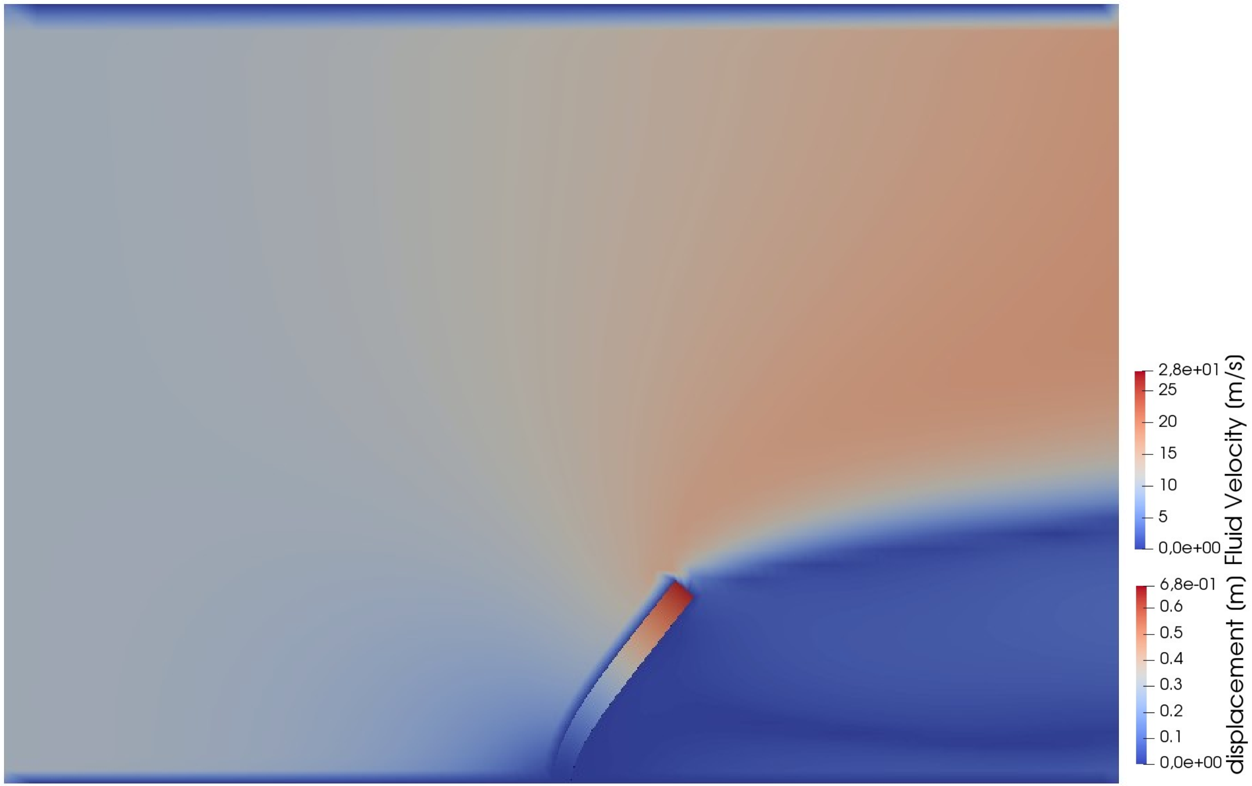
- Mass, energy conservation
- Value consistency

Complicated physics ⇒ Complex Software ⇒ Performance Nightmare

Surface Coupling, e.g. Fluid-Structure Interaction (FSI)







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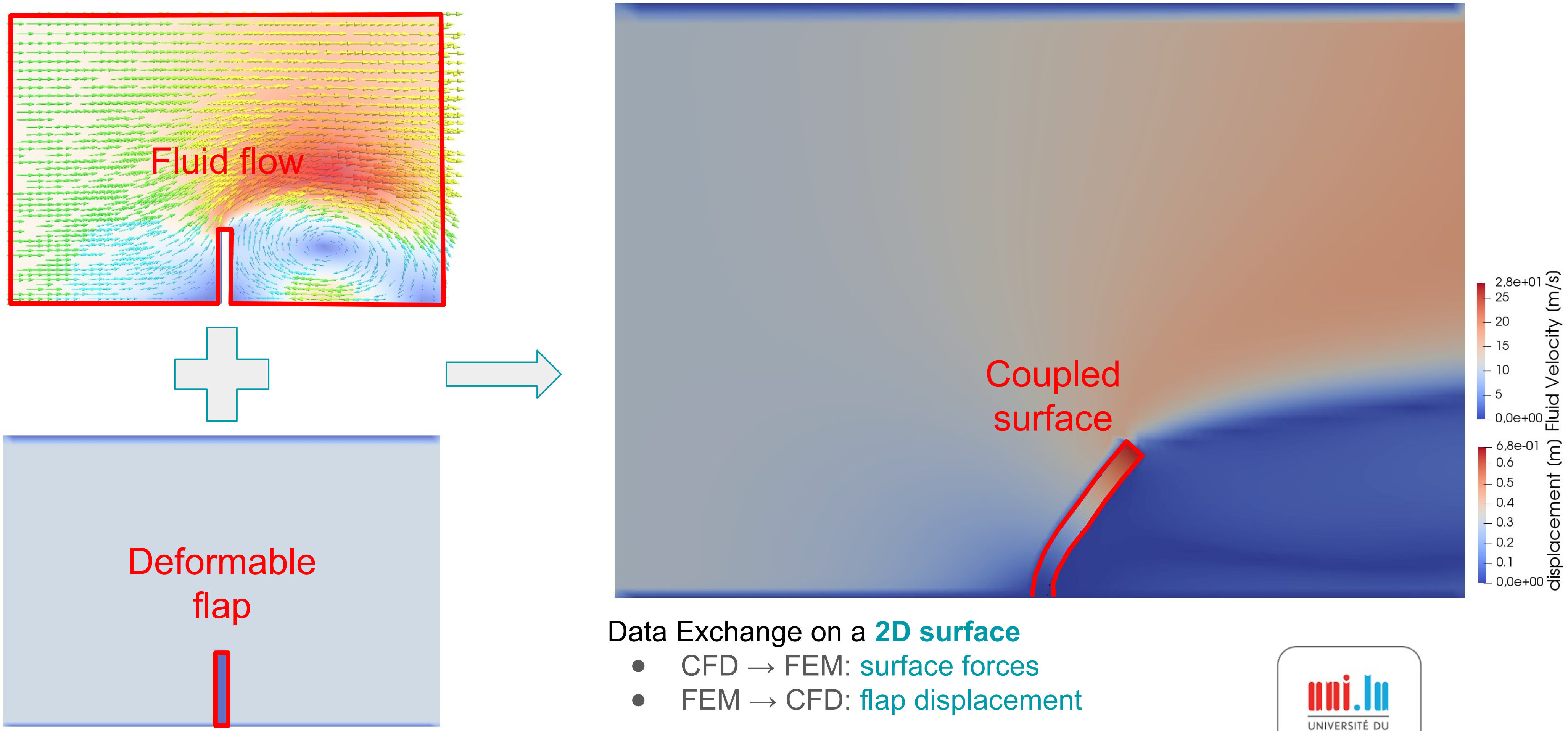
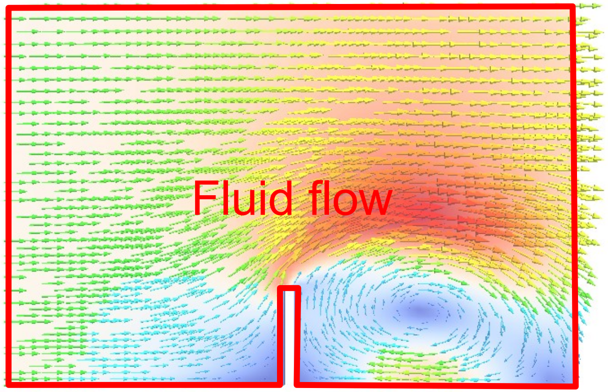
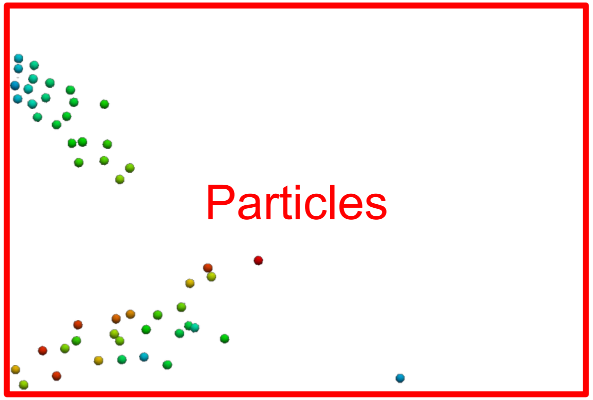


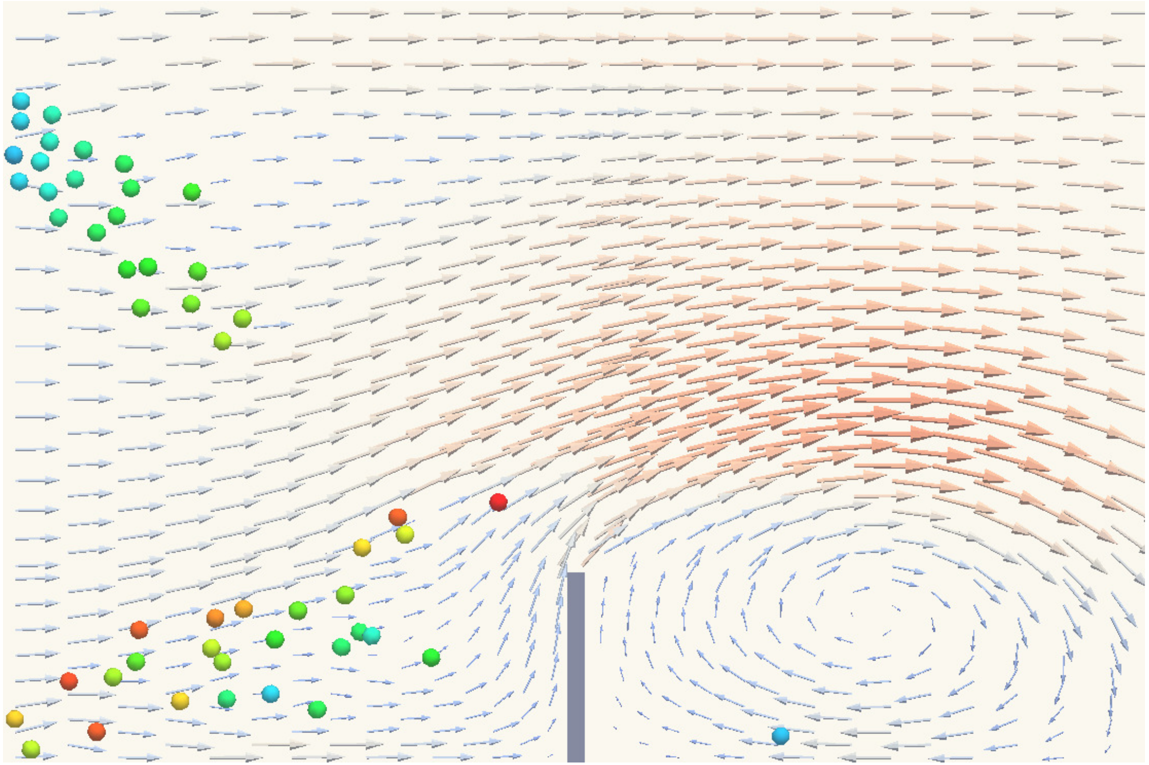
Data Exchange on a **2D surface**

- CFD → FEM: surface forces
- FEM → CFD: flap displacement

Volume Coupling, e.g. Fluid-Particles Interaction







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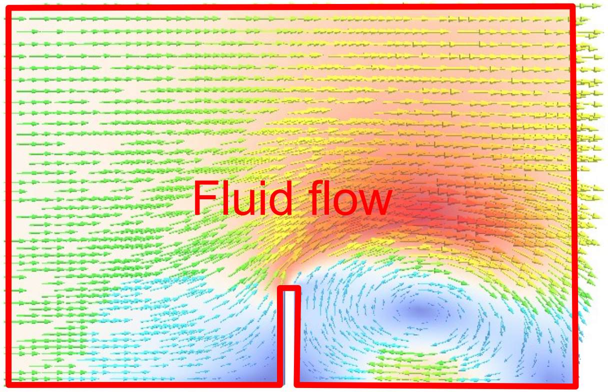

