Parallel Multi-Physics Coupled Simulation of a Midrex Blast Furnace

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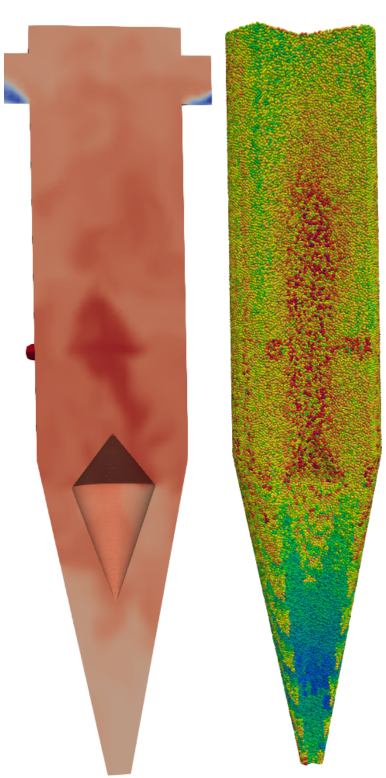


Context: Steelmaking Industry

Steelmaking Industry

- Blast furnaces are traditionally powered by coal
- Biggest source of CO_2 emissions (> 7% of global emissions)
- ➔ This must be addressed to mitigate global warming

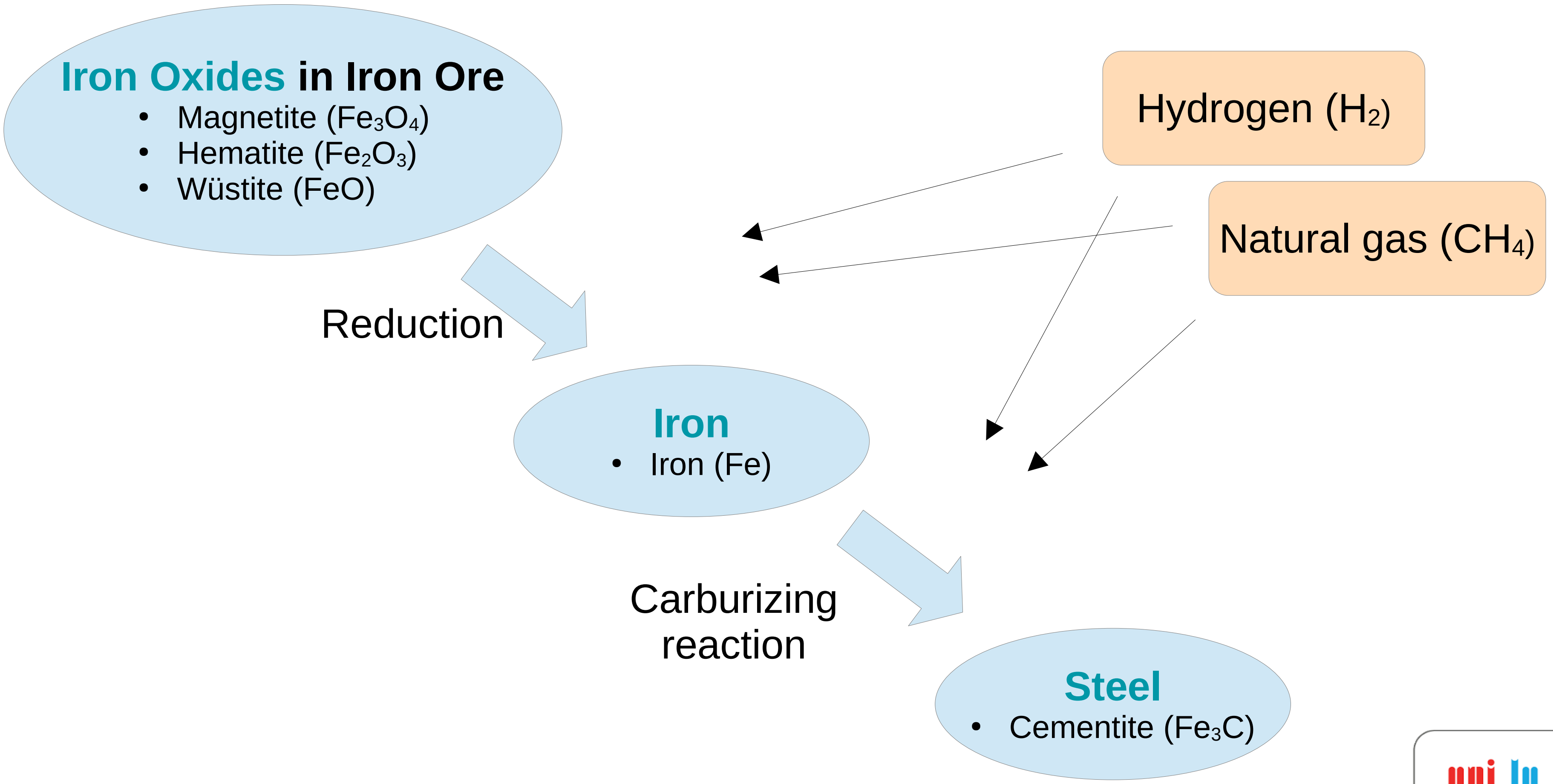
Green Steel

- Use of hydrogen as a reducing agent instead of carbon
- Furnaces to be powered by green electricity or green hydrogen

Our focus: Midrex Blast Furnace

- Introduced in the 70s
- Combine hydrogen and natural gas
- Not green, but lower carbon emission than coal-based traditional furnaces

From Iron Ore to Steel in the Midrex Blast Furnace



Research & Work Objectives

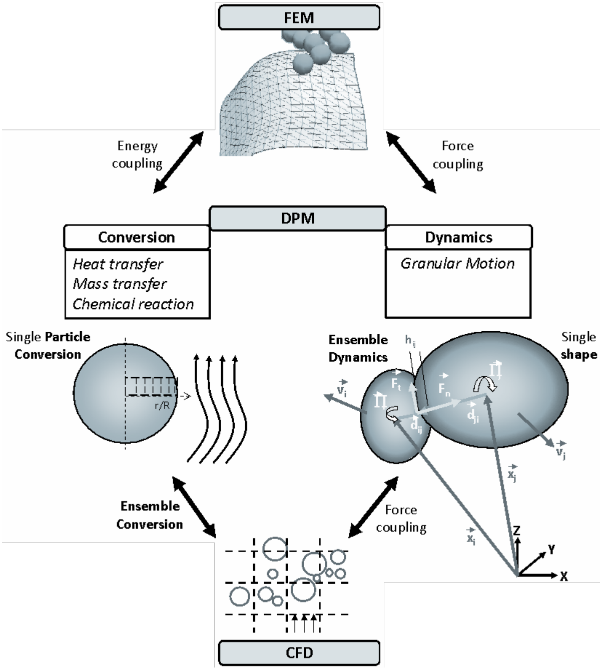
Multi-Physics Simulation of a Midrex Blast Furnace

