Development of an HPC Multi-Physics Biomass Furnace Simulation and Integration in a Cloud-based Workflow

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In collaboration with ENERSTENA GROUP

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MS97: Enabling Technologies and Simulation Practices for Advanced Scientific and Engineering Computation

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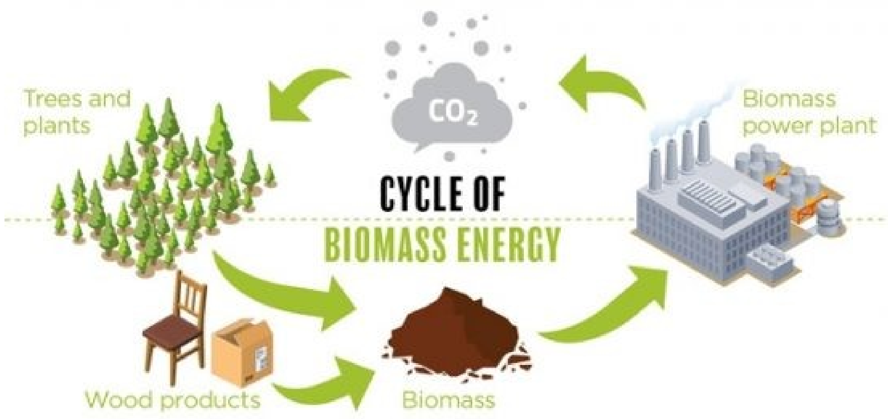
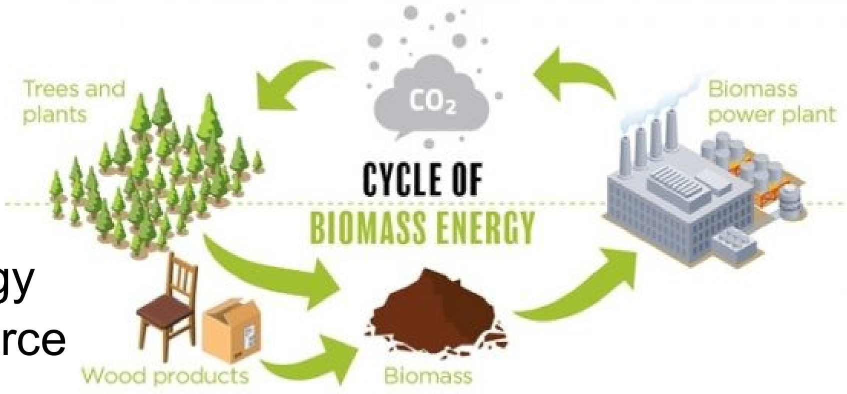
Introduction to Biomass Combustion



Biomass Combustion



Biomass combustion (e.g. wood chips)

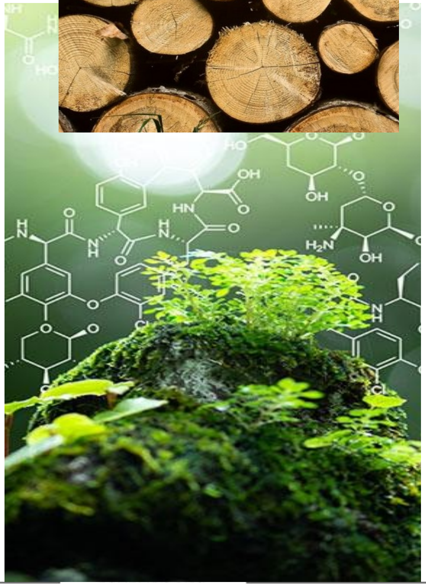
- widely used for generating electric and thermal energy
- renewable and potentially carbon-neutral energy source

Combustion process

- very complex
- requires advanced techniques to minimize harmful gas emissions

Alternative biomass

- wood waste, straw, bark, olive pits, nut shells, grain husks, bagasse, etc.
- can cause problems due to their chemical composition, ash melting temperature, humidity, ash content, calorific value and others.

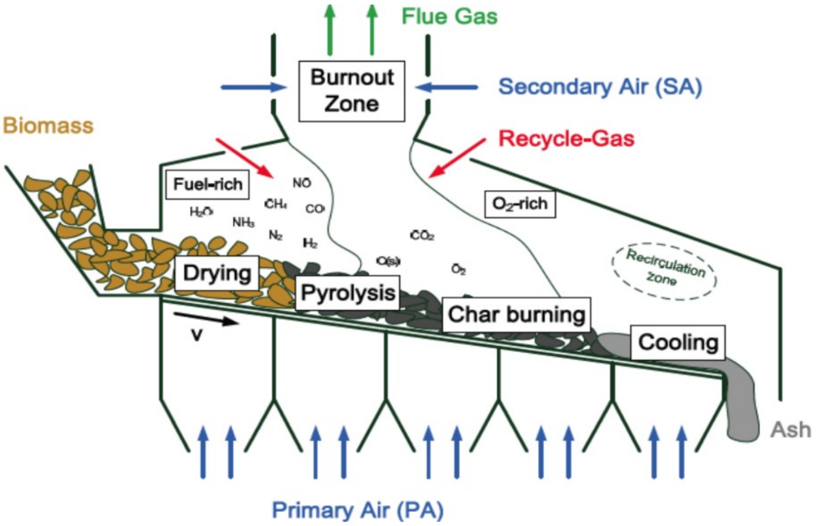


Combustion process in a biomass furnace

Combustion chamber of a biomass furnace
- forward acting grate
- transports the fuel through the furnace

The fuel undergoes a number of steps
- drying, pyrolysis, char burning, cooling in which it releases hydrocarbons
- hydrocarbons are burned in the gas phase

Use **numerical simulations**
- to study efficiency and performance
- and reduce the costs of experiments



Research & Work Objectives

Multi-Physics Simulation of a Biomass Furnace

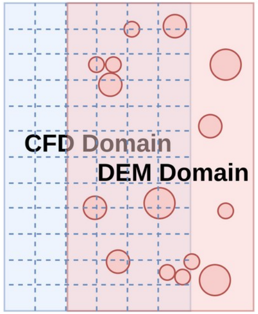
- Fluid phase with CFD
- Particulate phase with DEM
- Volume Coupling
- Momentum, Heat and Mass transfer
- Running on HPC

Seamless Cloud-based Workflow for SMEs

- Configurable Furnace Setup
  → specified by our industrial partner Enerstena UAB
- Fully automatic, from furnace specifications to simulation report

High Performance Biomass Furnace Simulation

- XDEM: eXtended Discrete Element Method
- CFD-DEM Volume Coupling
- Co-located Partitioning



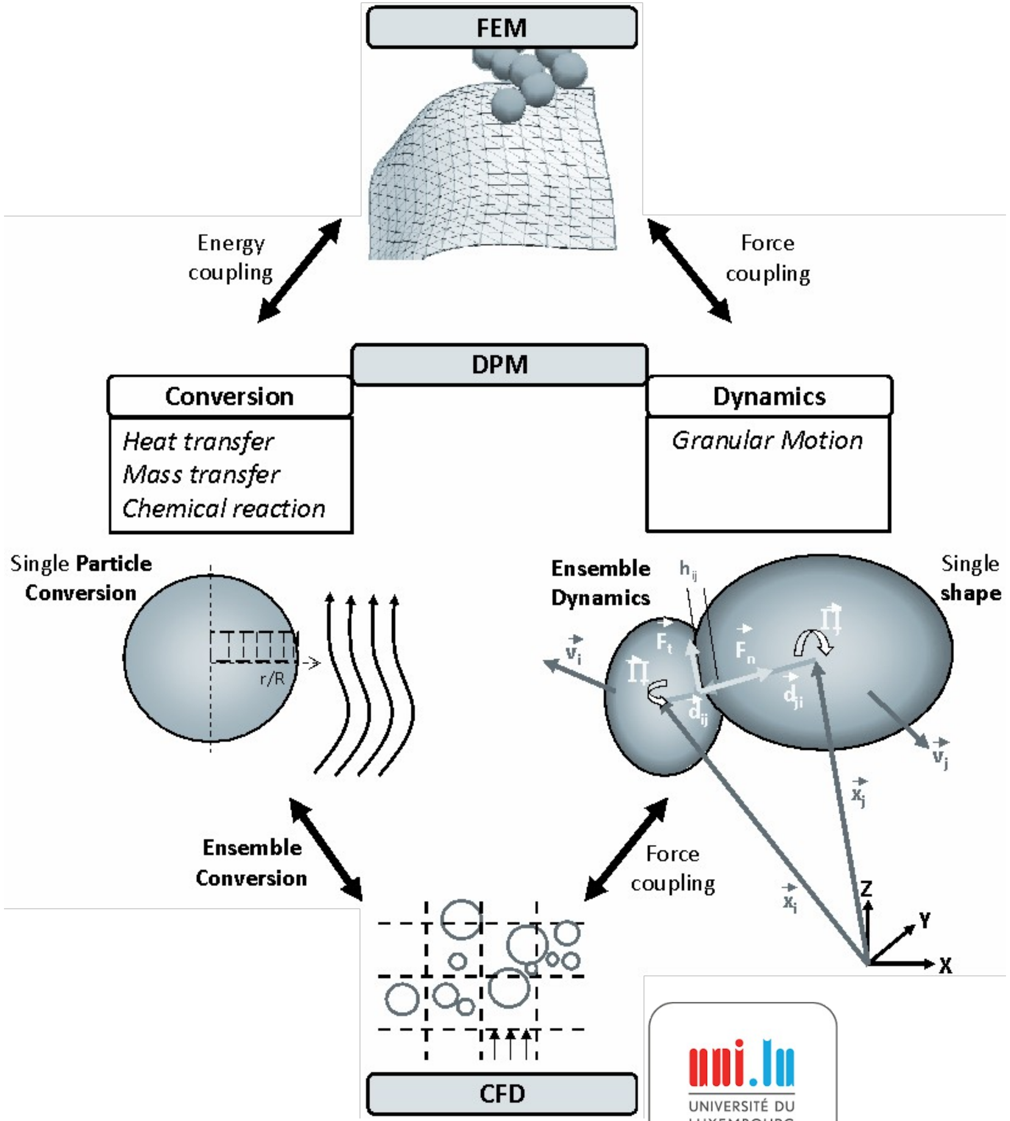
What is XDEM?