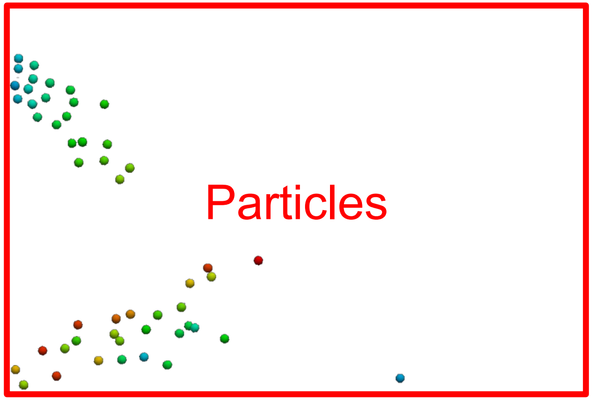

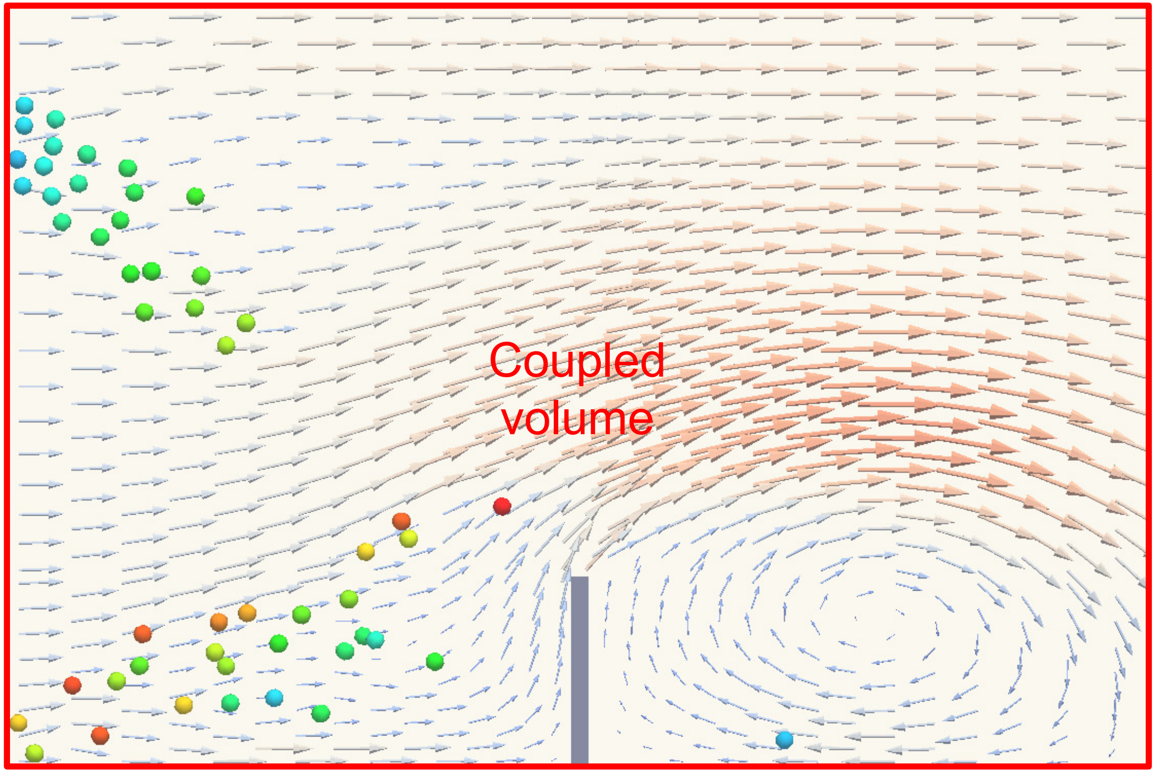

Data Exchange on a **3D volume**

- CFD → DEM: drag force, buoyancy
- DEM → CFD: porosity, particle momentum

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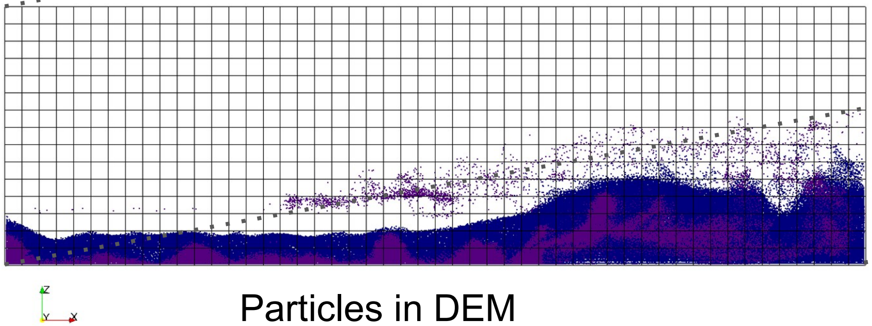
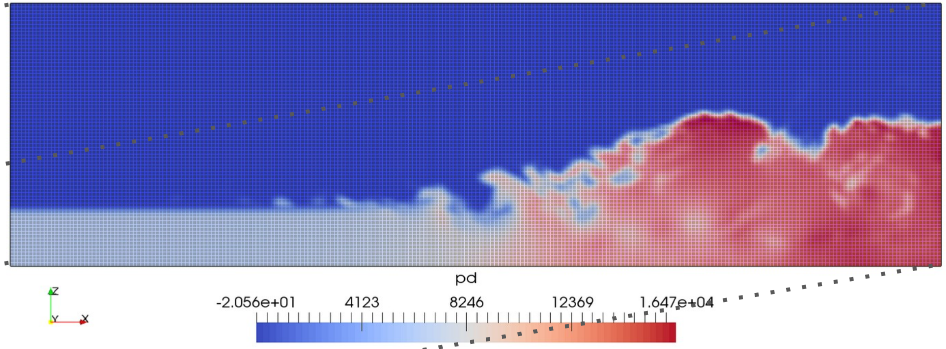
CFD-DEM
Volume Coupling

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

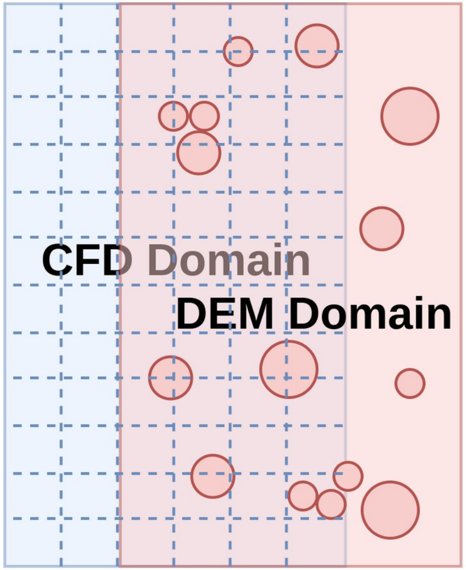
From DEM to CFD

- Porosity
- Particle source of momentum

CFD ⟷ XDEM

- Heat transfer
- Mass transfer

CFD-DEM Parallel Coupling: Challenges

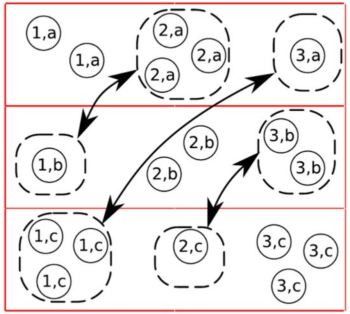


Challenges in CFD-XDEM parallel coupling

- Combine different independent software
- Volume coupling ⇒ Large amount of data to exchange
- Different distribution of the computation and of the data
- DEM data distribution is dynamic
- Data interpolation between meshes

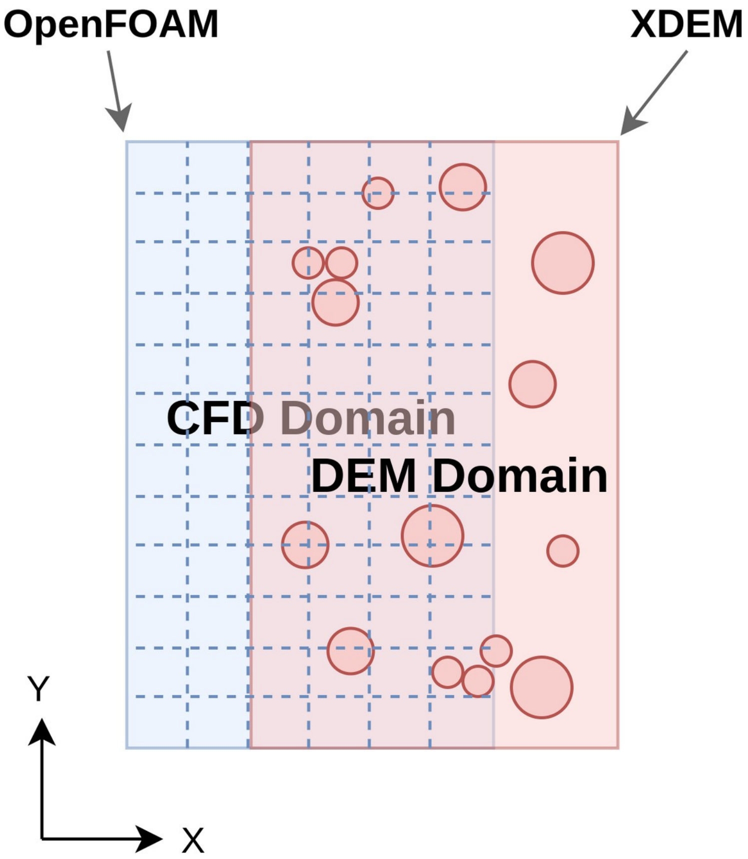
Classical Approaches

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



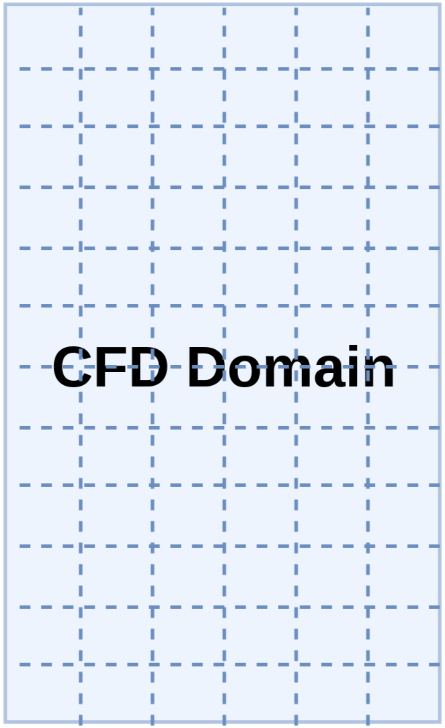
SediFoam [Sun2016]