- Fluid phase with Computational Fluid Dynamics (CFD)
- Particulate phase with Discrete Element Method (DEM)
- Volume Coupling
- Momentum, Heat and Mass transfer

Parallel Simulation on a Midrex Blast Furnace on HPC

- Performance evaluation on an industrial setup
- Understand the behavior of the coupled execution
- Highlight the challenges related to the load-balancing

Numerical Modelling of the Midrex Blast Furnace with the **eXtended Discrete Element Method (XDEM)**



Interactions Particles ↔ Gas

Reduction with hydrogen:

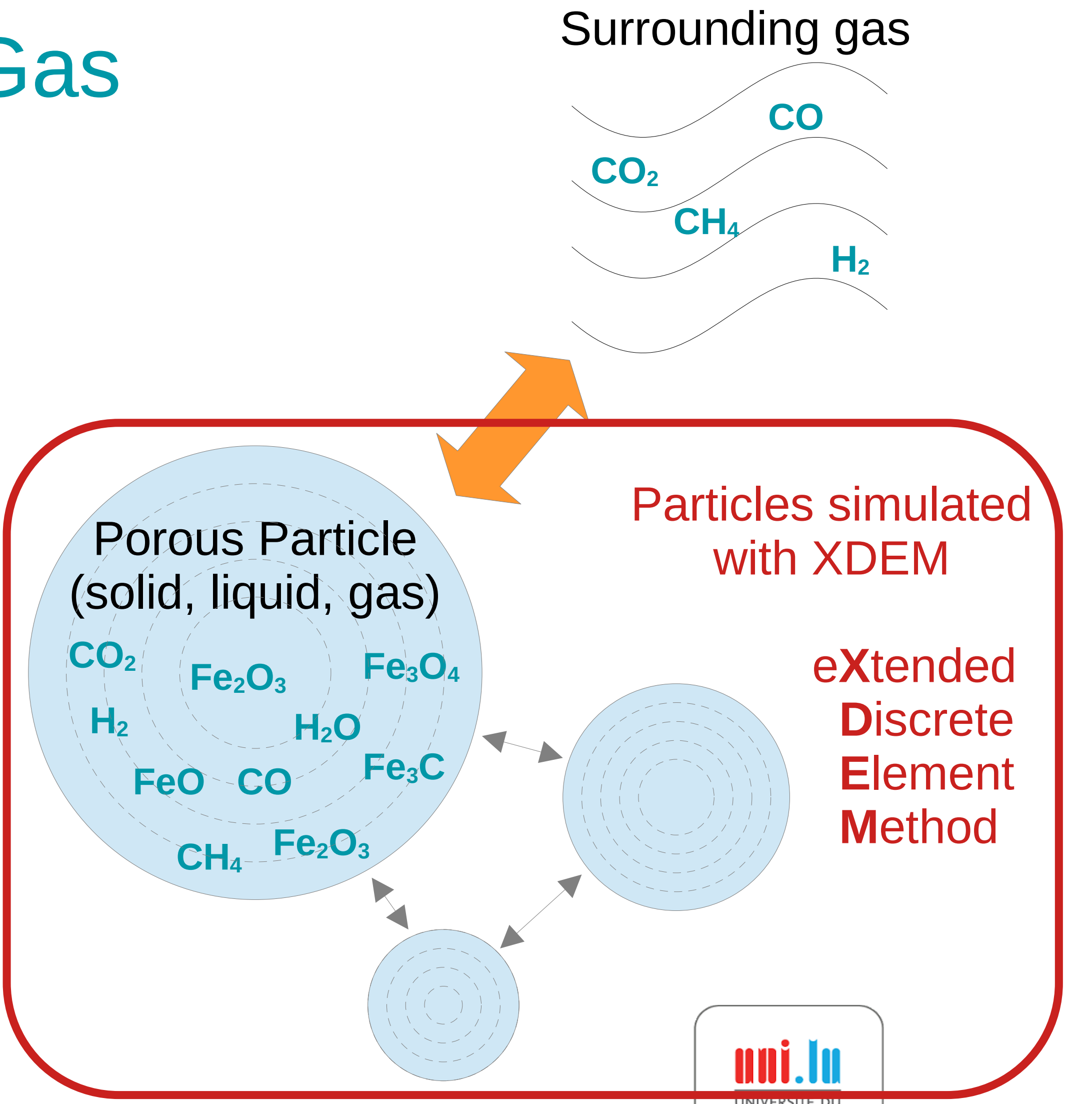
$$3Fe_2O_3 + H_2 \leftrightarrow 2Fe_3O_4 + H_2O$$
$$Fe_3O_4 + H_2 \leftrightarrow 3FeO + H_2O$$
$$FeO + H_2 \leftrightarrow Fe + H_2O$$

Reduction with carbon monoxide:

$$3Fe_2O_3 + CO \leftrightarrow 2Fe_3O_4 + CO_2$$
$$Fe_3O_4 + CO \leftrightarrow 3FeO + CO_2$$
$$FeO + CO \leftrightarrow Fe + CO_2$$

Carburizing reaction:

$$3Fe + CH_4 \leftrightarrow Fe_3C + 2H_2$$



Validation of Particle Conversion in XDEM

with experimental data

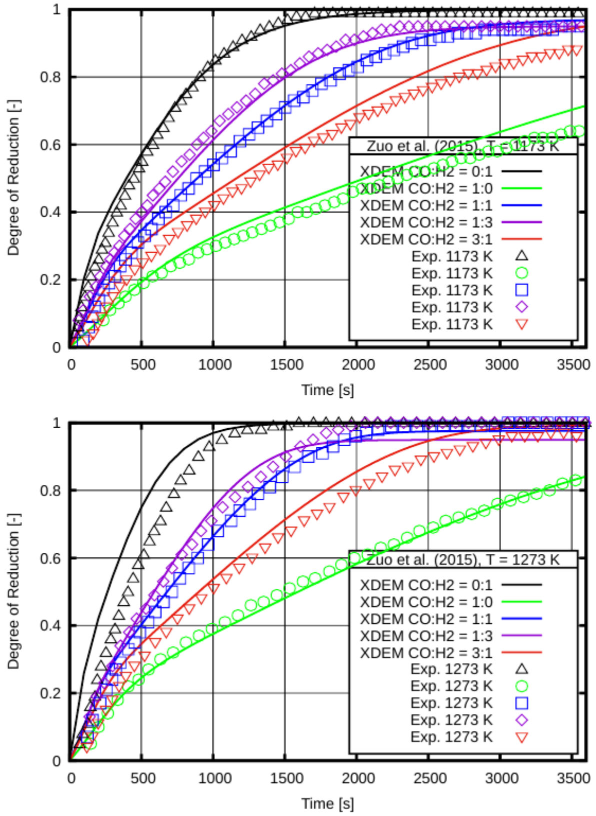


Figure 4: Validation of reducing reactions 1 to 3 for temperatures of 1073 K, 1173 K and 1273 K for different compositions of hydrogen and carbon monoxide in comparison with experimental data from [85].