eXtended Discrete Element Method

Particles Dynamics
- Force and torques
- Particle motion

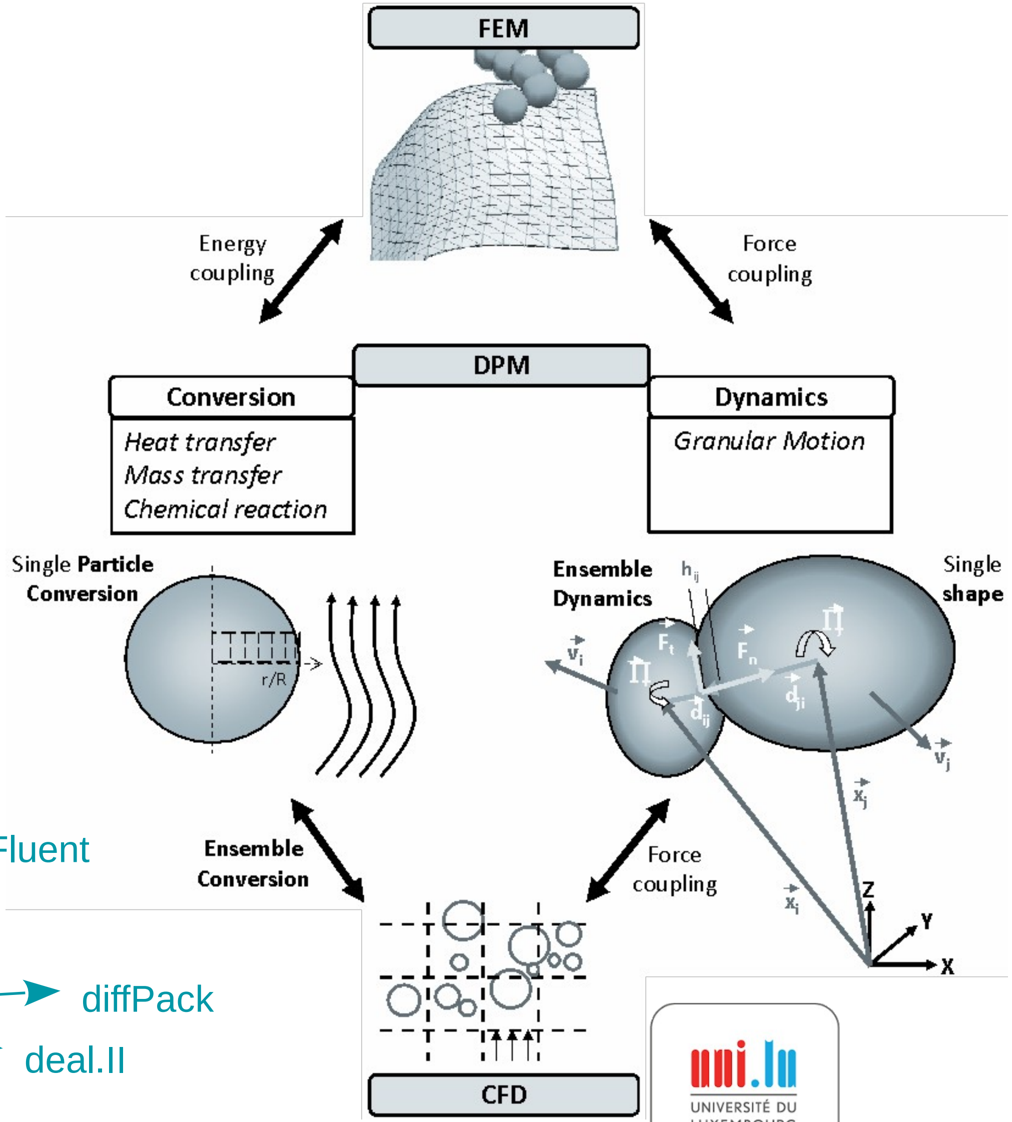
Particles Conversion
- Heat and mass transfer
- Chemical reactions

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



What is XDEM?

eXtended **D**iscrete **E**lement **M**ethod



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

Numerical Approach for Biomass Furnace: **Multi-Physics Simulation**

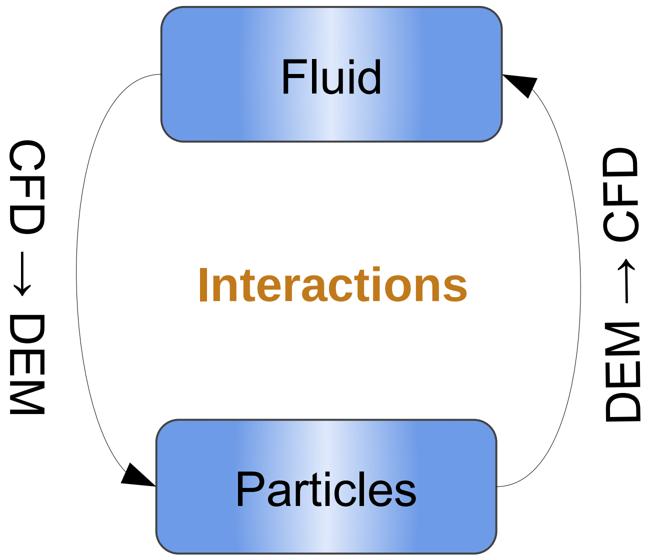
Two-way coupling between Discrete Element Method (DEM) and Computational Fluid Dynamics (CFD)

XDEM (Lagrangian) for:

- Motion and collisions of biomass particles
- Conversion of biomass particles

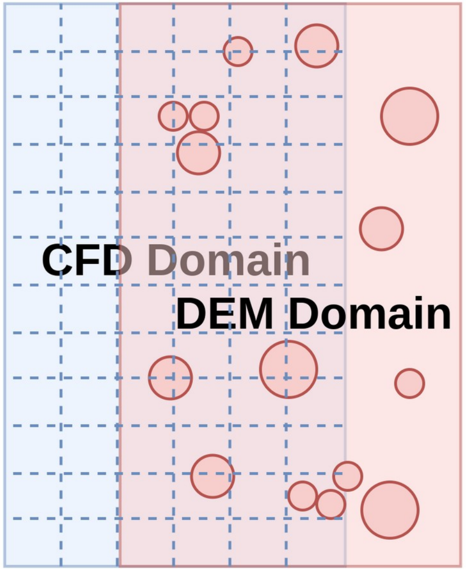
OpenFOAM (Eulerian) for:

- Flow of gas phase
- Reactions in the gas phase



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

CFD-DEM Parallel Coupling: Challenges

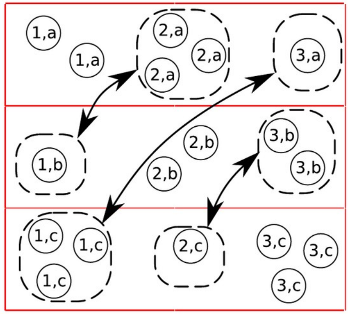


Challenges in CFD-XDEM parallel coupling

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

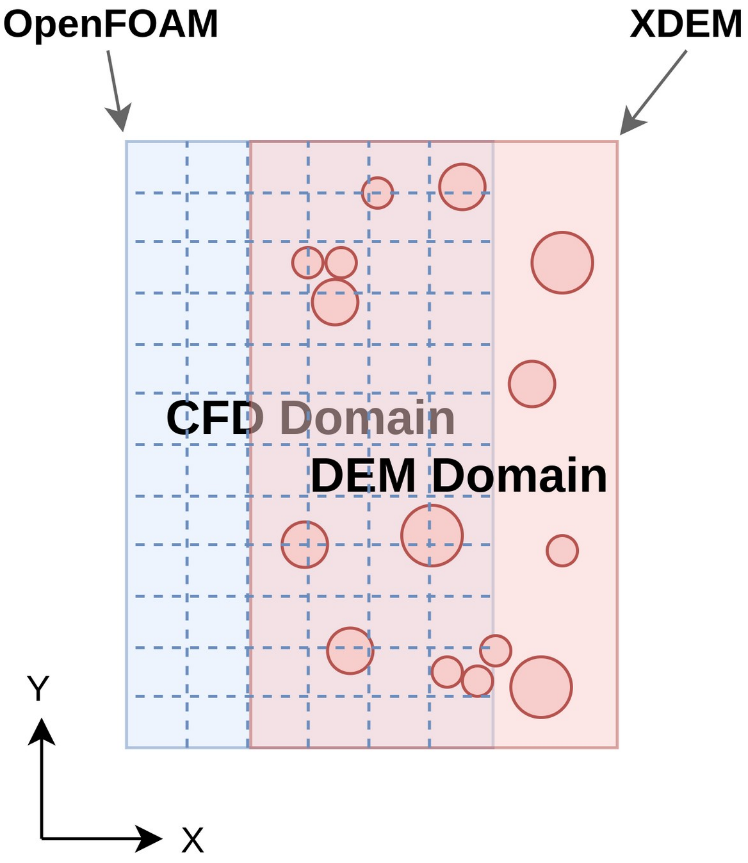
Classical Approaches

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



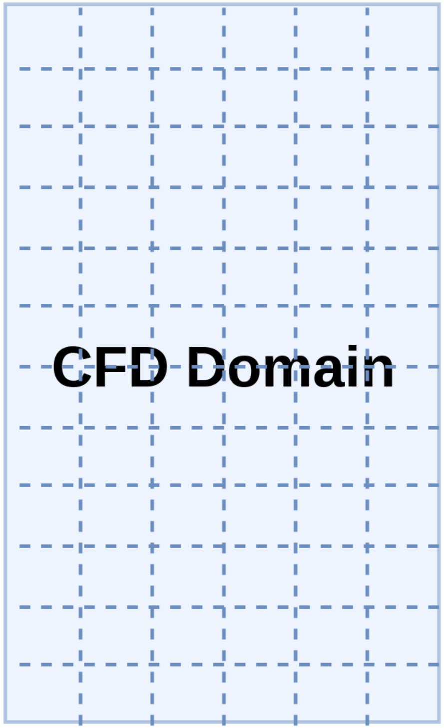
SediFoam [Sun2016]