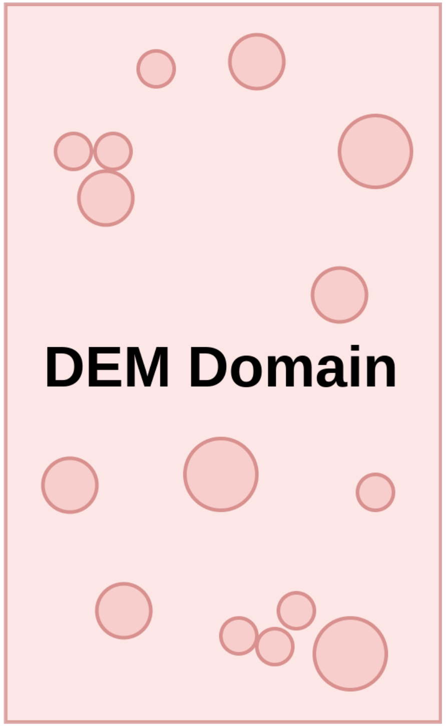
CFD-DEM Parallel Coupling: Challenges



The domains overlap in space

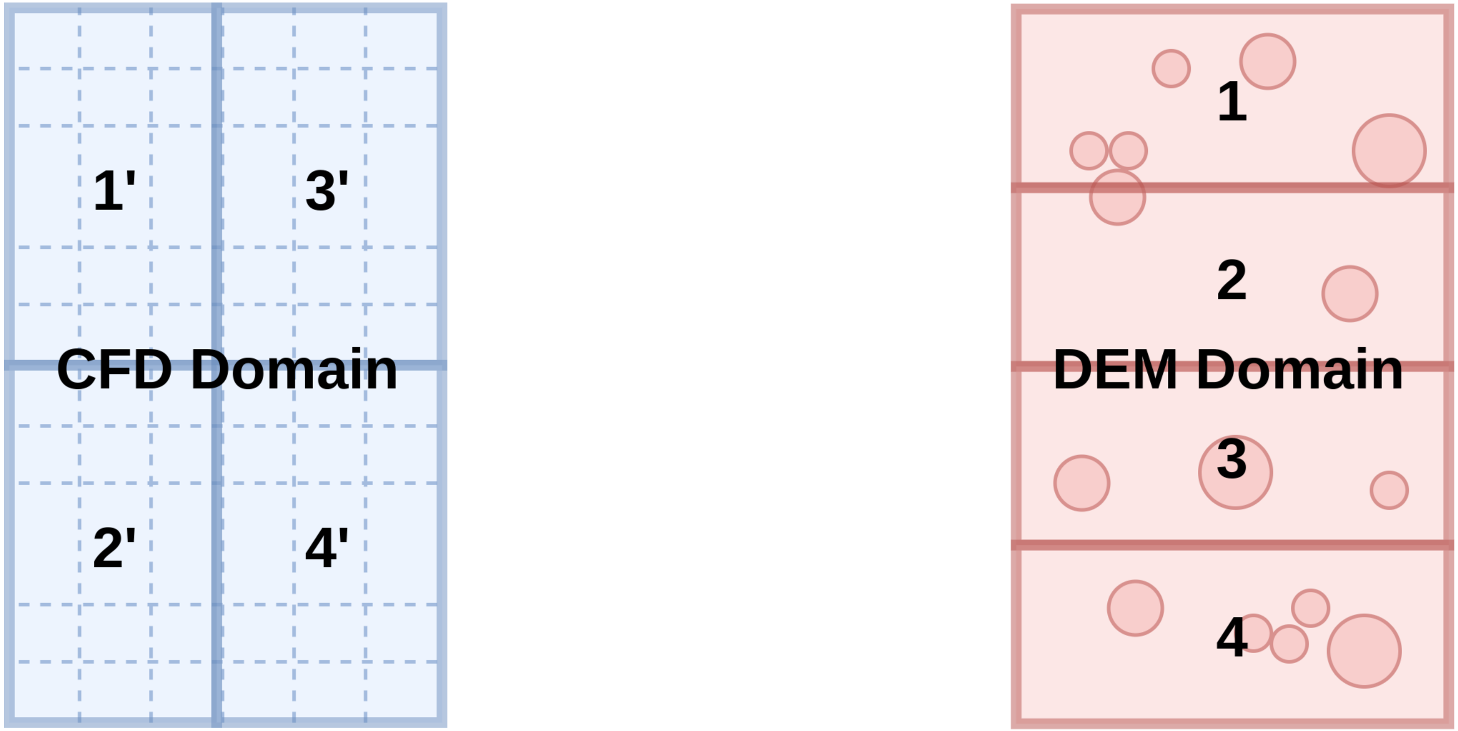
CFD-DEM Parallel Coupling: Challenges





CFD-DEM Parallel Coupling: Challenges

Classical Approach: the domains are partitioned independently



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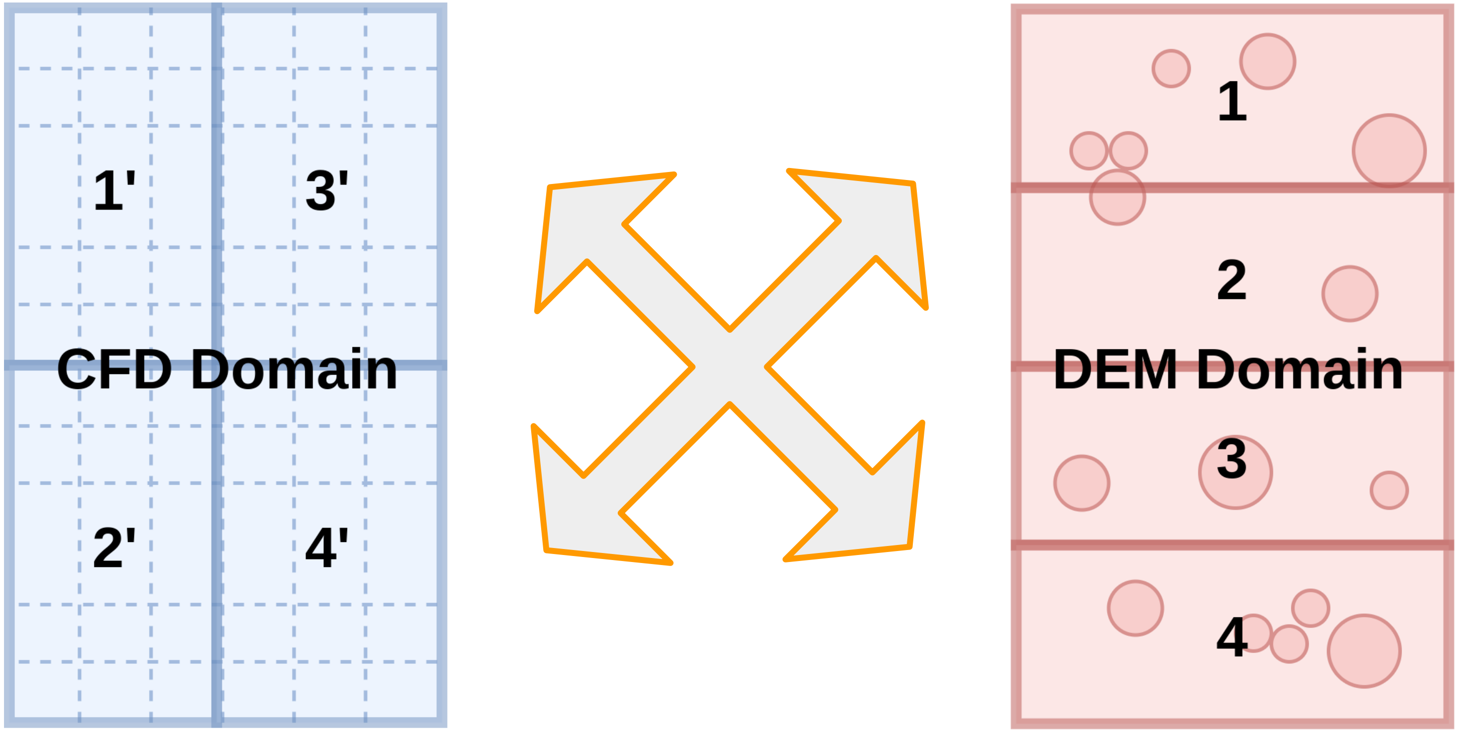
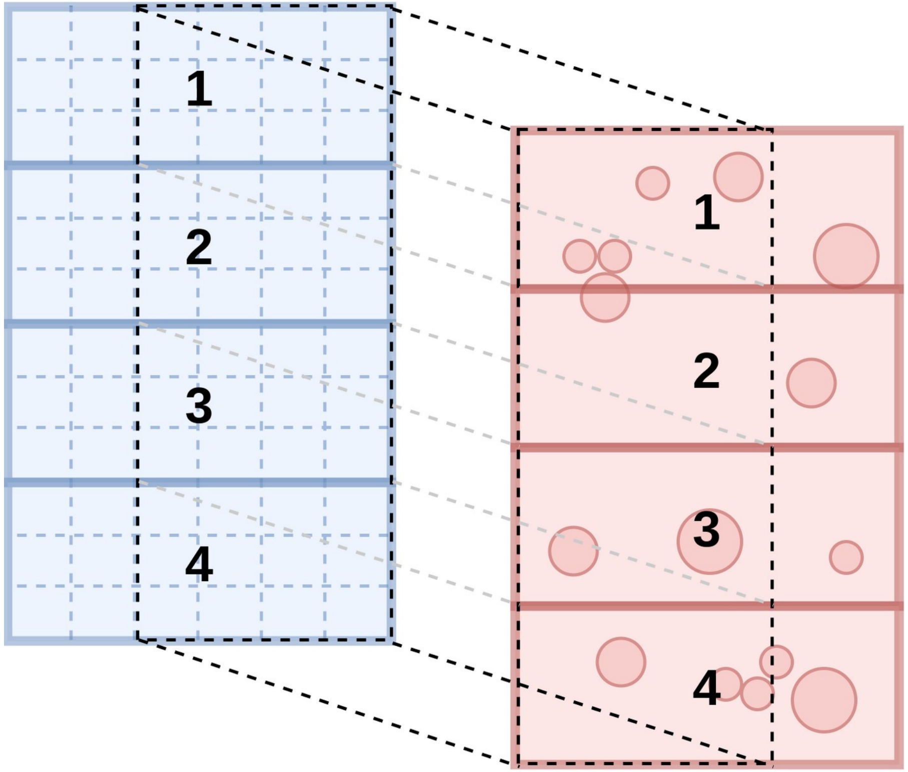


Complex pattern and large volume of communication

Co-located Partitioning Strategy

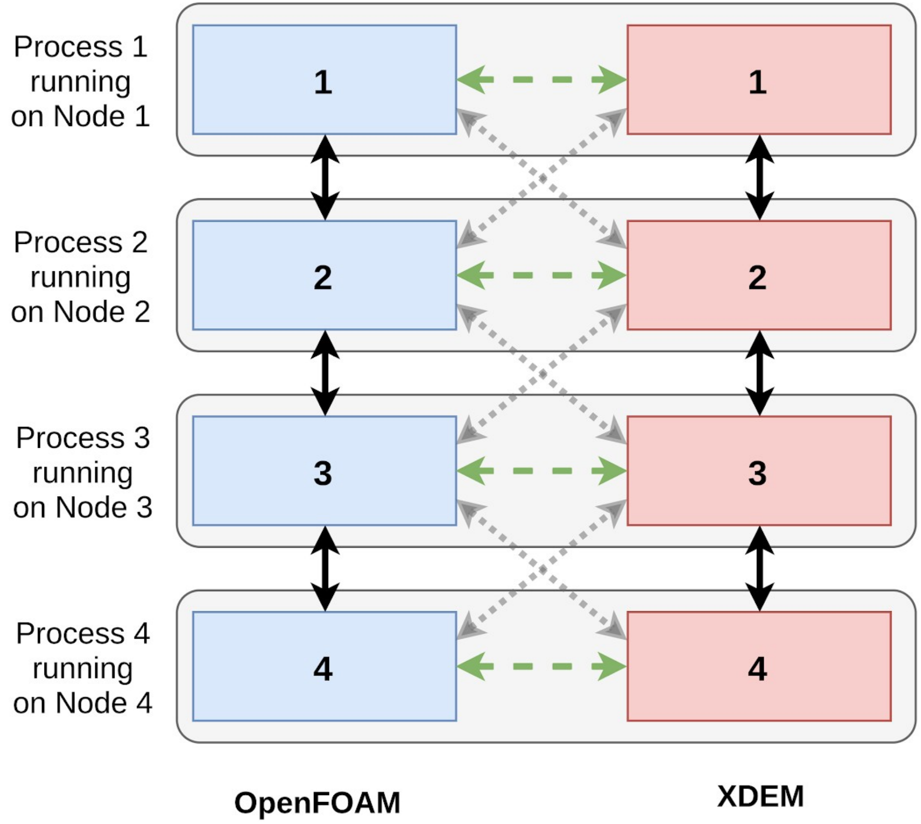
A co-located partitions strategy for parallel CFD–DEM couplings
G. Pozzetti, X. Besseron, A. Rousset and B. Peters
Journal of Advanced Powder Technology, December 2018
https://doi.org/10.1016/j.apt.2018.08.025

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

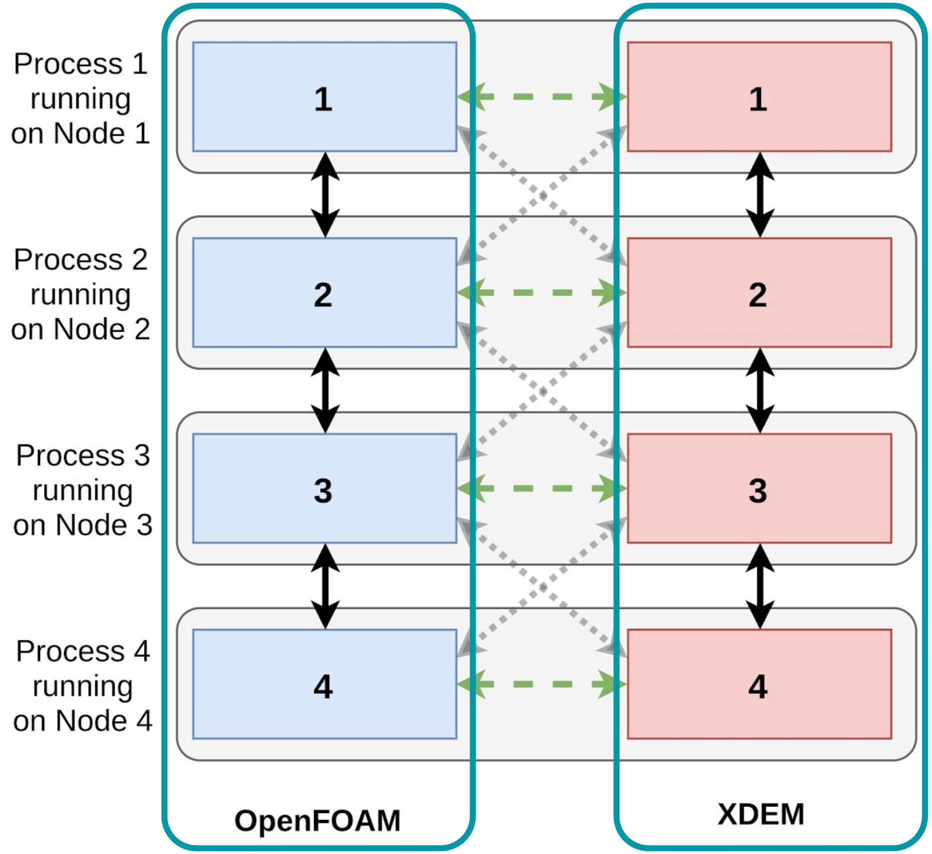
Inter-partition intra-physics Data Exchange using MPI communication layer
with native implementation in OpenFOAM and XDEM

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

Co-located Partitioning Strategy: communication



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With native implementation of each sotfware