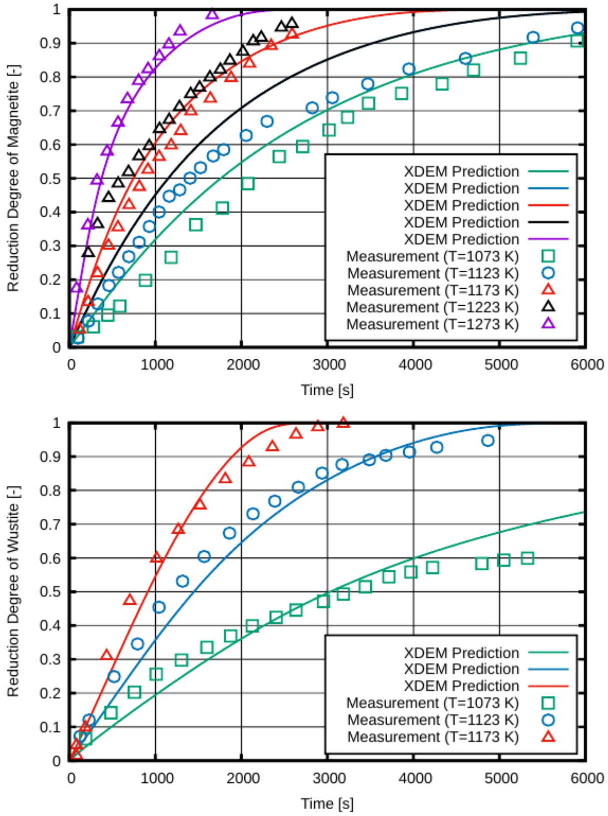


Figure 5: Validation of reducing reactions of Hematite, Magnetite and Wüstite for different temperatures in a pure carbon monoxide atmosphere according to reactions 4 to 6 in comparison with experimental data from [41].

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Coupling XDEM and OpenFOAM:
→ Multi-Physics Simulation of the Midrex Furnace

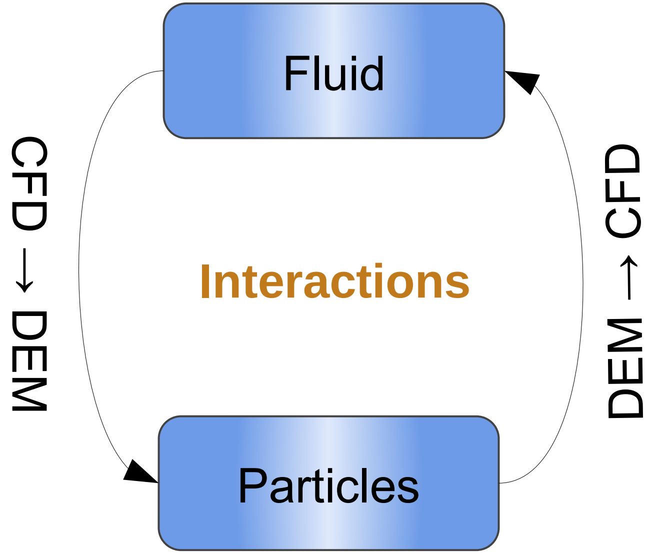
Two-way **volume coupling** between
Discrete Element Method (DEM) and
Computational Fluid Dynamics (CFD)

XDEM (Lagrangian) for:

- Motion and collisions of particles
- Thermodynamic Conversion of particles

OpenFOAM (Eulerian) for:

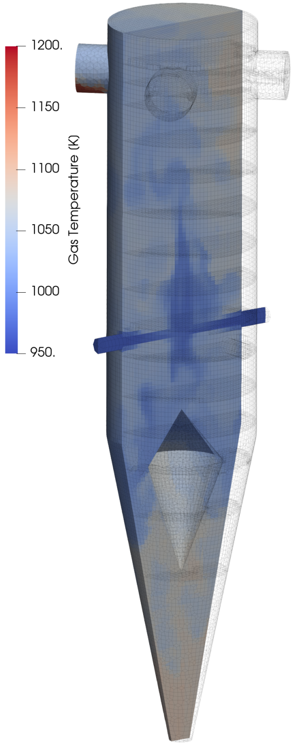
- Flow of gas phase
- Reactions in the gas phase



CFD-DEM coupling is required to capture the physics of the blast furnace and offers unprecedented insight.

Volume Coupling and Momentum, Heat and Mass transfer

Computational Fluid Dynamics



Fluid phase in **OpenFOAM**

- Fluid velocity, density, dynamic viscosity
- Pressure Gradient
- Temperature
- Thermal conductivity
- Heat
- Species mass fractions (CH_4, CO_2, CO, H_2, H_2O, N_2, O_2)

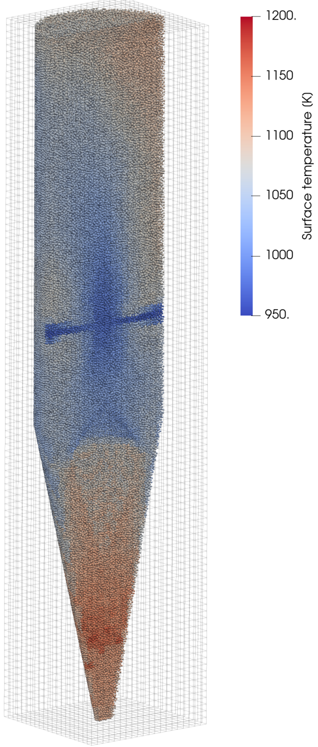
OpenFOAM to **XDEM**

Volume coupling
with
preCICE
coupling library

XDEM to **OpenFOAM**

- Porosity
- Momentum source (explicit and implicit terms)
- Heat source
- Mass sources (CH_4, CO_2, CO, H_2, H_2O, N_2, O_2)