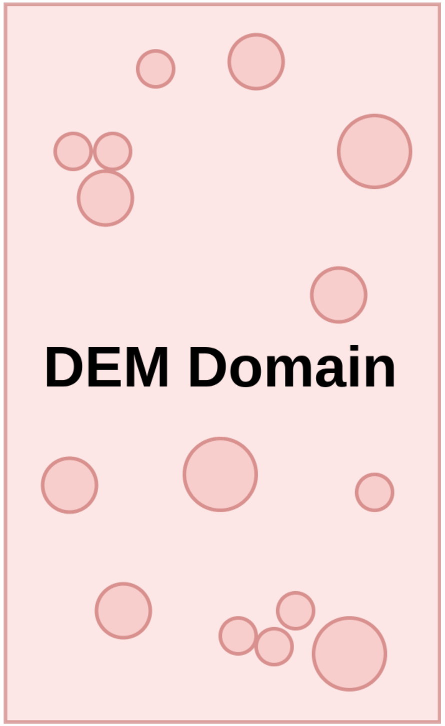
CFD-DEM Parallel Coupling: Challenges



The domains overlap in space

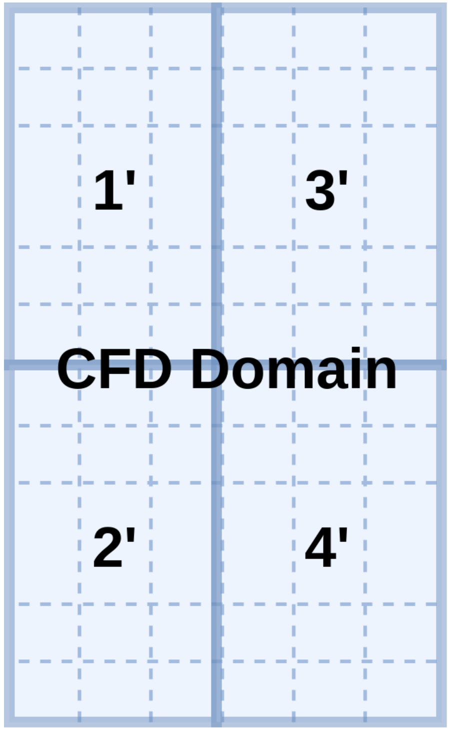
CFD-DEM Parallel Coupling: Challenges

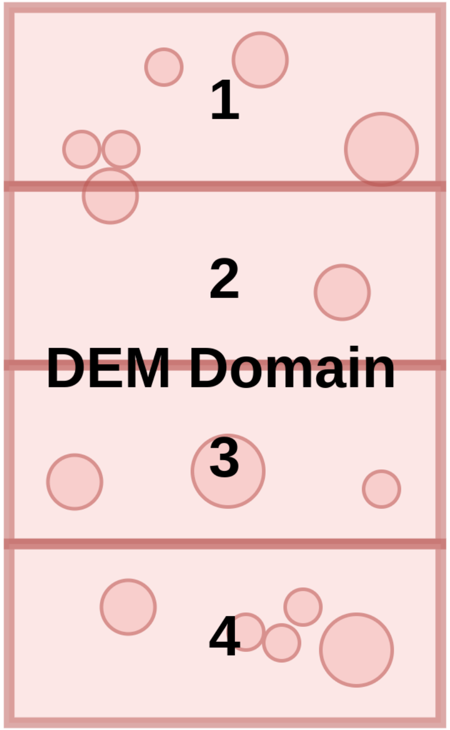




CFD-DEM Parallel Coupling: Challenges

Classical Approach: the domains are partitioned independently





CFD-DEM Parallel Coupling: Challenges

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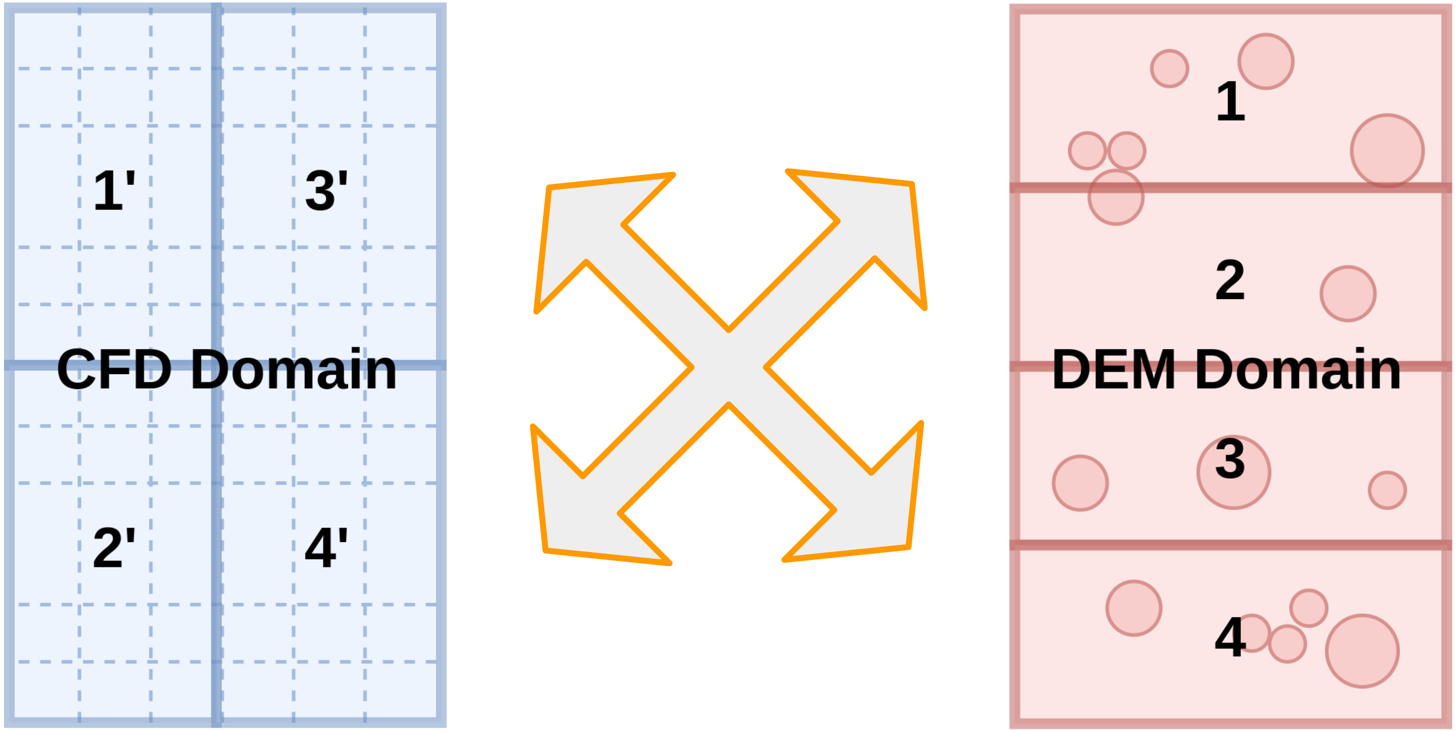
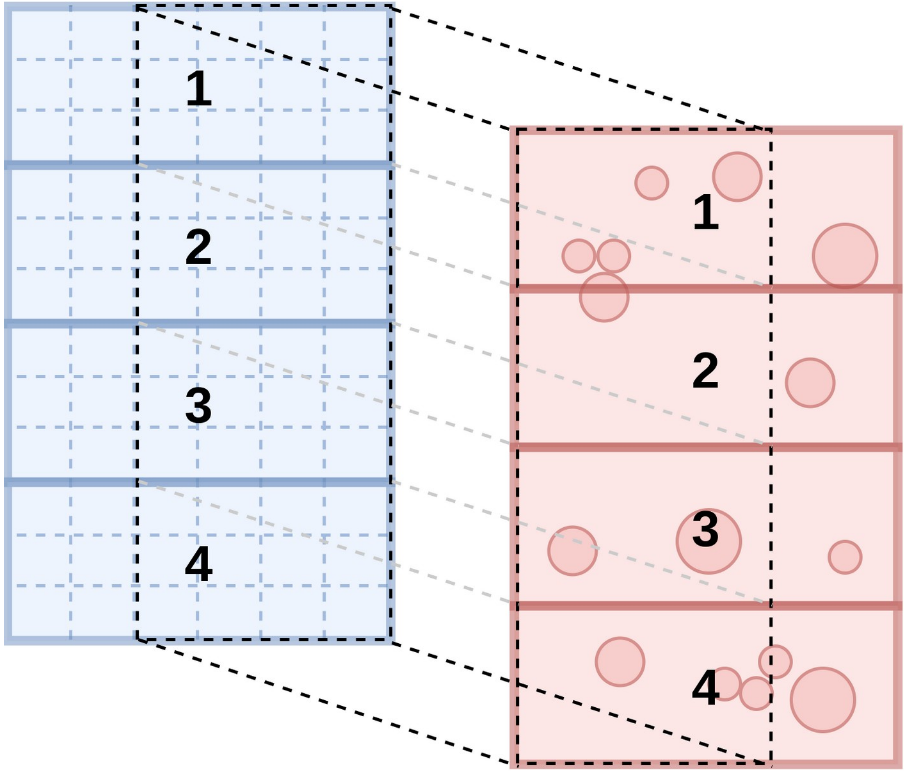