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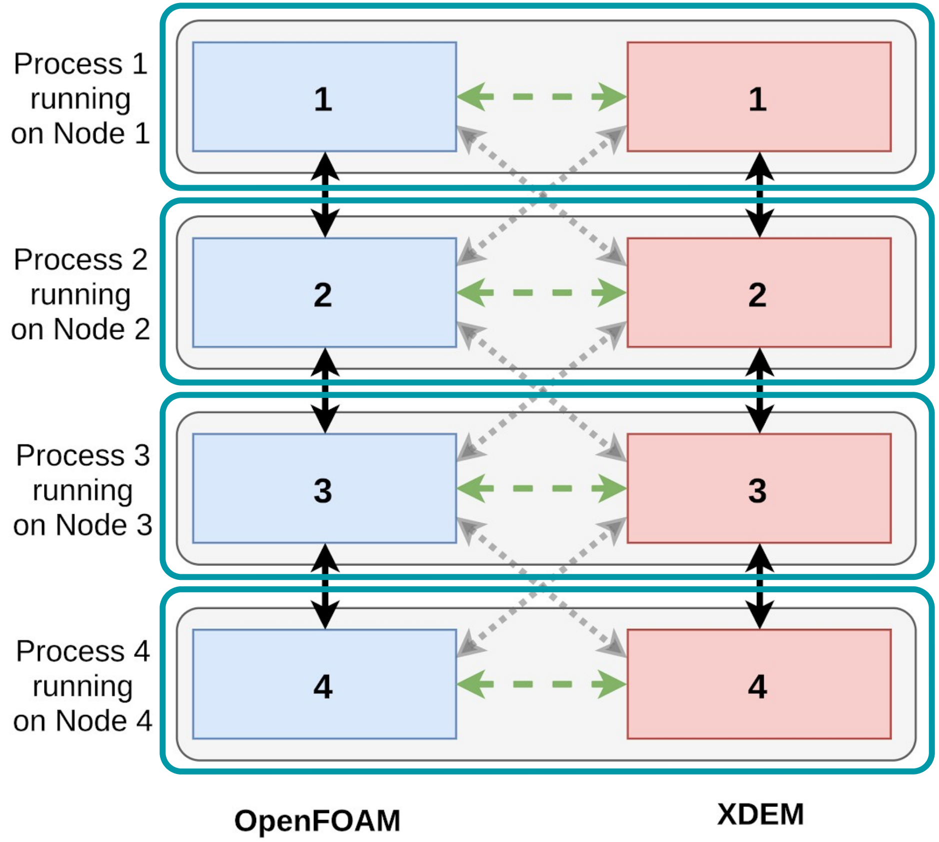
Co-located Partitioning Strategy: communication



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Use direct intra-proces memory access if the two software are linked into one executable,

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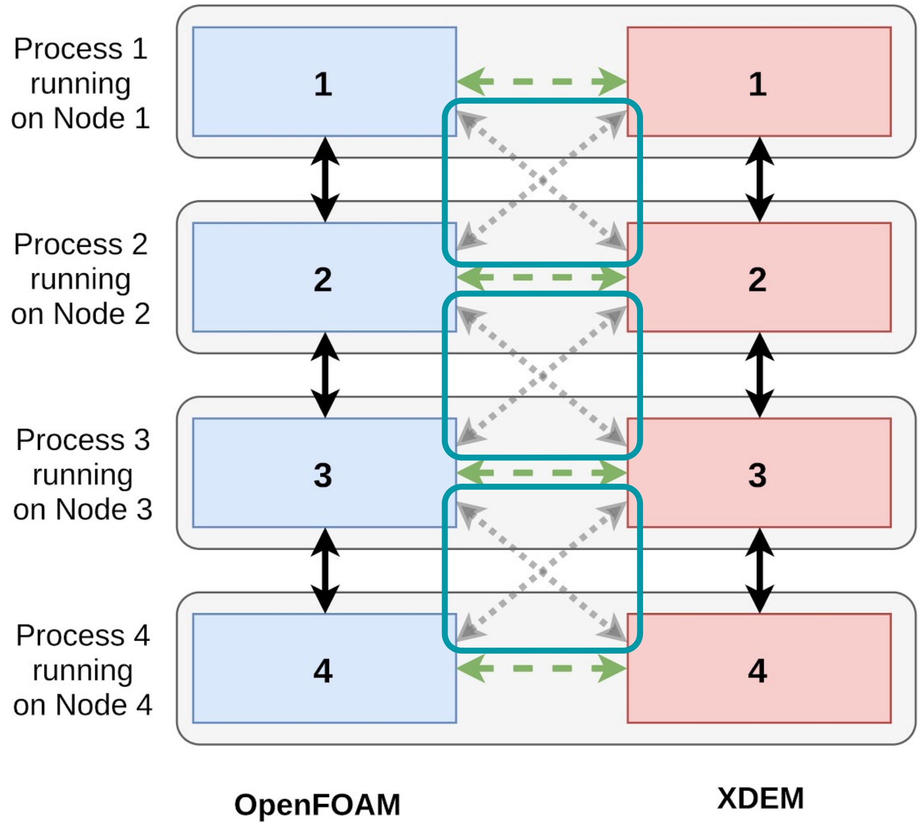
Co-located Partitioning Strategy: communication



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

Can be non-existing if partitions are perfectly aligned

Dual-Grid Multiscale Approach

A multiscale DEM-VOF method for the simulation of three-phase flows

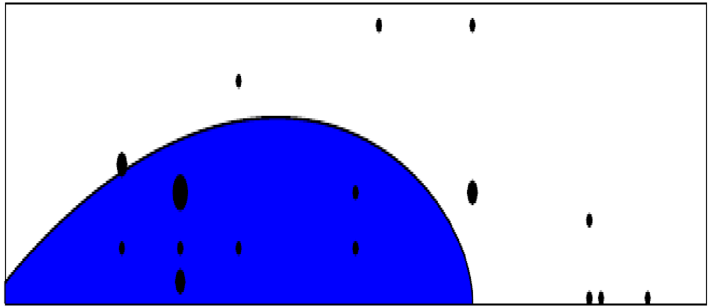
G. Pozzetti and B. Peters

International Journal of Multiphase Flow, February 2018

https://doi.org/10.1016/j.ijmultiphaseflow.2017.10.008

Advantages of the dual-grid multiscale

Bulk coupling scale



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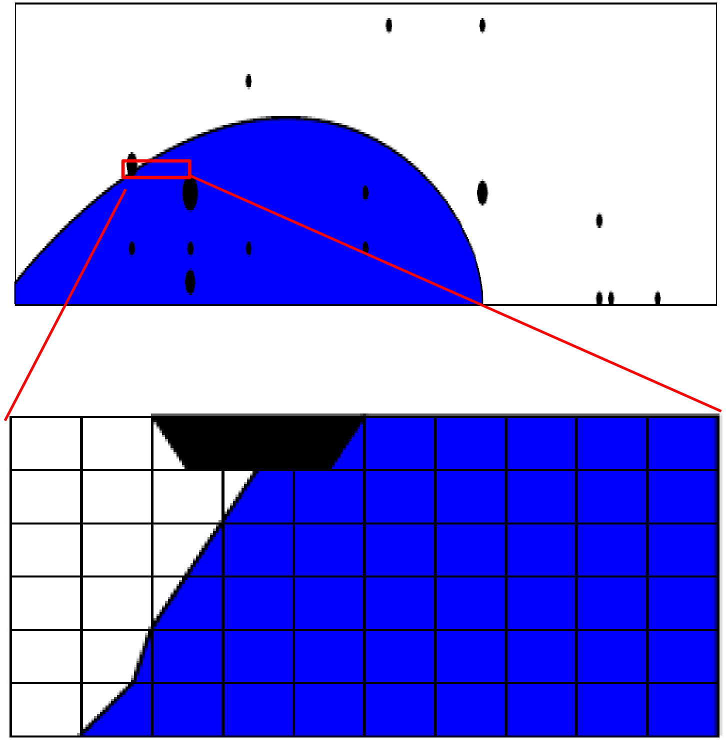

Fluid fine scale

Advantages of the dual-grid multiscale

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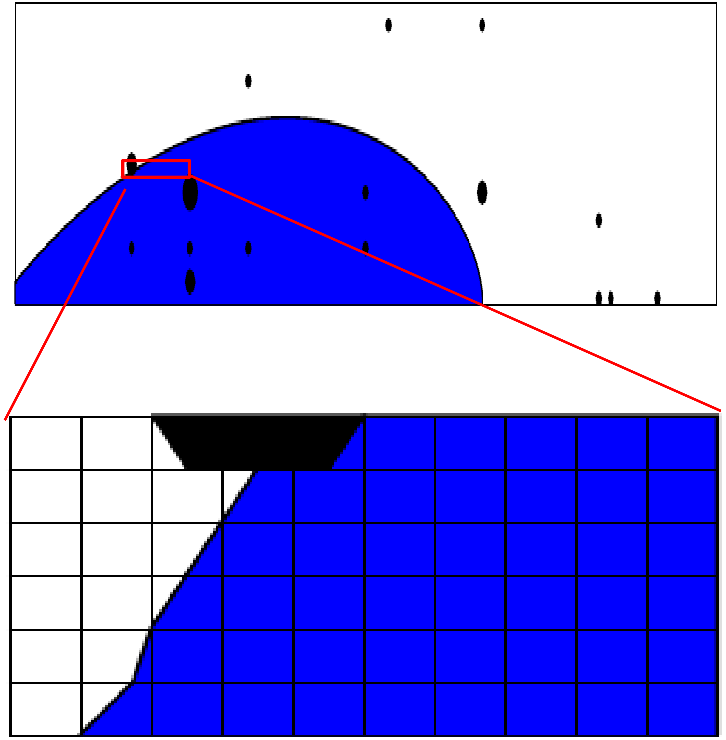

Fluid fine scale

Coarse Mesh

Averaging
Fluid-Particle
interaction

Advantages of the dual-grid multiscale

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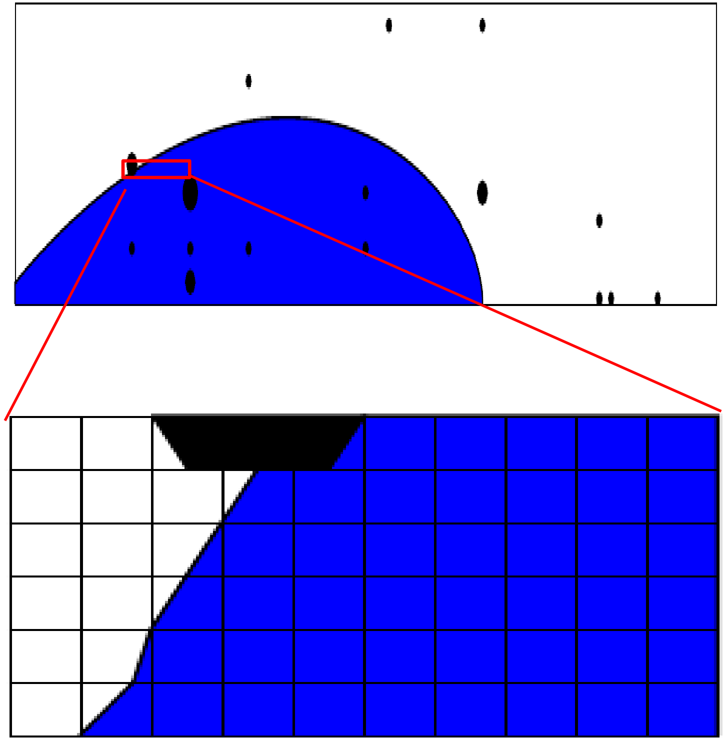


Fluid fine scale

Coarse Mesh

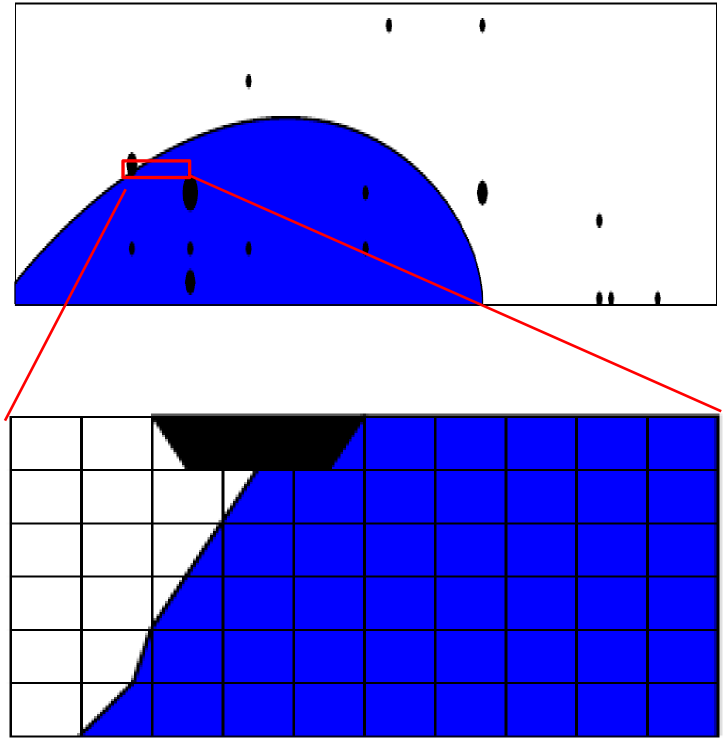
Averaging Fluid-Particle interaction

Fine Mesh

Solving fluid fine-scale

Advantages of the dual-grid multiscale

Bulk coupling scale



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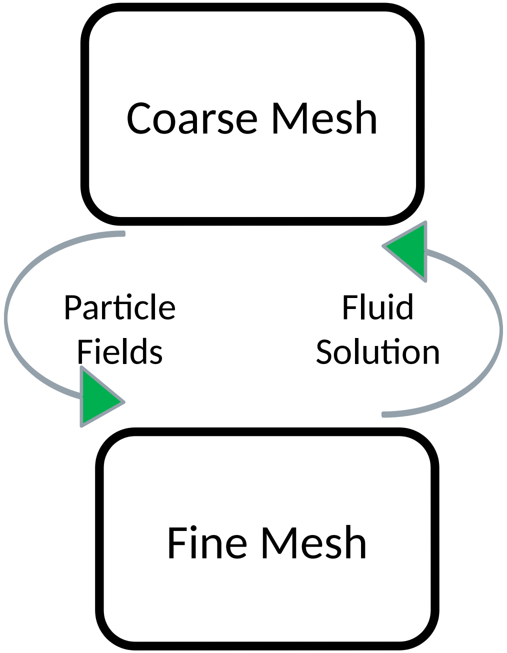
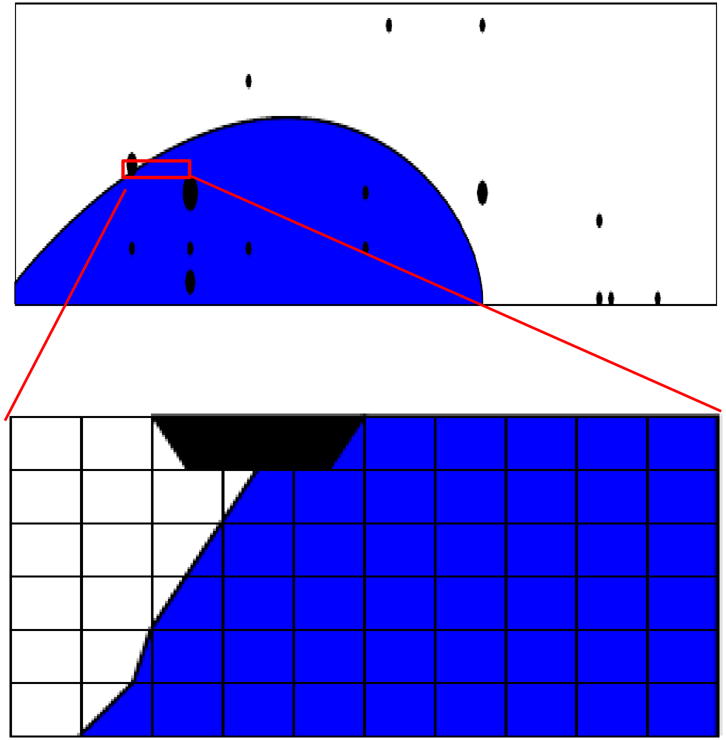