Extended Discrete Element Method



Particle phase in **XDEM**

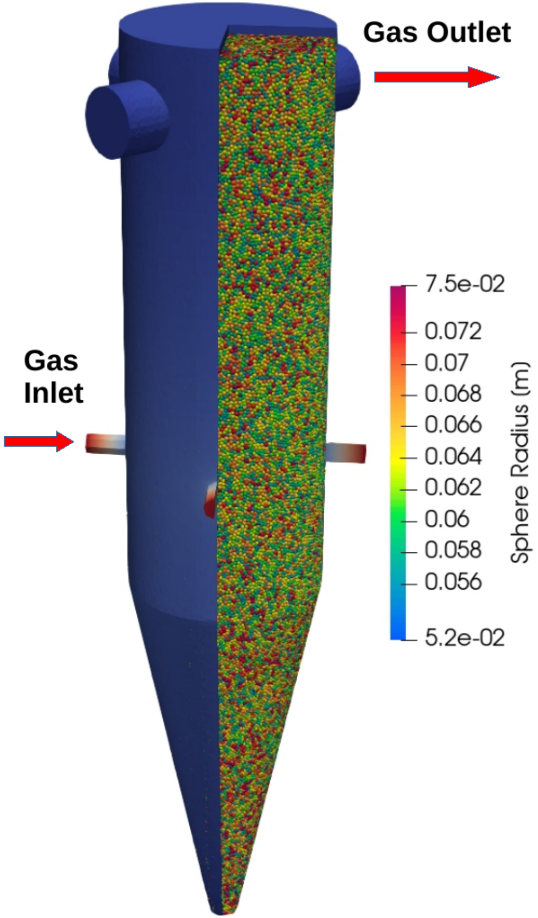
Midrex Blast Furnace Setup

Furnace

- Height: 32m and Diameter: 6.5m
- 4 gas inlet mid-height
- 4 gas outlet at the top
- CFD mesh with 133.559 cells

Iron Ore

- 485,336 spherical particles
- Radius between 4.5cm and 7.5cm
- 12 solid and gaseous species
- Scaling factor of 10 (Representative Particle Method)
- Particle motion is disabled
- Thermodynamics and chemical conversion is enabled



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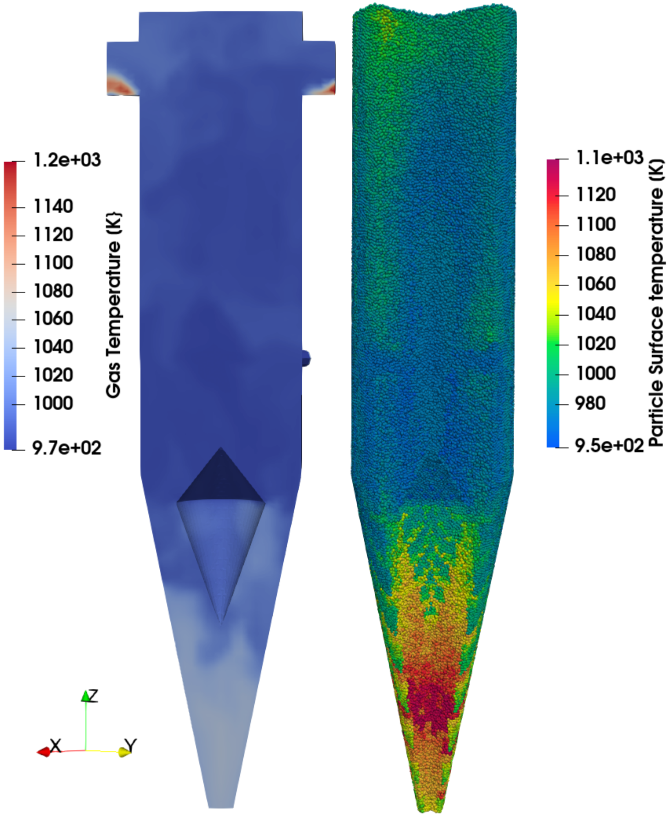
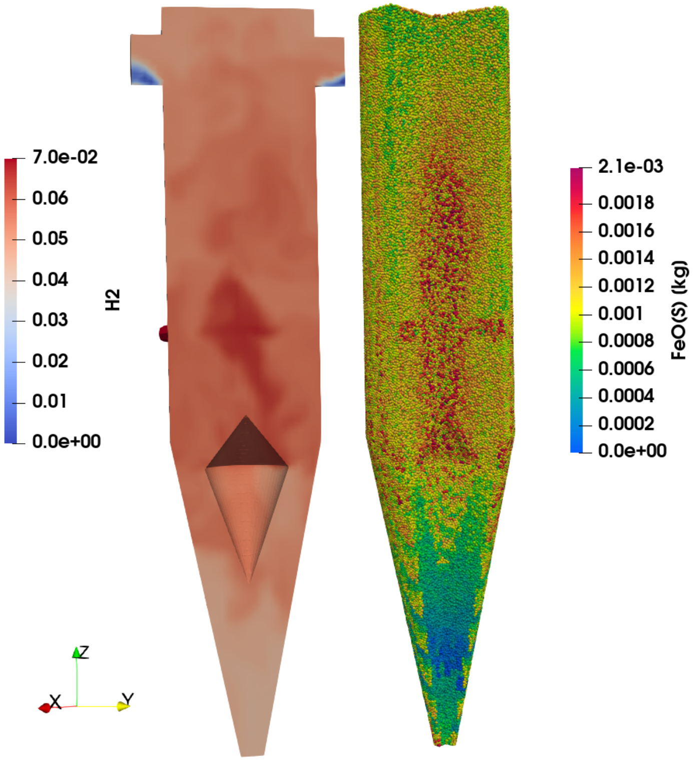
Numerical Results: Monitoring the Reduction Progress

Gas and Particle Temperature



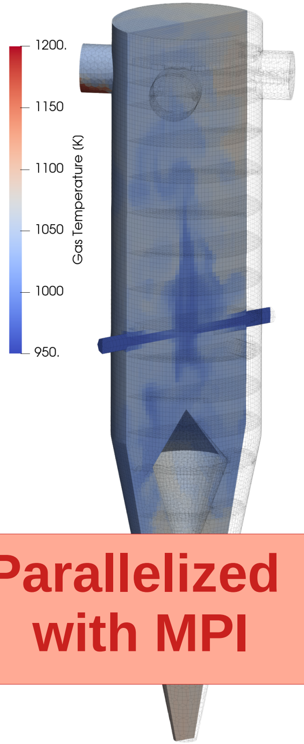
Distribution of H_2 in the Gas phase
Iron Oxide (FeO) in the Particles



Parallel Simulation of a Multi-Physics Midrex Blast Furnace

Parallel Coupling for MidRex Blast Furnace Simulation

Computational Fluid Dynamics



Parallelized with MPI

Fluid phase in **OpenFOAM**

- Fluid velocity, density, dynamic viscosity
- Pressure Gradient
- Temperature
- Thermal conductivity
- Heat
- Species mass fractions (CH_4, CO_2, CO, H_2, H_2O, N_2, O_2)

OpenFOAM to **XDEM**

Volume coupling
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XDEM to **OpenFOAM**