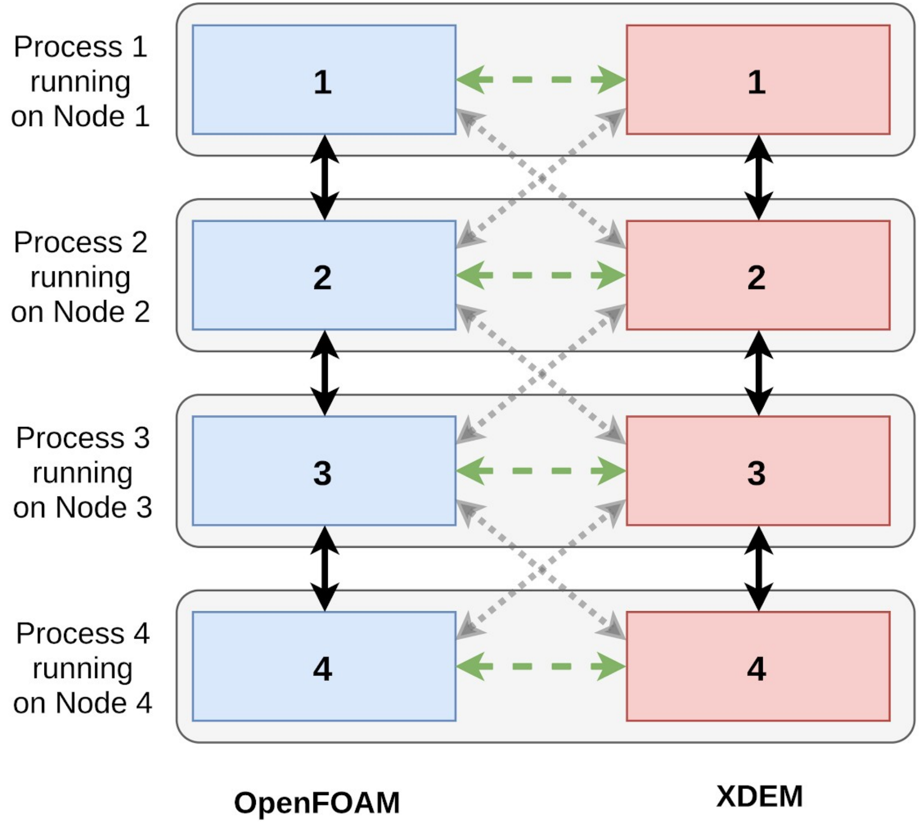
Complex pattern and large volume of communication

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

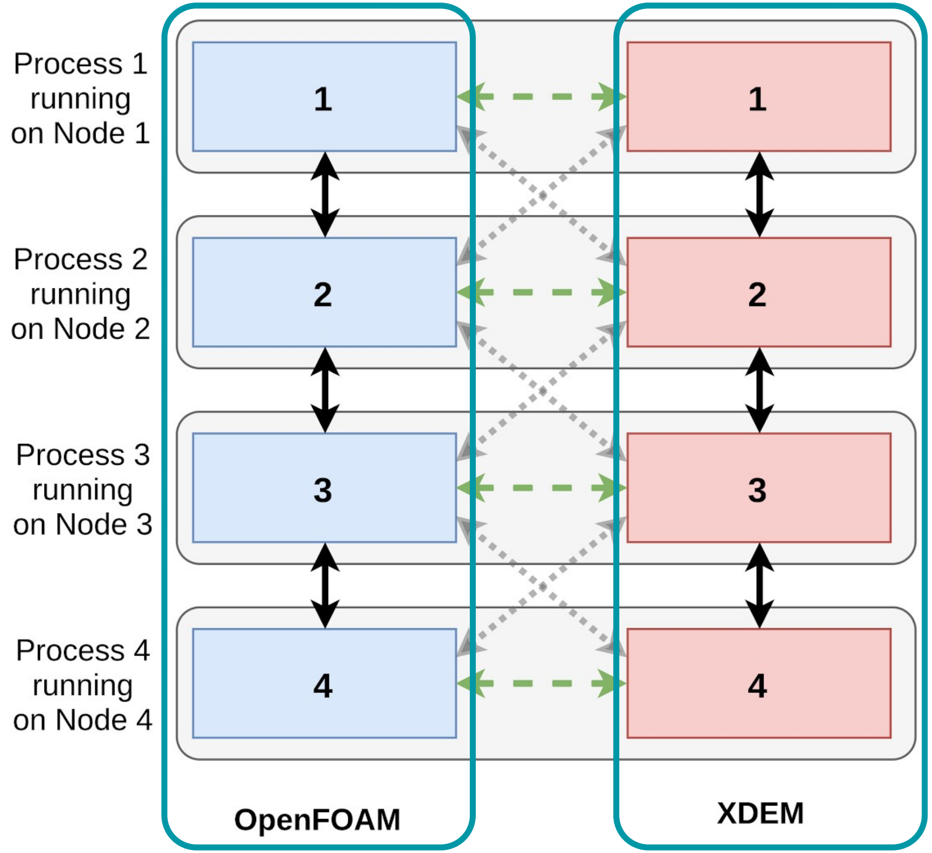
Inter-partition intra-physics Data Exchange using MPI communication layer
with native implementation in OpenFOAM and XDEM

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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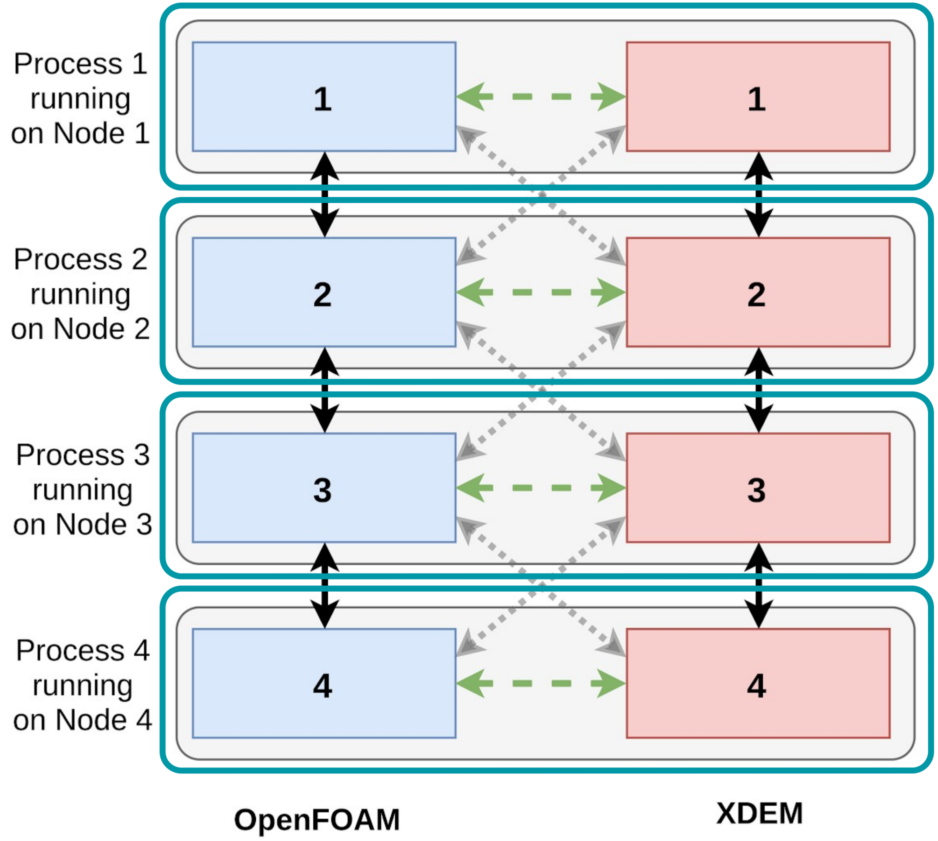
With native implementation of each sotfware

Co-located Partitioning Strategy: communication



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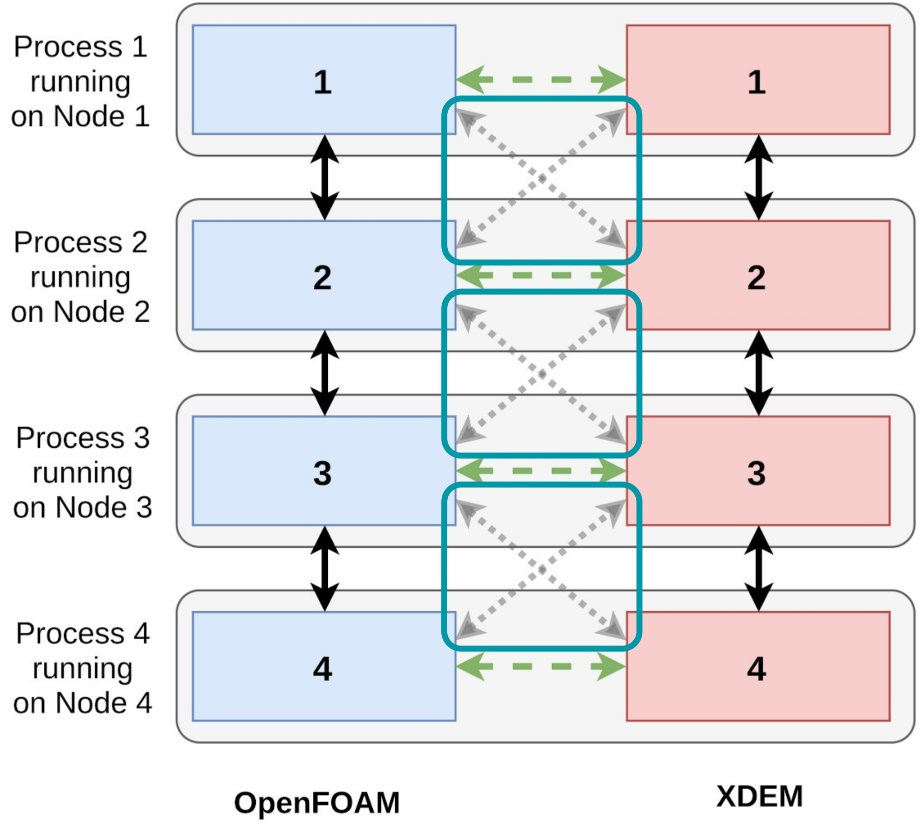
Use direct intra-proces memory access
if the two software are linked into one executable,