Averaging Fluid-Particle interaction

Solving fluid fine-scale

Advantages of the dual-grid multiscale

Bulk coupling scale



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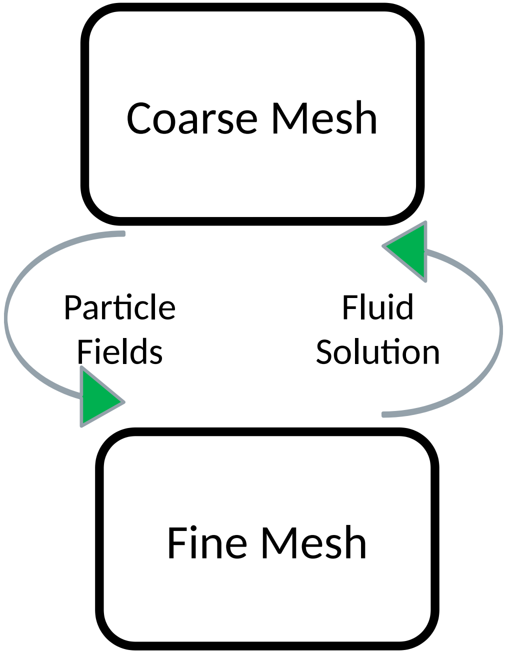

Averaging Fluid-Particle interaction

Solving fluid fine-scale

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

Co-located Partitioning Strategy
+
Dual-Grid Multiscale Approach

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
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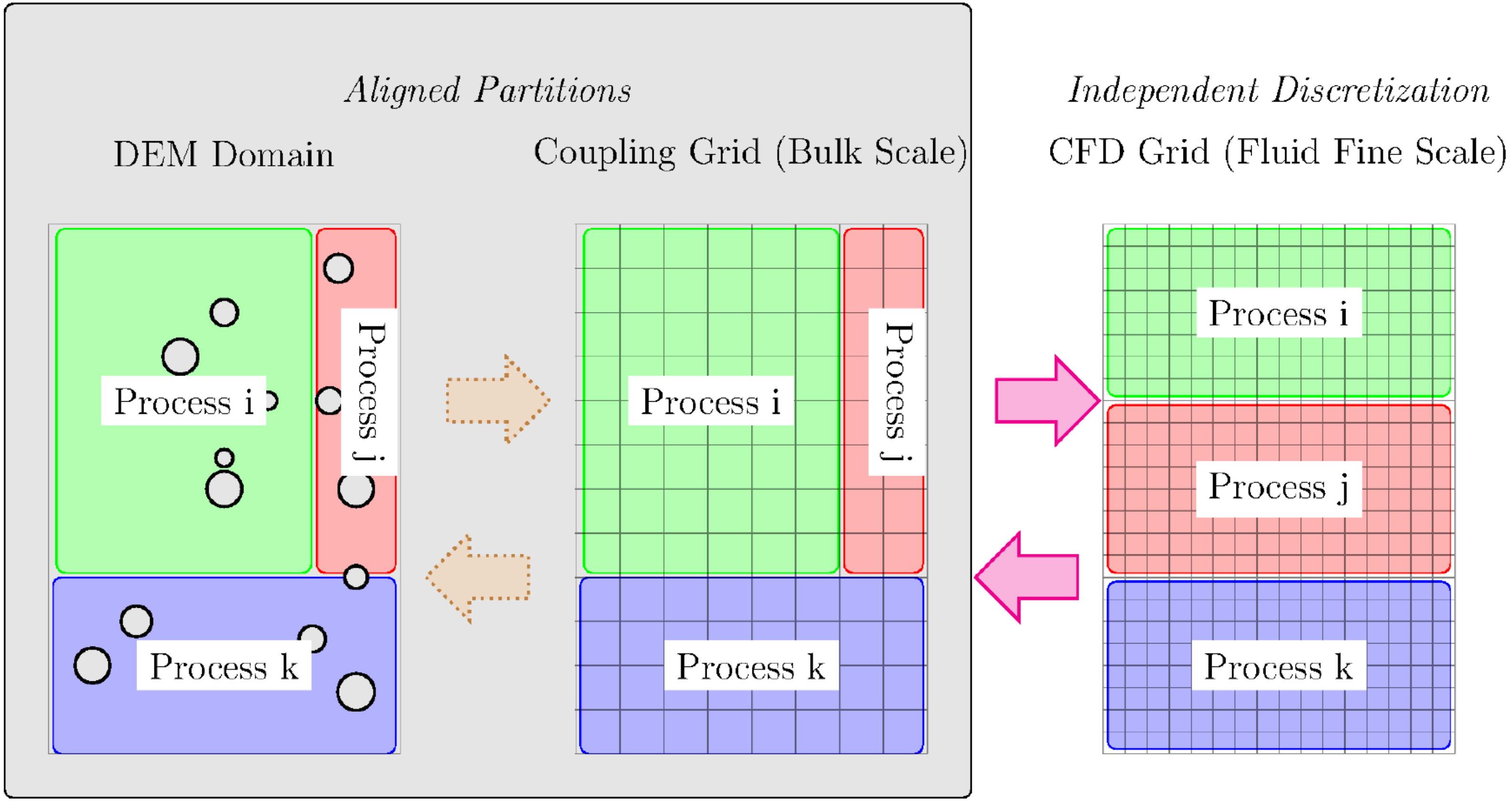
Dual grid and co-located partitioning



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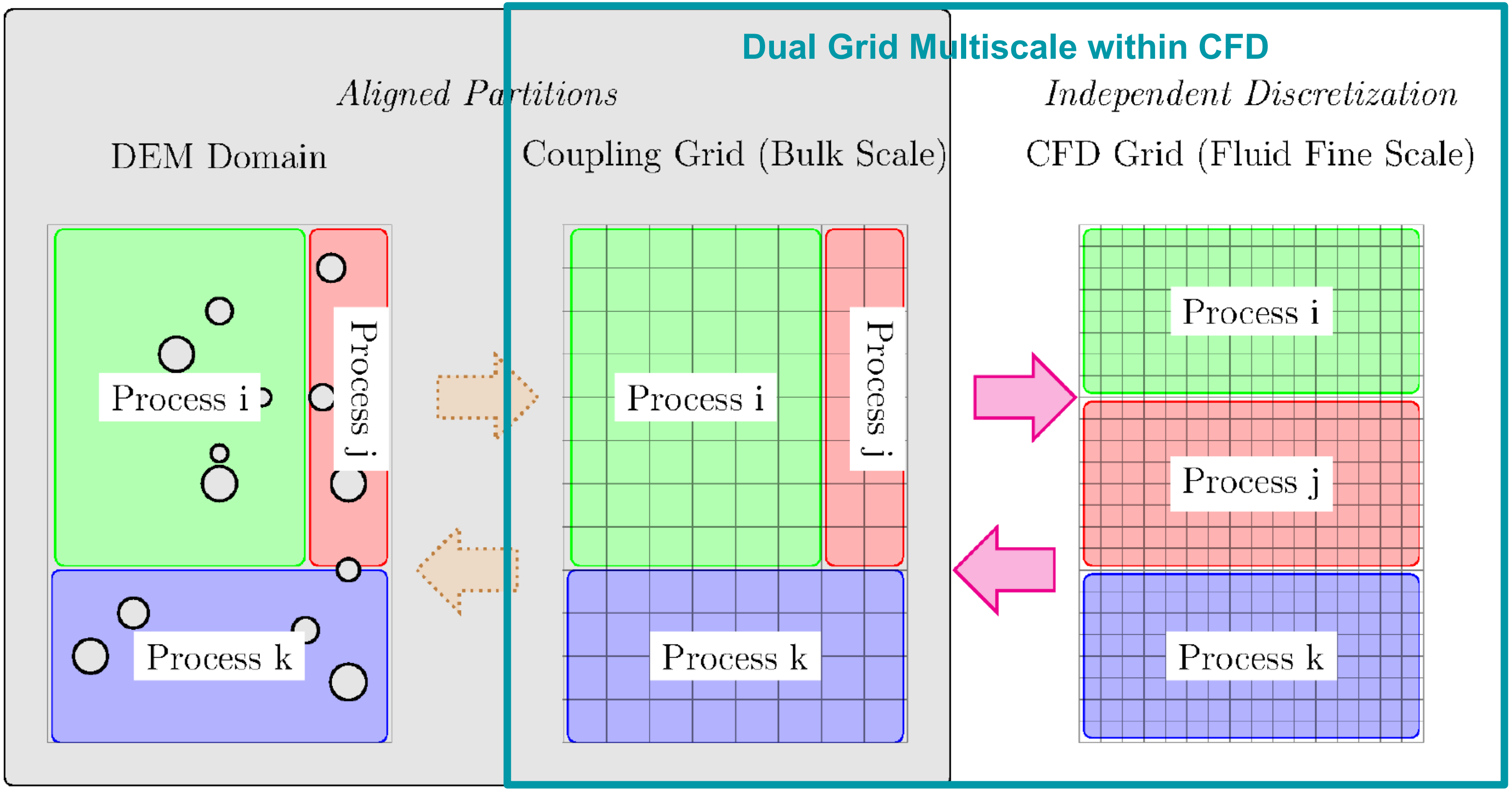
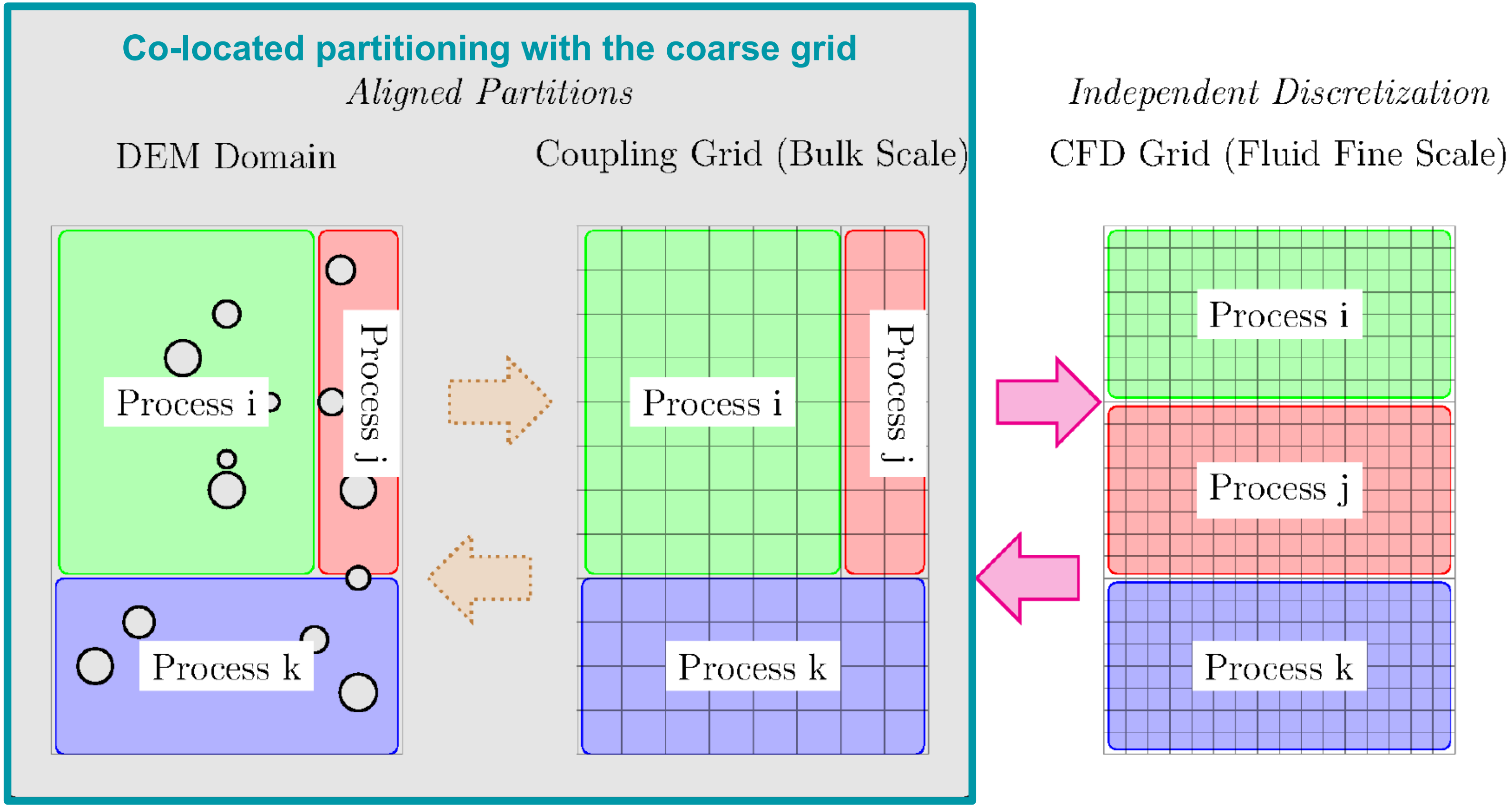