- Porosity
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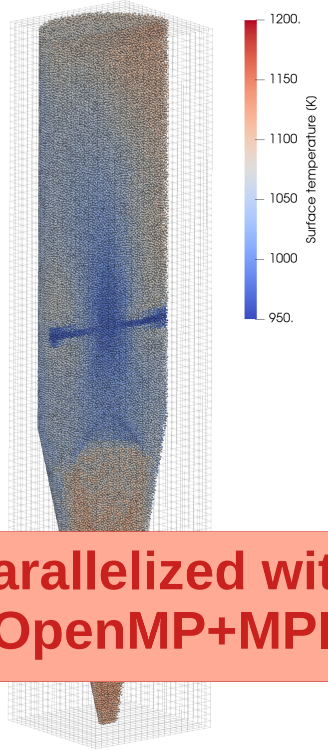
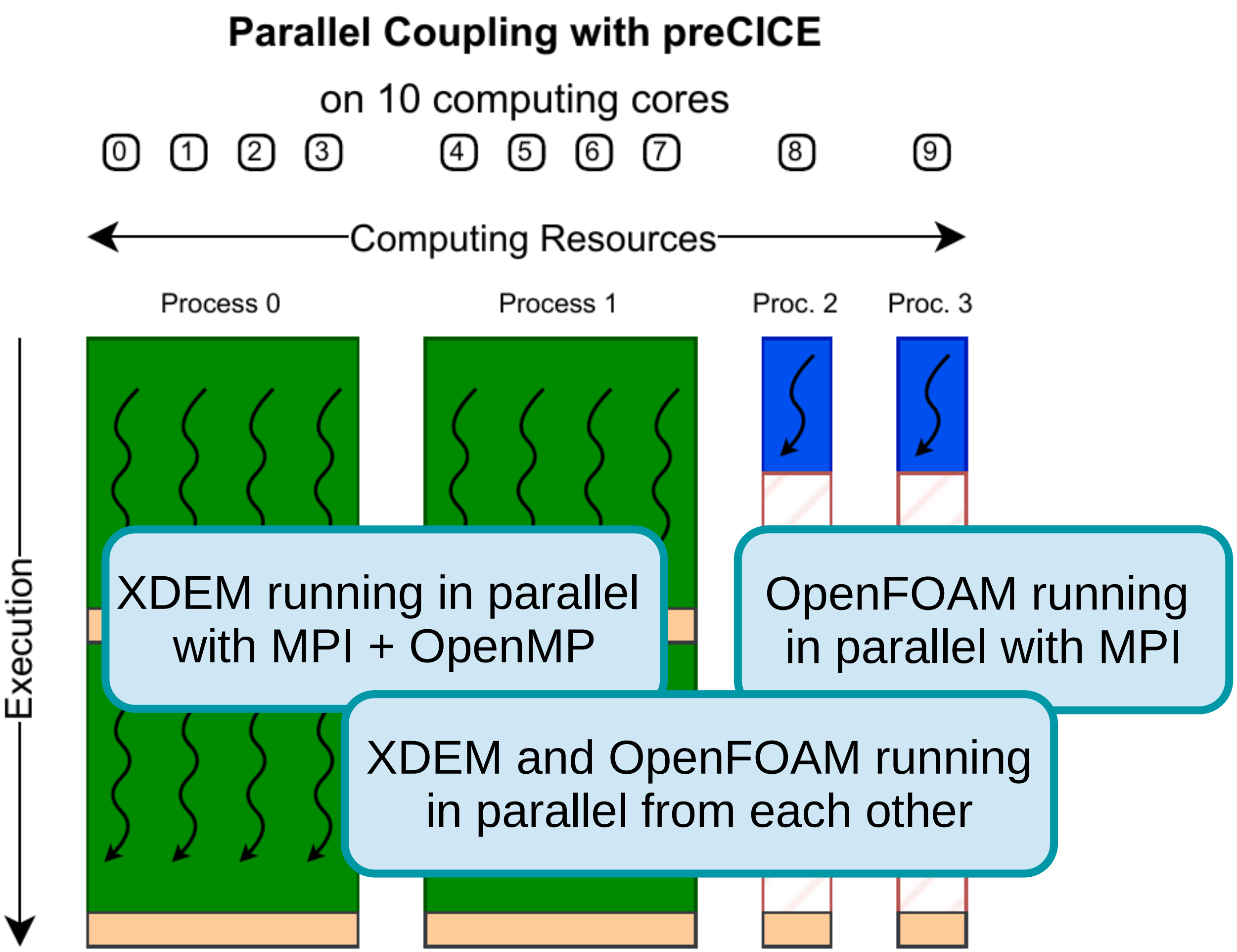
Extended Discrete Element Method



Parallelized with OpenMP+MPI

Particle phase in **XDEM**

Coupling Execution Strategy



Legend

- DEM with XDEM
- CFD with OpenFOAM
- Coupling communication with preCICE
- Unused computing time
- Computing threads