Co-located Partitioning Strategy: communication



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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

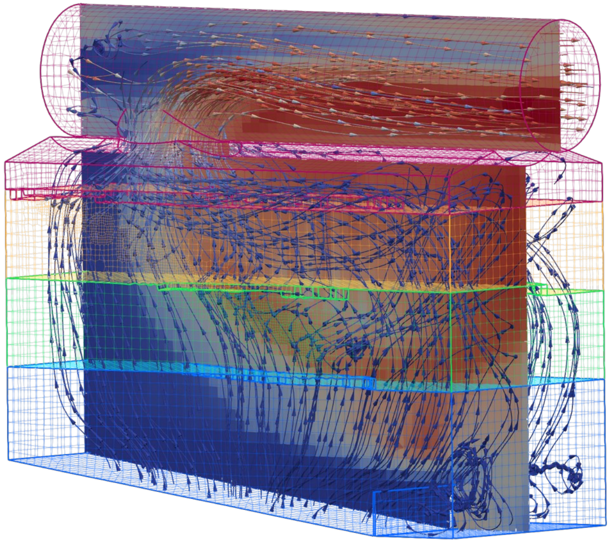
Can be non-existing if partitions are perfectly aligned

Volume Coupling for Biomass Furnace Simulation

Momentum, Heat and Mass transfer

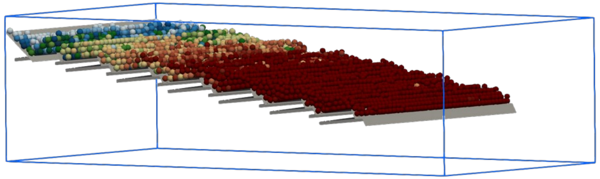
CFD to DEM

- Fluid velocity, density, dynamic viscosity
- Pressure Gradient
- Temperature
- Thermal conductivity
- Specific heat
- Diffusivity
- Species mass fraction (CH_4, CO_2, CO, H_2, H_2O, N_2, O_2, Tar)



Fluid phase in OpenFOAM

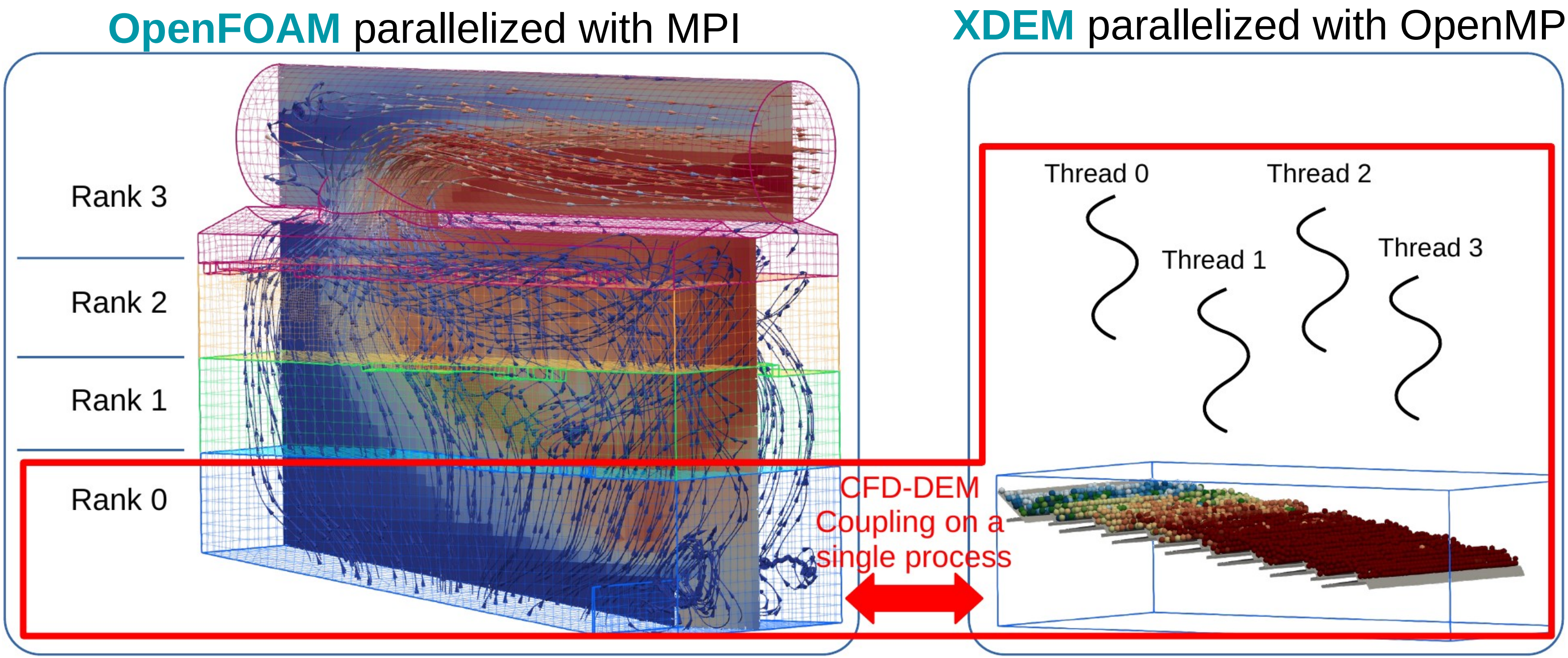
- Porosity
- Momentum source (acceleration, omega)
- Heat source
- Mass sources (CH_4, CO_2, CO, H_2, H_2O, N_2, O_2, Tar)



Particles in XDEM

DEM to CFD

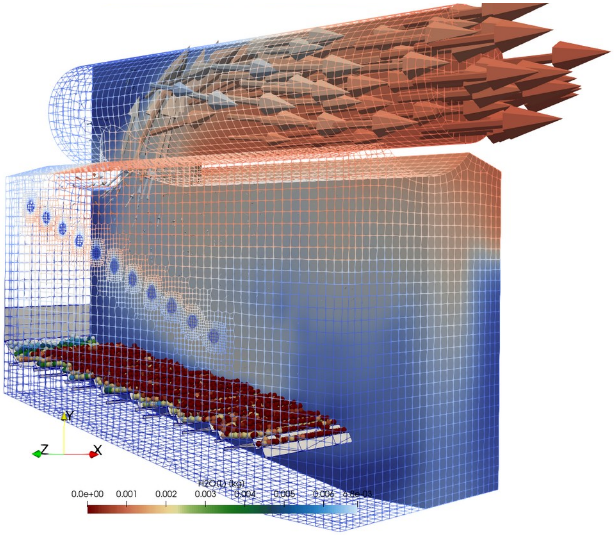
Parallelization approach for Biomass Furnace Simulation



Overlapping domains are co-located ⇒ No inter-partition inter-physics communication
Solvers linked as one executable ⇒ Fast intra-partition inter-physics data exchange

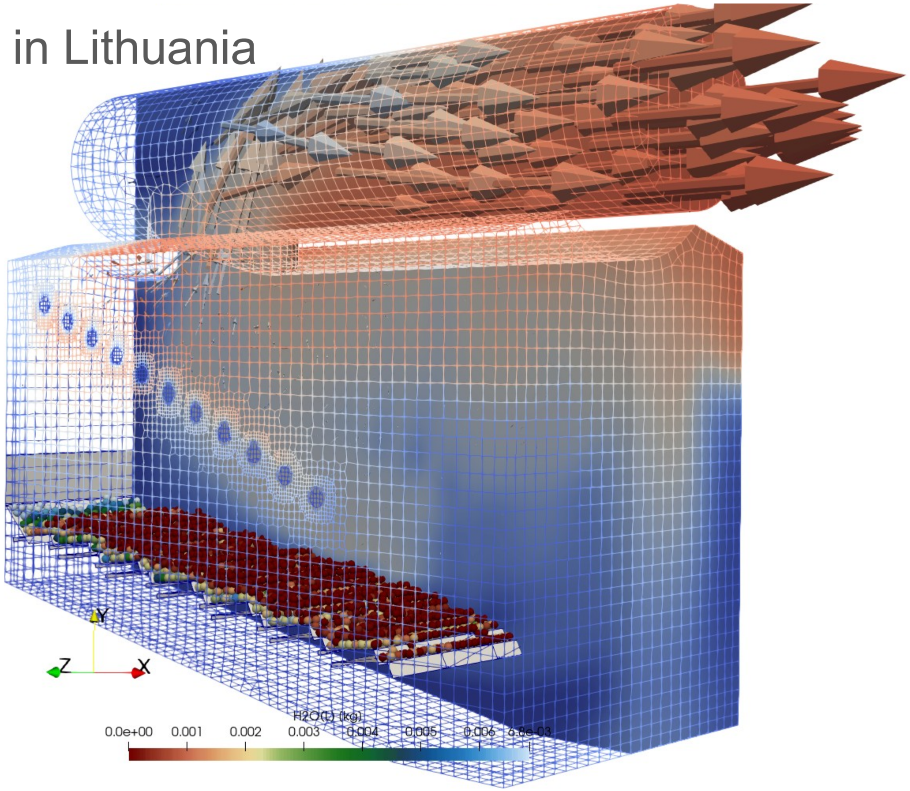
High Performance
Biomass Furnace Simulation

Simulation and performance results



Biomass Furnace Setup

based on an experimental furnace at Enerstena UAB in Lithuania



Furnace

- Dimensions of 2.51m × 1.14m × 2.07m (L × W × H)
- Top exhaust pipe of 0.6m diameter
- 6 primary air inlets from the bottom
- 11 secondary air inlets on each side
- 1 tertiary air inlet on the exhaust pipe

Grates

- 8 static grates and
- 6 moving grates with an
- average slope of 7.5 degrees

Fuel bed

- Initial fuel bed heigh is 10cm
- Wood particles of 3cm diameter with 40% humidity
- Injected at the top side of the grates at a rate of 439kg/h

- CFD mesh with 60,001 cells
- 9,141 particles initially

Performance measurements were performed on the *Barbora* cluster of the IT4Innovations HPC platform.