- No constraint on the partitioning of the fine mesh ⇒ better load-balancing for CFD

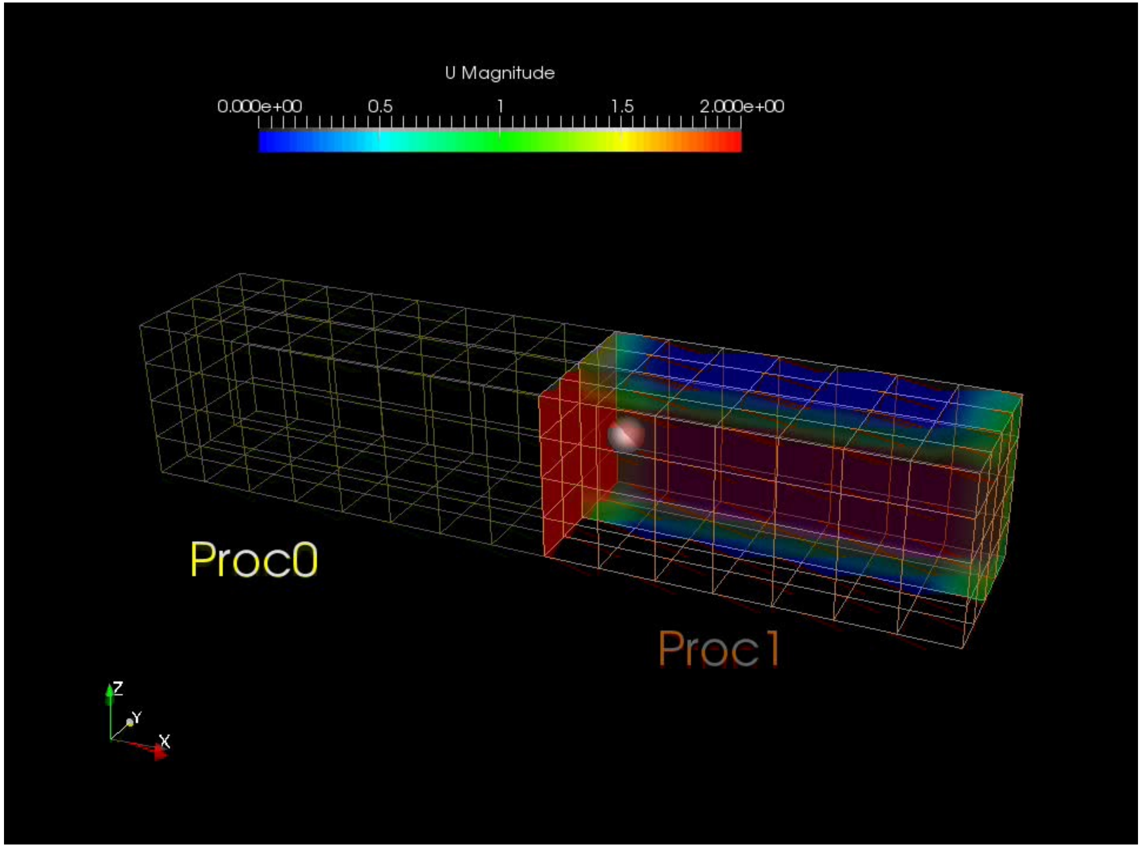
Dual grid and co-located partitioning



- 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

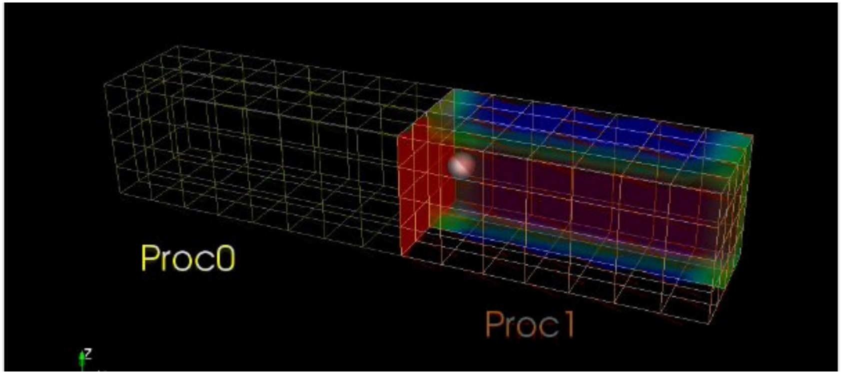
One particle crossing process boundaries