based on preCICE

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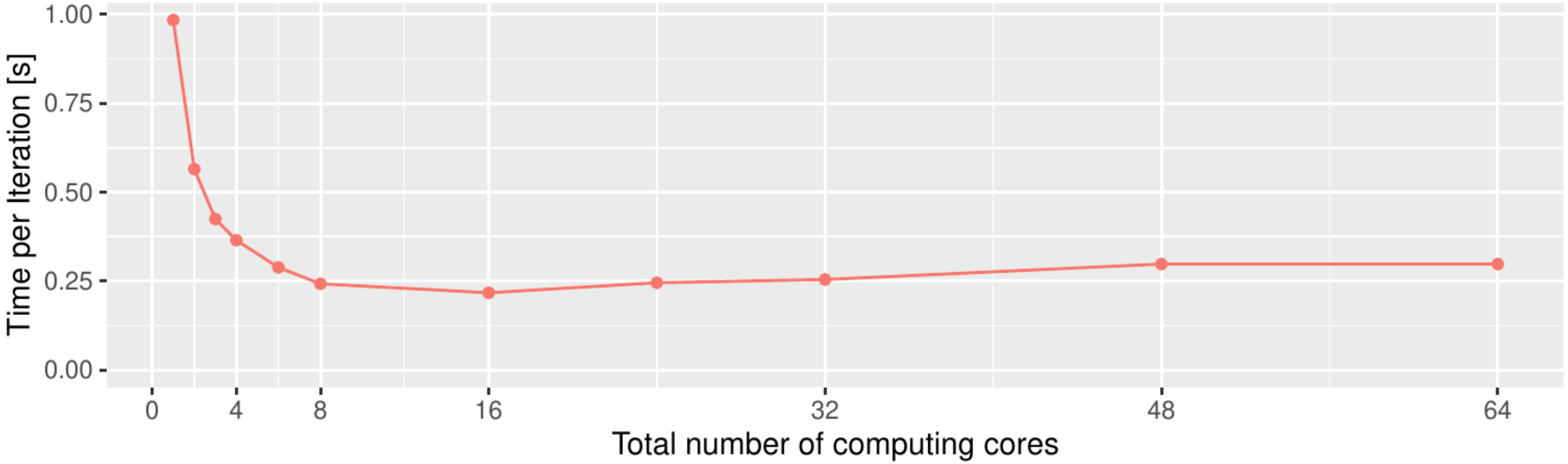
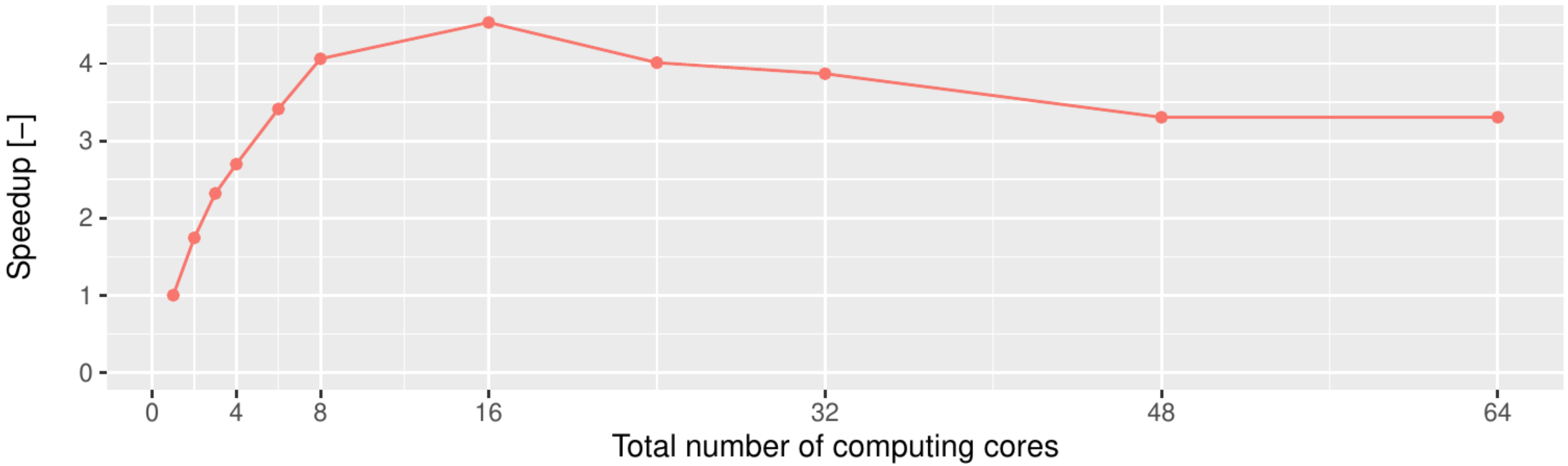
Performance Evaluation

Individual Scalability of OpenFOAM

- Coupled execution
- Time spent in OpenFOAM solver



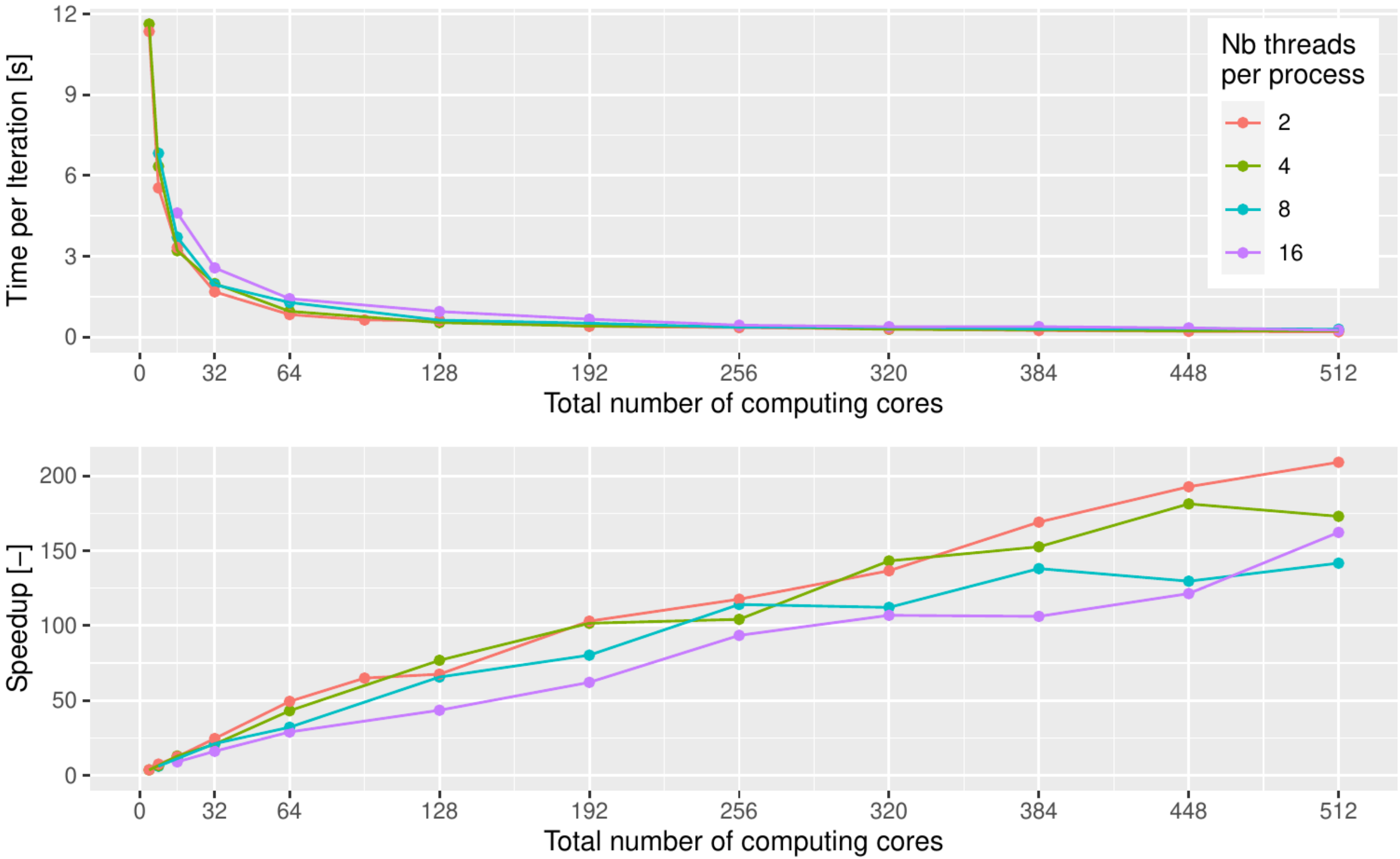
Time per iteration in sequential = 0.98 s