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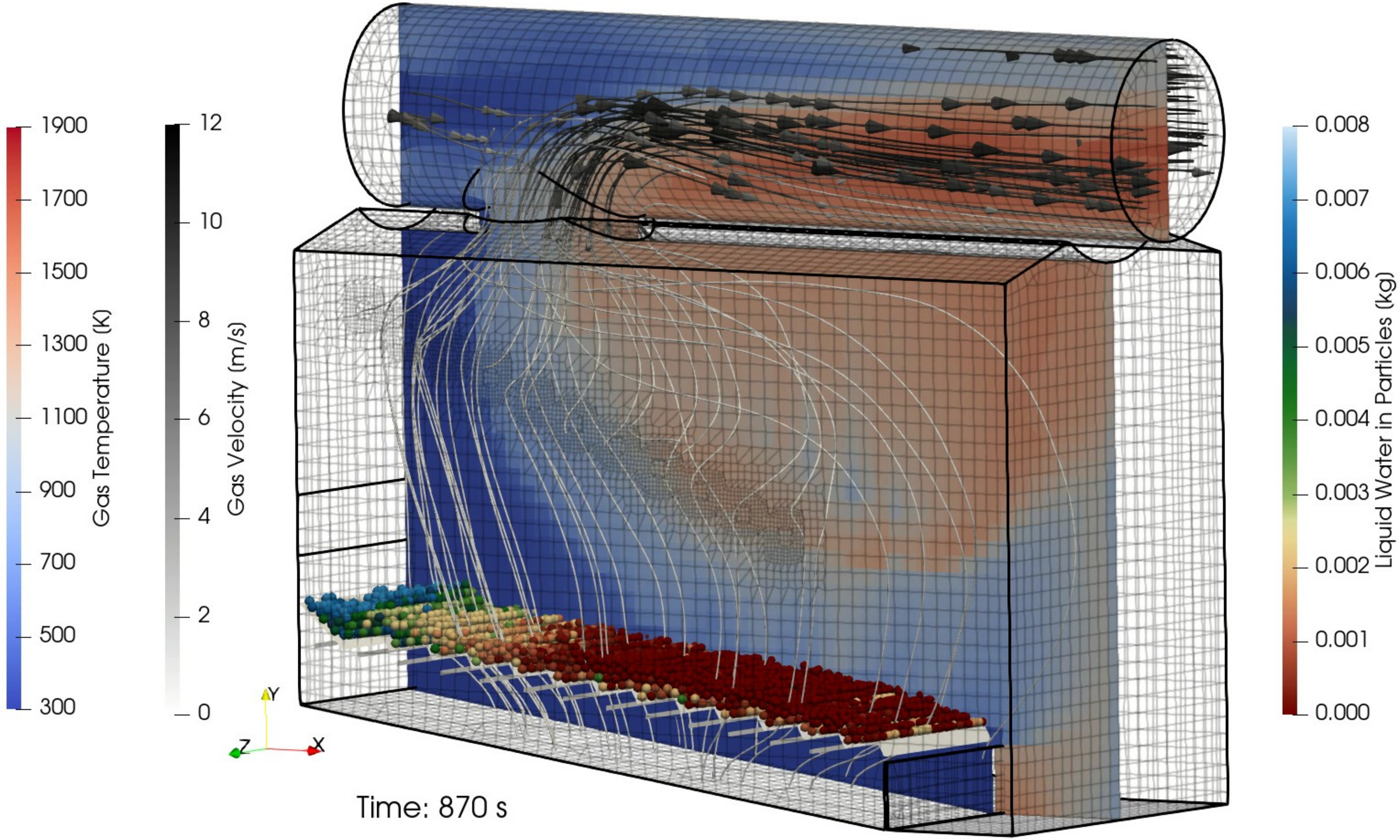
Biomass Furnace simulation using XDEM+OpenFOAM



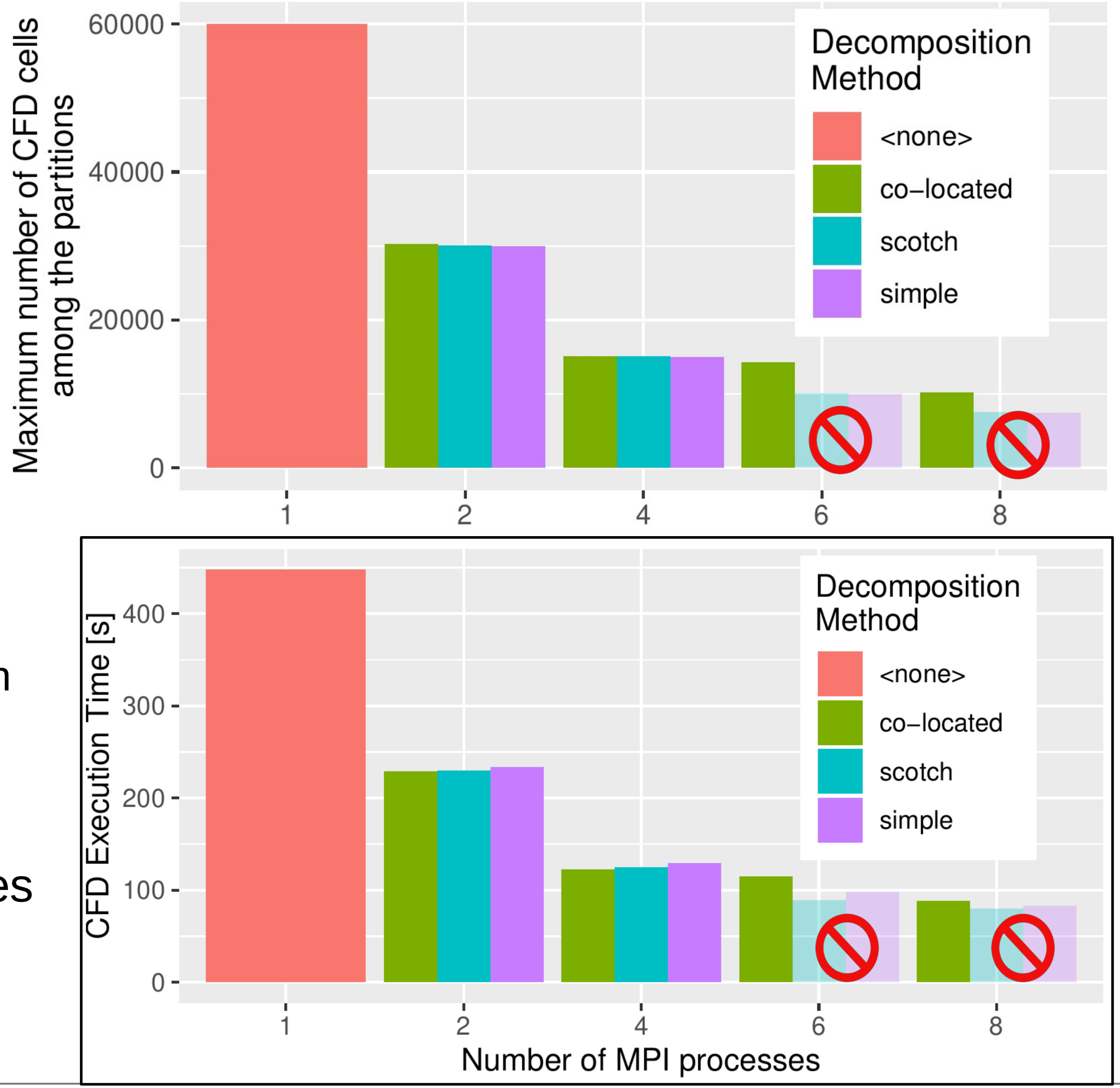
OpenFOAM decomposition and scalability

- Execution of the coupled problem, but looking only at the CFD part

- OpenFOAM case is relatively small: only 60k cells

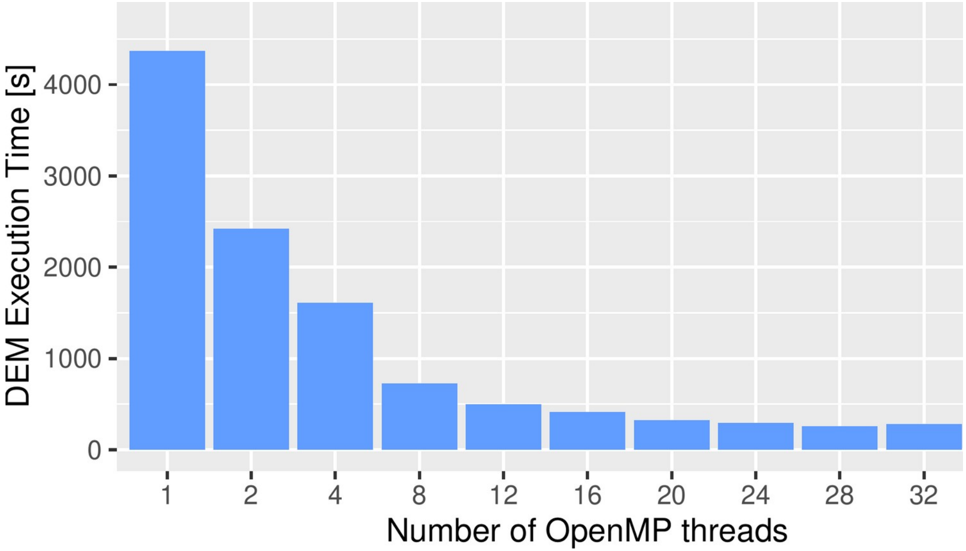
- Execution time for the first 10s of simulation