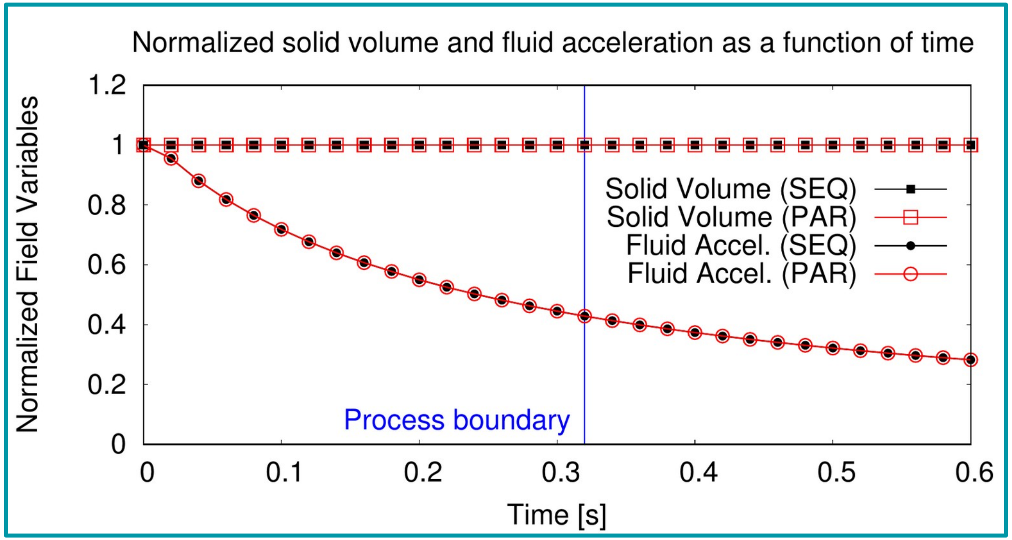


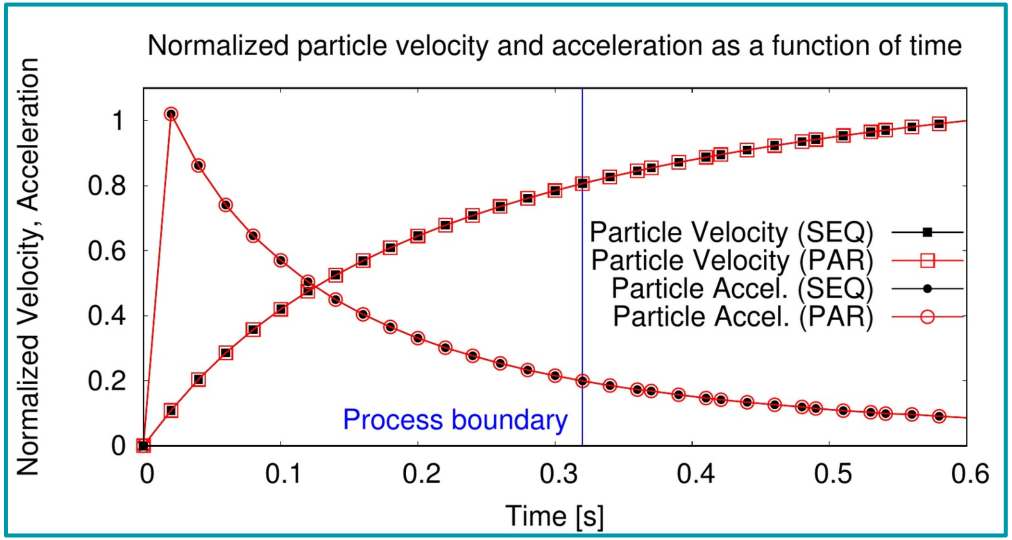
Setup

- 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

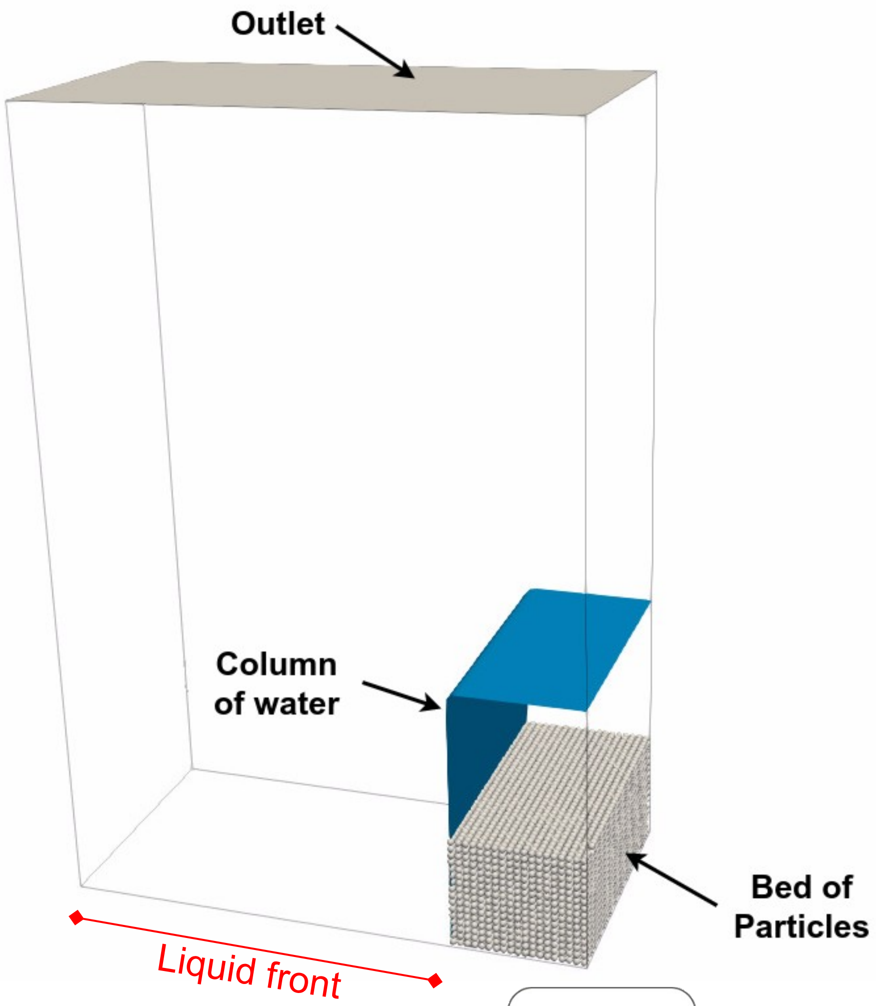
Liquid Front in a Dam Break

Setup

- colunm of water
- falling with particles

Results

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



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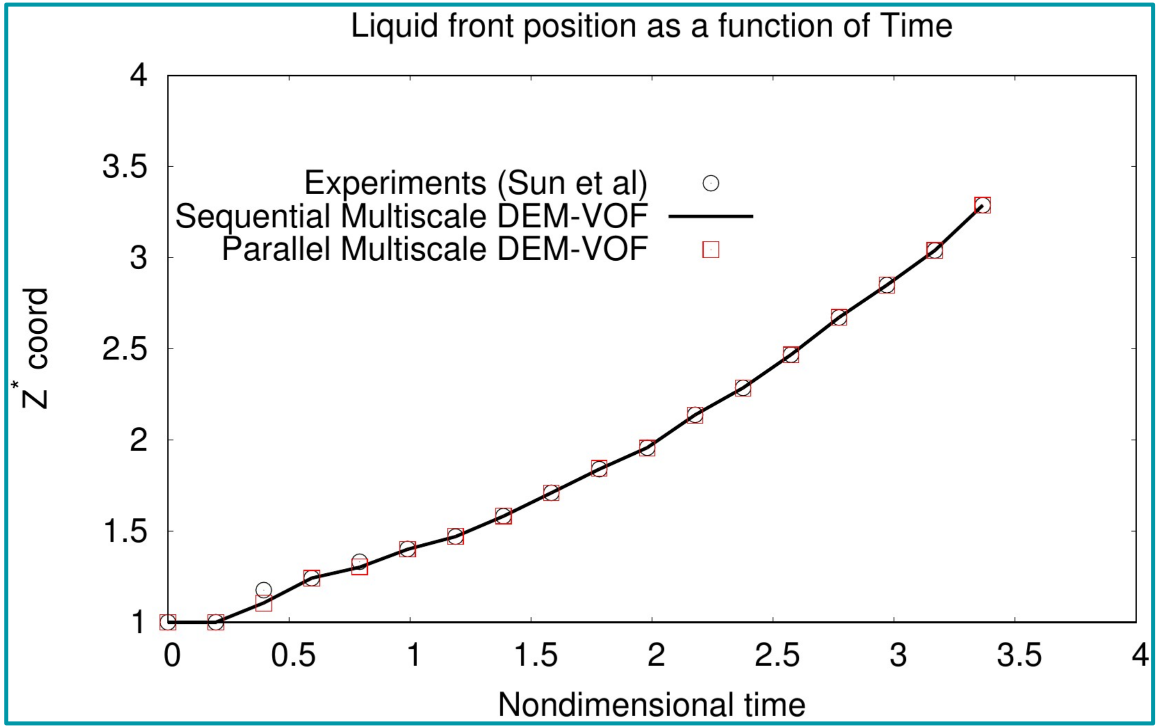
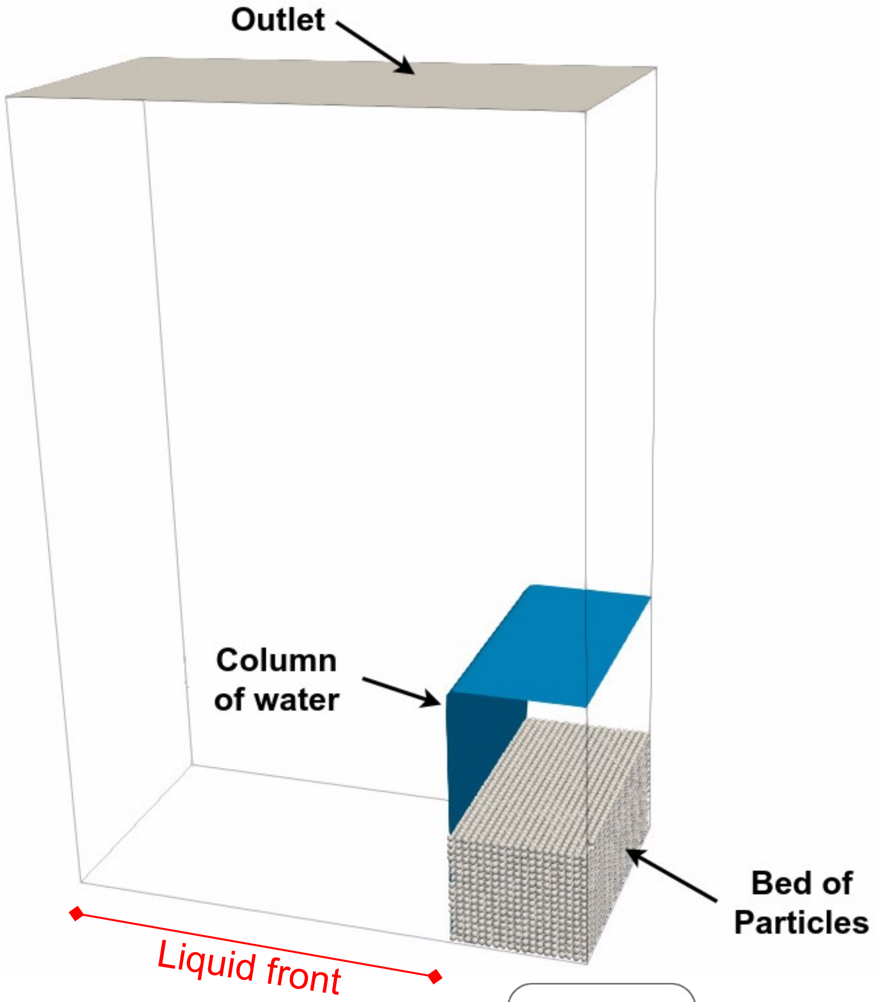




- position of the liquid front
- identical between sequential and parallel
- identical with experimental data

Performance Evaluation

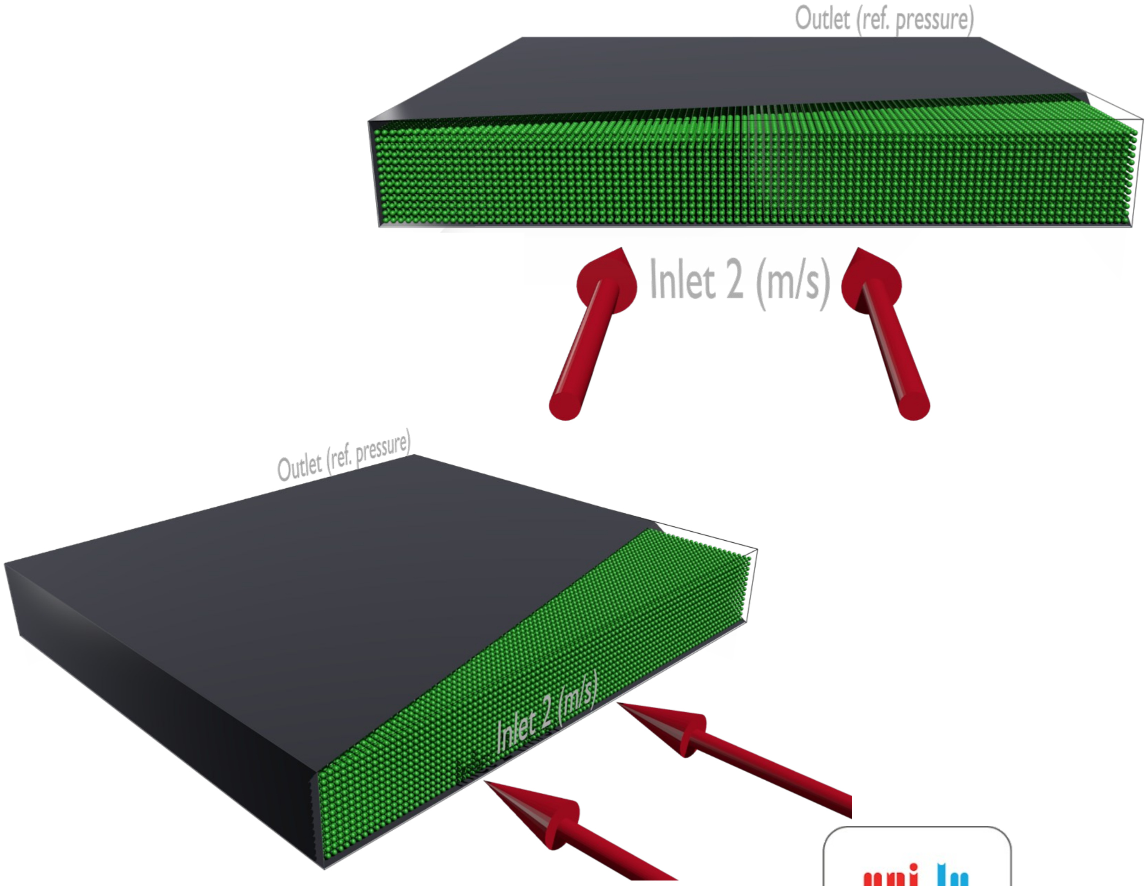
Scalability results (co-located only)

Setup

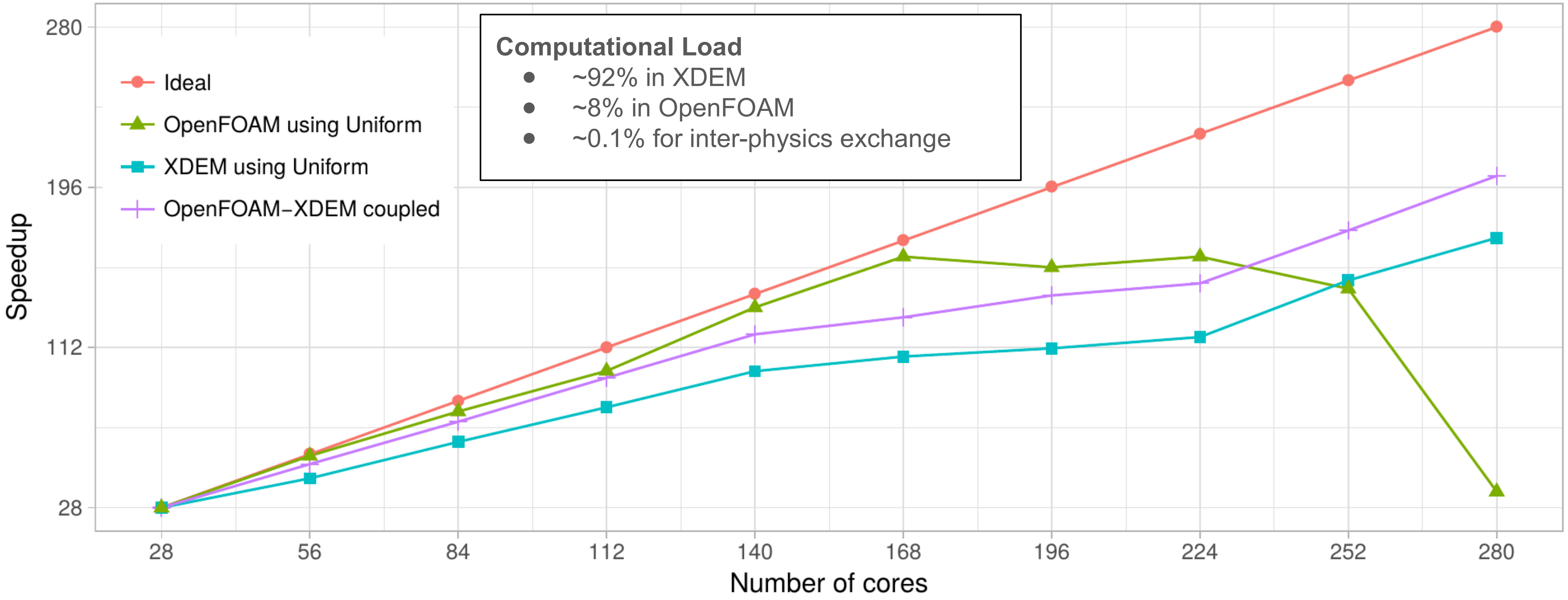
- 10 million particles
- 1 million CFD cells
- CFD mesh and DEM grid are aligned
- Uniform distribution
- From 1 to 10 nodes

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

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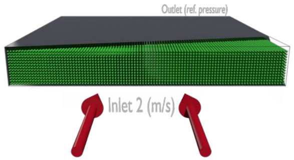
Weak Scalability / Communication Overhead

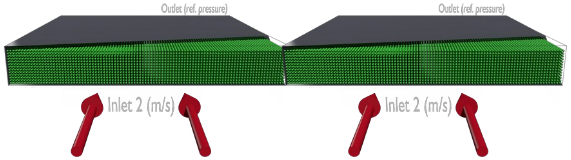
Setup

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

On 10 nodes

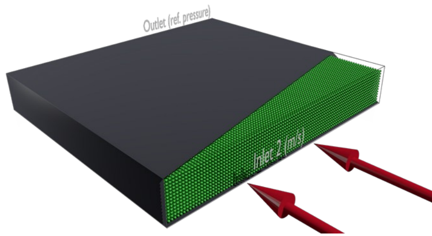


On 20 nodes



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)

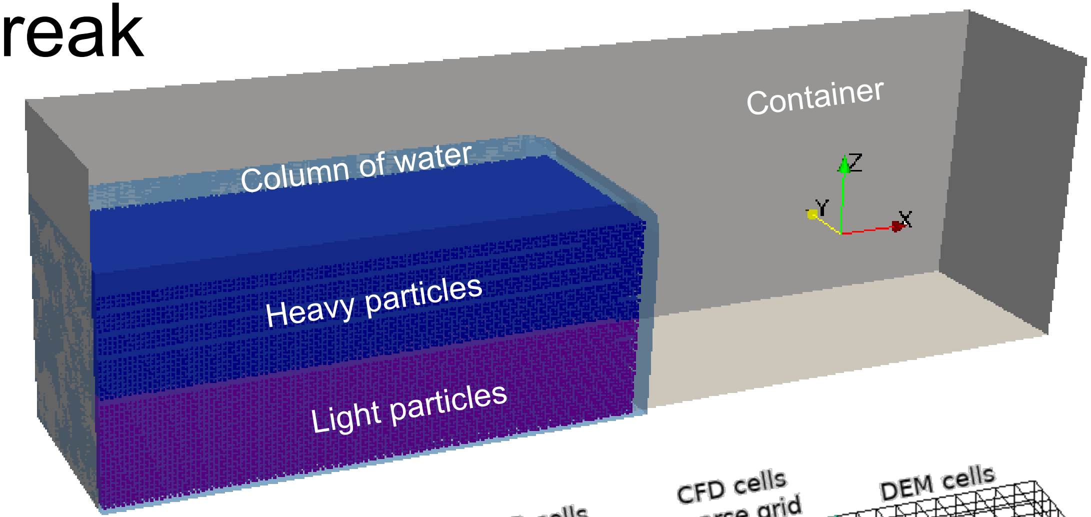
- **MFIX:** +160% overhead from 64 to 256 processes [Gopalakrishnan2013]
- **SediFoam:** +50% overhead from 128 to 512 processes [Sun2016]