Scalability limited by the number of CFD cells

Individual Scalability of XDEM

- Coupled execution
- Time spent in XDEM solver

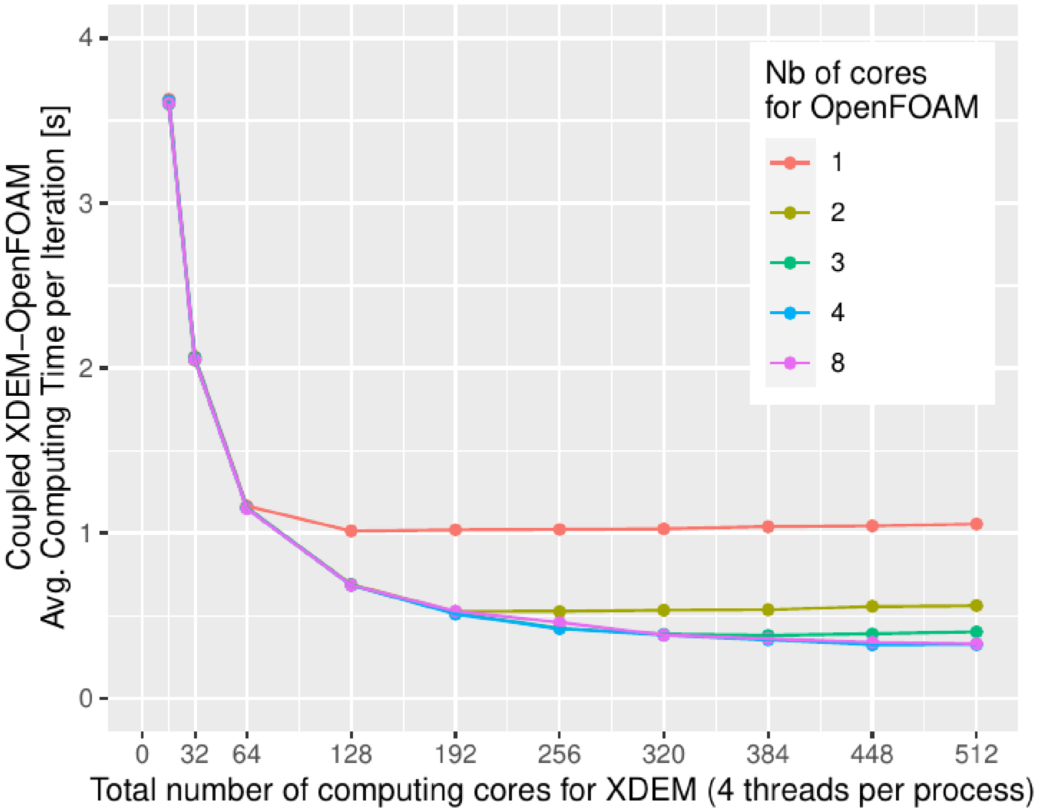


Time per iteration in sequential = 41.2 s

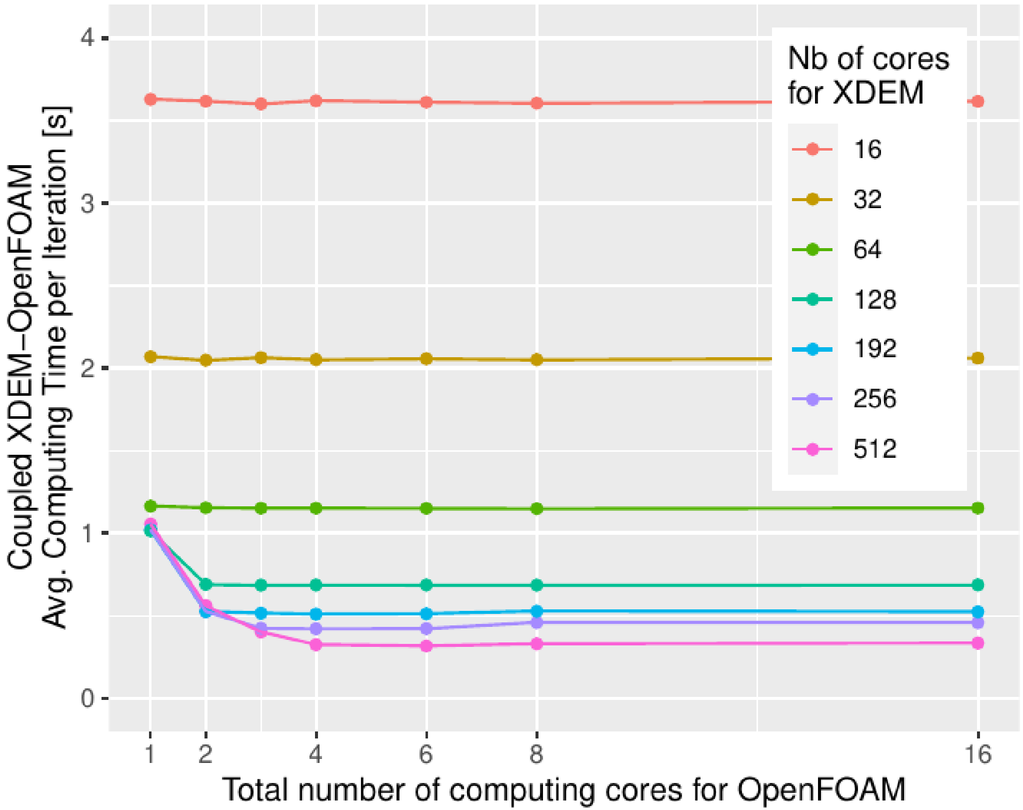
The load of XDEM is about 42 times the load of OpenFOAM