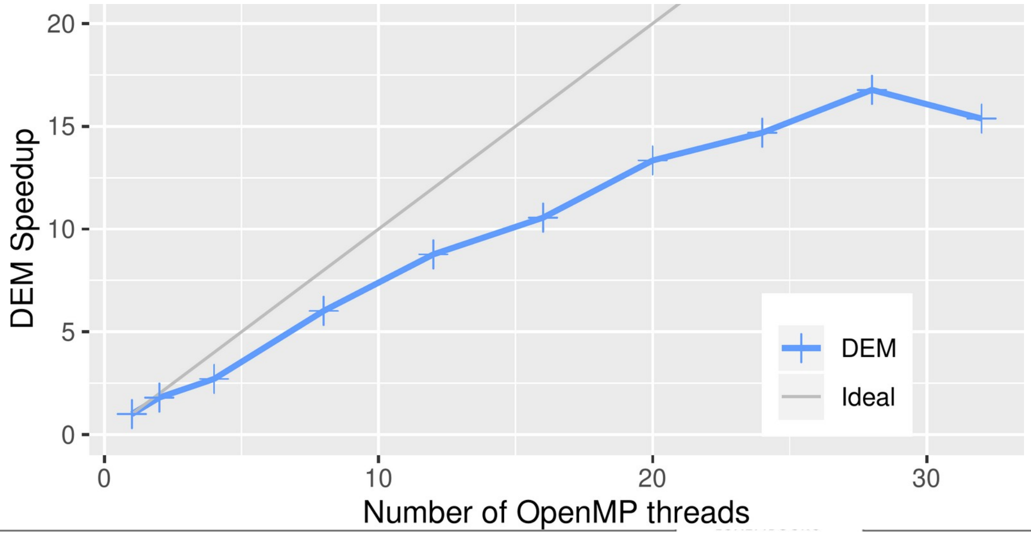
Only the co-located partitioner guarantees the correct results beyond 4 processes due the coupling constraints



XDEM Scalability

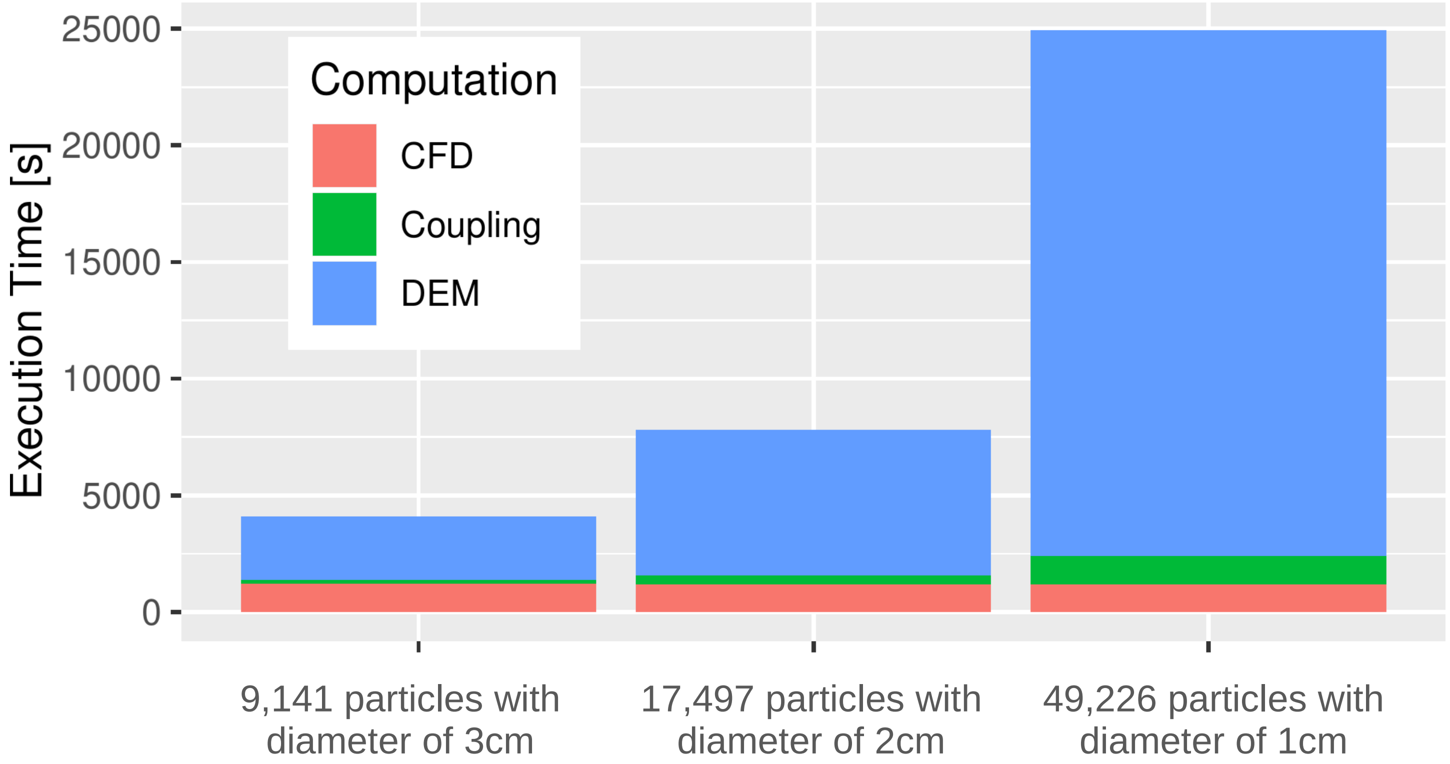
- Execution of the coupled problem, but looking only at the DEM part
- Around 9k particles
- Execution time for the first 10s of simulation



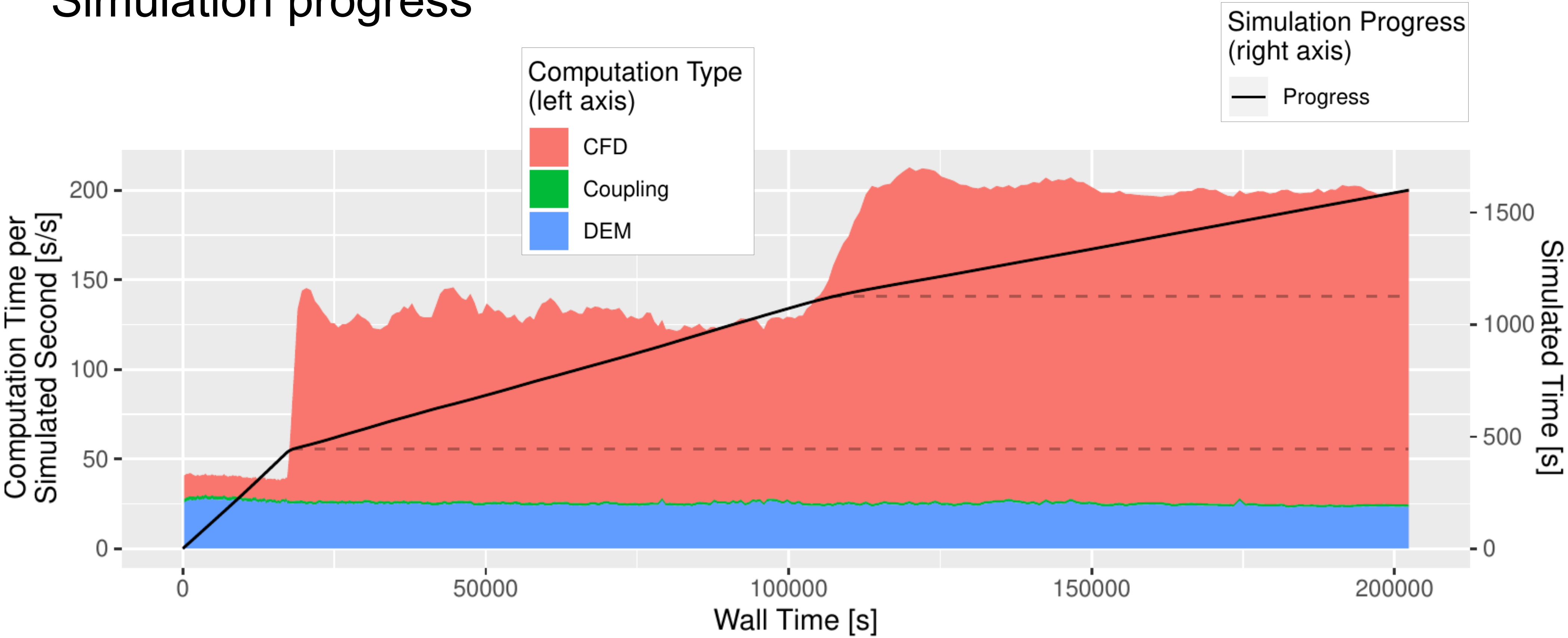


Influence of the number of particles

Same furnace settings and bed height, only changing the size of wood particles



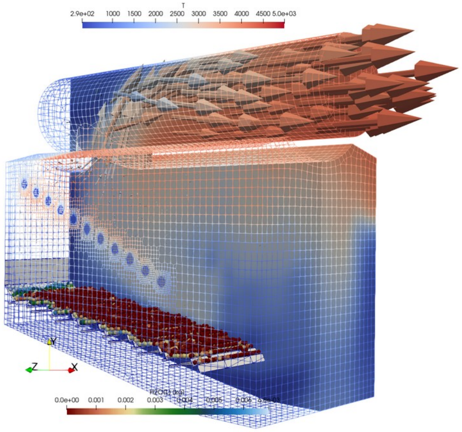
Simulation progress

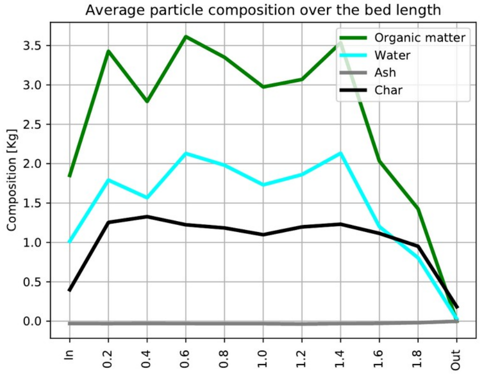


- At 445s of simulated time, lighting-up of the furnace
- Around 1125s, furnace reaches the steady state (all hot gases are burning)