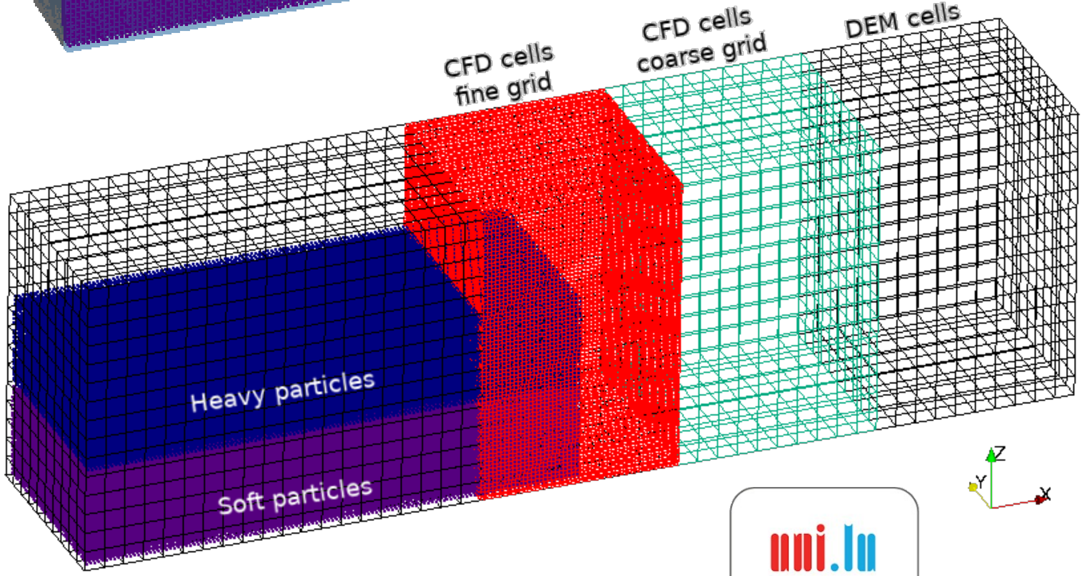
→ due to large increase of process-to-process communication

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

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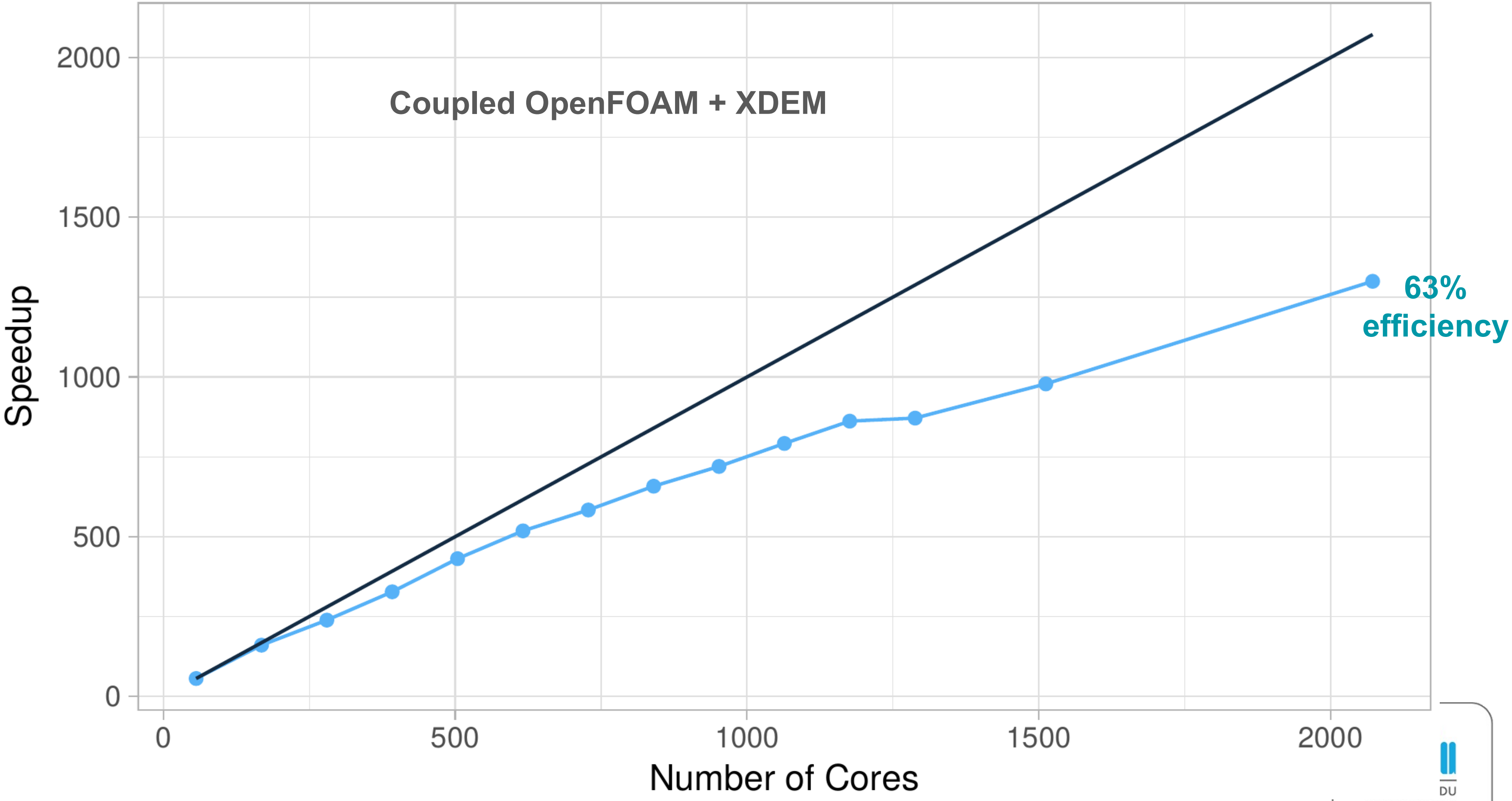
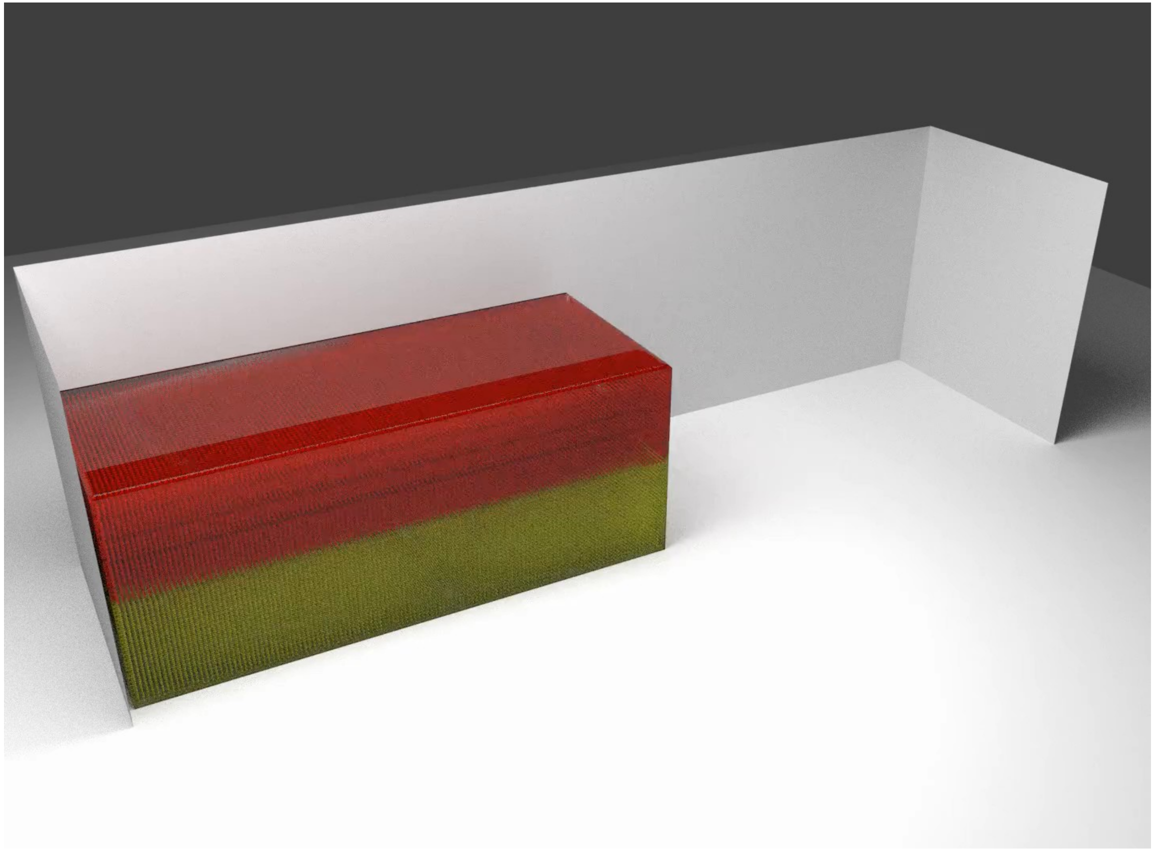
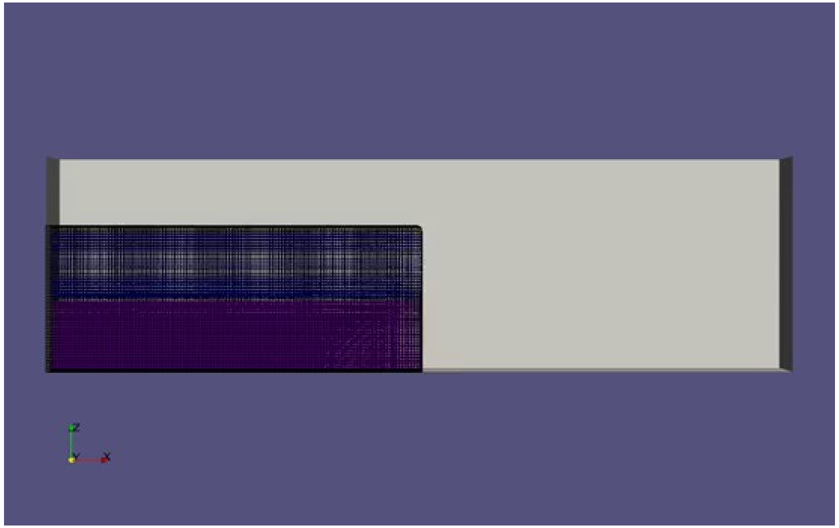
Dam Break scalability



Realistic Testcase: Dam Break





OpenFOAM
- 10M CFD cells

XDEM
- 1.18M light particles
- 1.18M heavy particles

Conclusion

Summary: Parallel Coupling of CFD-DEM Simulations

Leveraging 2 ideas

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

Next step in XDEM

- Support for heat and mass transfer in dual-grid / colocated strategy
  - Energy and mass conservation

Open issues

- Multiphysics-aware partitioner
  - Unequal load distribution between software
  - Data distribution
  - Dynamics load distribution
- Dynamics load-balancing / re-partitioning
  - To be supported by each physics module
- Resolve constraints on the mesh
  - Interpolation for arbitrary meshes
  - Inter-partitions inter-physics communication
  - Moving mesh
  - Use a generic coupling framework? eg **preCICE**, **OpenPALM/CWIPI**

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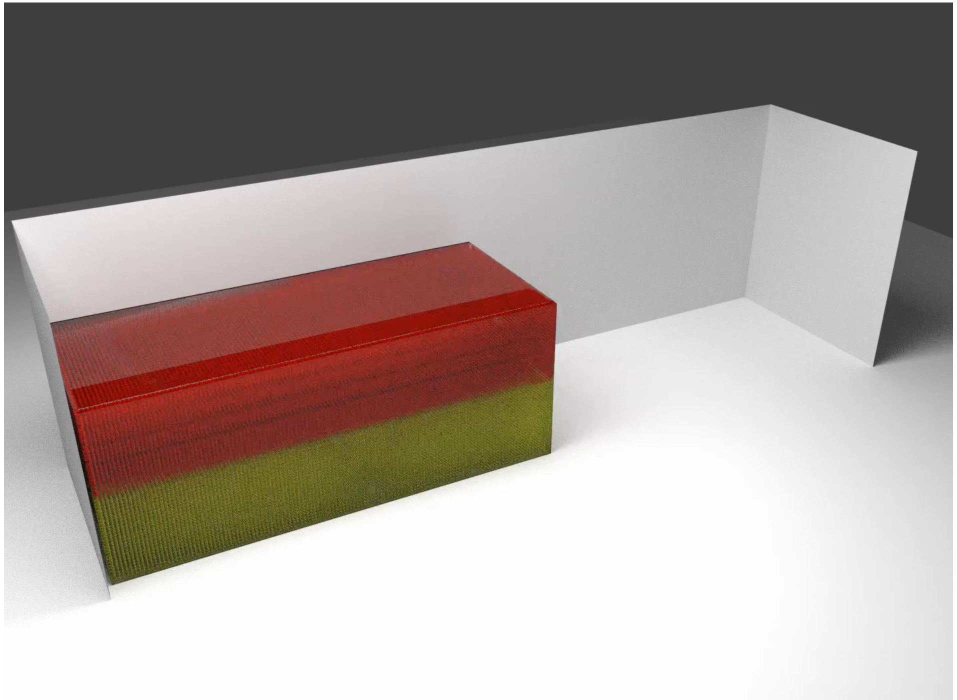
Thank you for your attention!

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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