Good scalability up to 512 cores

Scalability of Coupled XDEM-OpenFOAM



Increasing number of cores assigned to XDEM



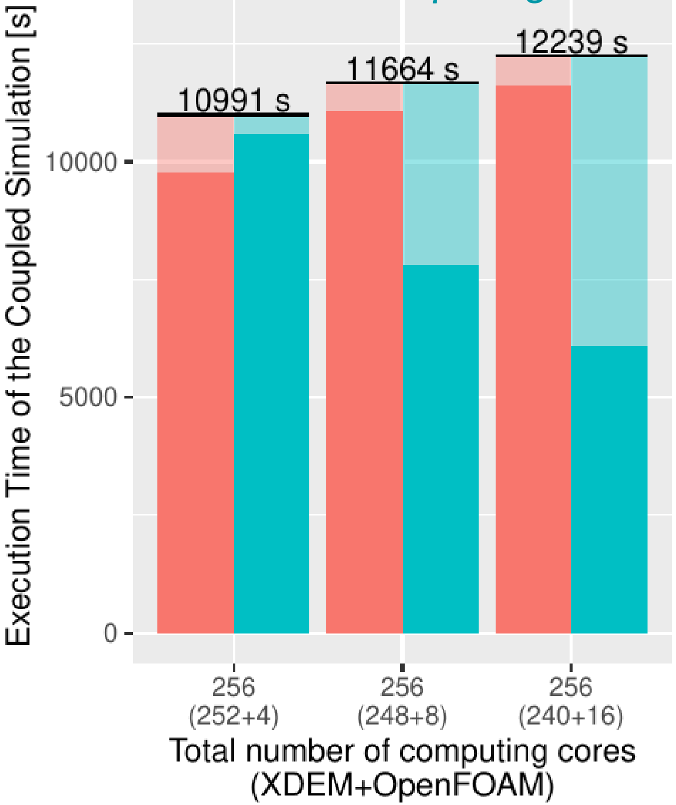
Increasing number of cores assigned to OpenFOAM

→ Performance are limited by the slowest solver

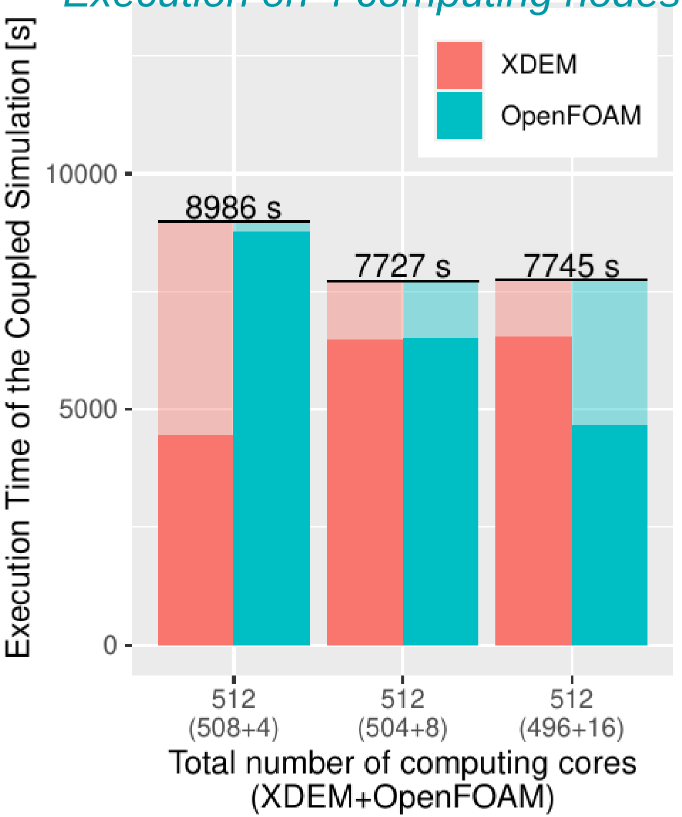
Complete Simulation of the Midrex Blast Furnace

500 simulated seconds

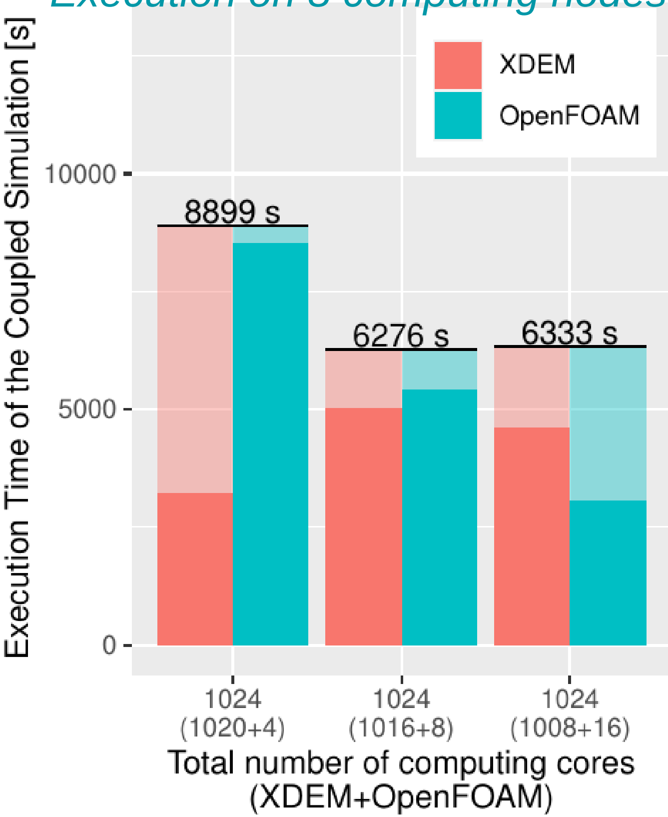
Execution on 2 computing nodes



Execution on 4 computing nodes



Execution on 8 computing nodes



- 500s simulation of Midrex Blast Furnace in 1h45 (config 1016+8)
- Coupling cost (communication+synchronization) up to 27% (config 1008+16)

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Beyond the Midrex Blast Furnace

What did we learn on the
Load Balancing of Multi-Physics Coupled Simulations ?

- The slowest solver limits the performance
- We must balance the load **within solvers** and **between solvers**
- The slowest solver can change when new resources are added
  - → Load balancing needs a **performance model of each solver**
- **Coupling cost** can represent a large part of time at larger scale
  - → Load balancing needs a **cost model for the coupling**

Furthermore, solver load can change with the time

→ Update of the performance model + Dynamic load balancing

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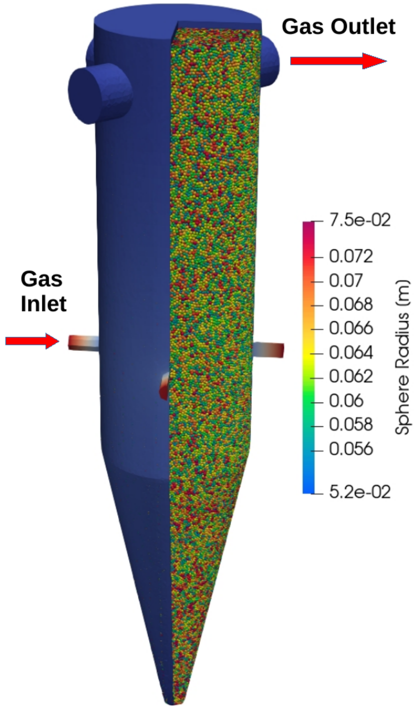

Thank you for your attention!

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Fonds National de la Recherche Luxembourg

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