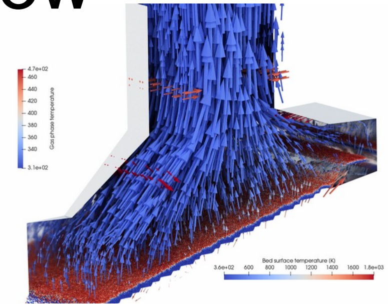
Cloud-based Workflow for Biomass Furnace Simulation

Objectives

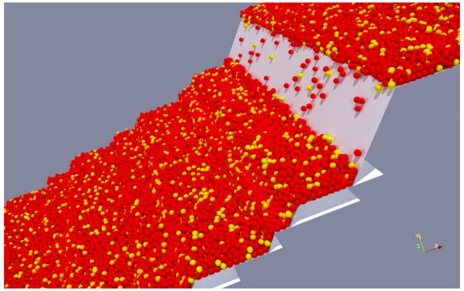




Complexity of biomass furnace simulation workflow

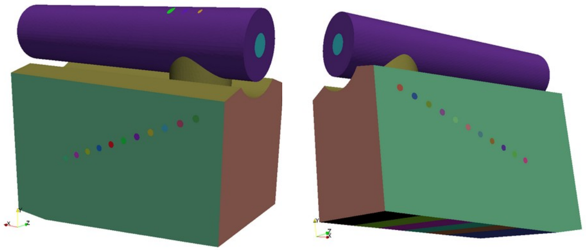


The setup, execution and post-processing of biomass furnace simulations is challenging.



The necessary steps include:

- Generation of furnace and grate geometry
- CFD mesh generation and CFD case setup
- Calculation of the initial particle bed
- DEM case setup
- Calculation of fuel properties from ultimate analysis



This complexity is a serious obstacle, in particular for SMEs

- The adoption of such technologies requires substantial investment in computer hardware, software licenses and training of engineering staff.

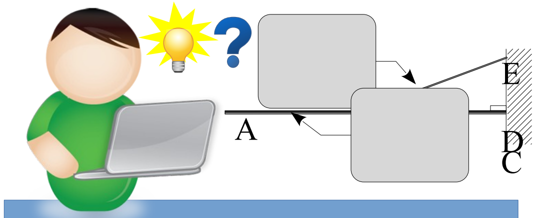
CloudiFacturing Overview

https://www.cloudifacturing.eu

- Support manufacturing SMEs and their needs for advanced cloud- or HPC-based ICT solutions
- Open solutions, empowering different stakeholders to become members of the community
- Services offered based on a pay-per-use or subscription business model with a unified billing process

Objective: a simple user workflow

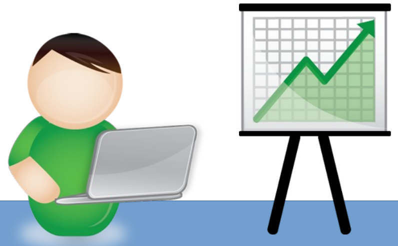
From the spreadsheet to the report



Prepare Input File
- define the geometry and the settings of the furnace
- based on a Spreadsheet

Submit Input File
- via the CloudiFacturing web portal

Run the Simulation
- on the HPC platform
- no interaction needed from the user



Visualize the results
- download archive from the web portal
- pre-generated report

Cloud-based Workflow for Biomass Furnace Simulation

Under the hood

How to much input is required?

Furnace and grate design

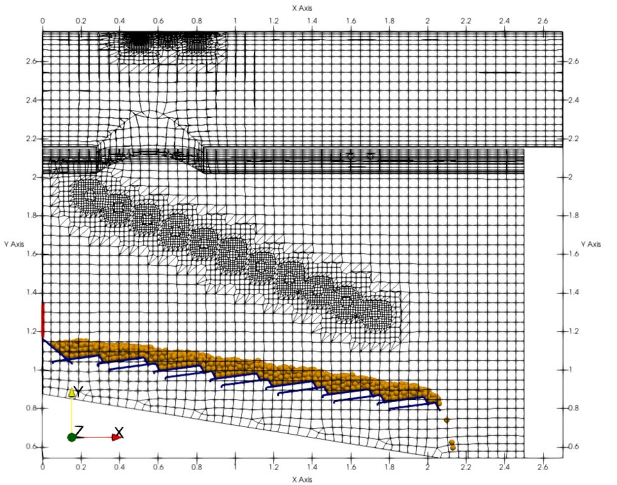
- parametrised with a few numbers
- geometry is generated automatically

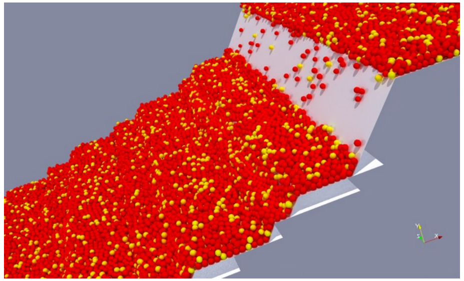
Fuel / Wood chip

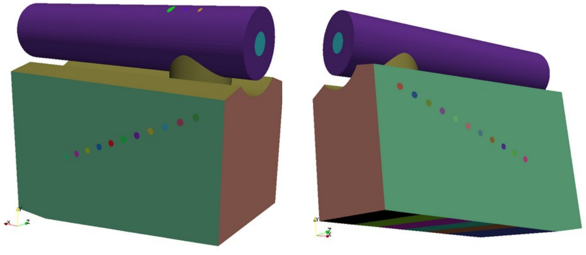
- characterised by ultimate analysis
- thermo-physical values obtained from standard experiments

Air inlets

- can be placed at any position
- require the full composition when recirculation is used



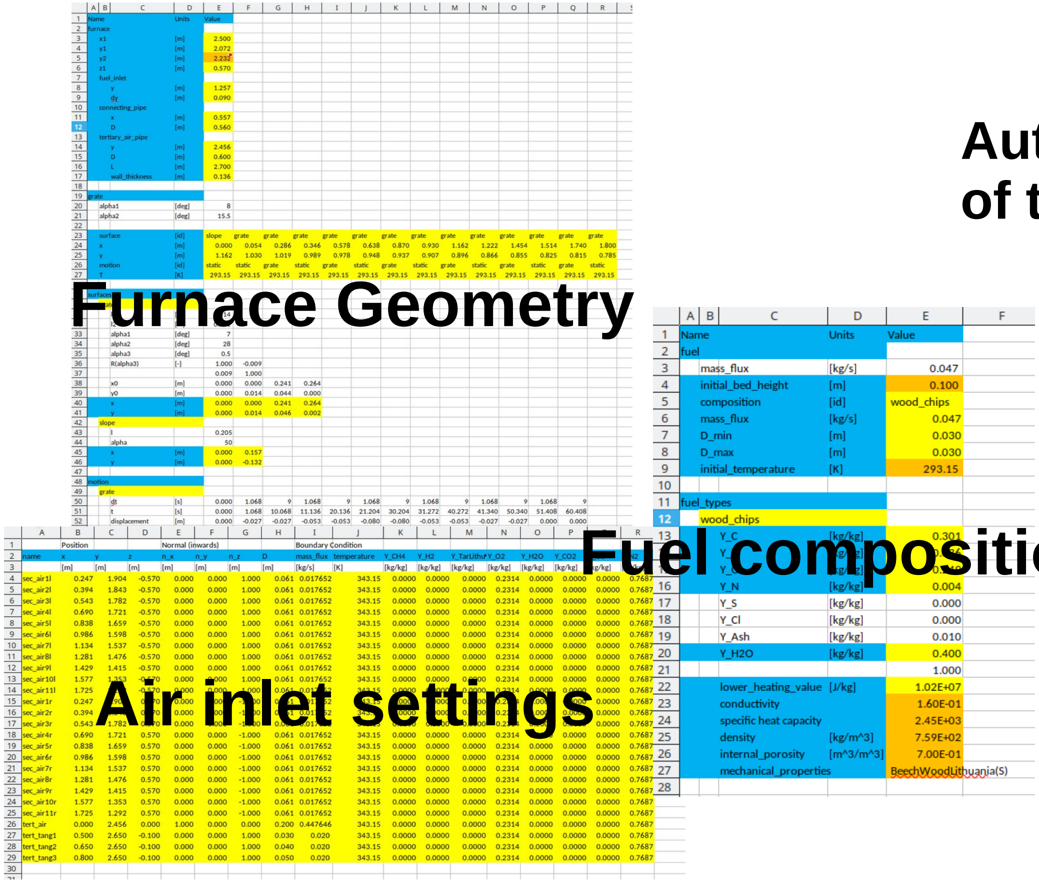




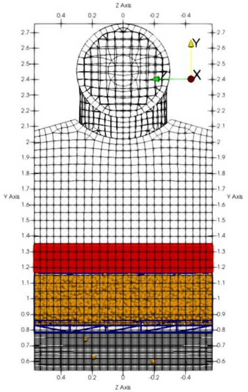
→ A few hundred degrees of freedom!

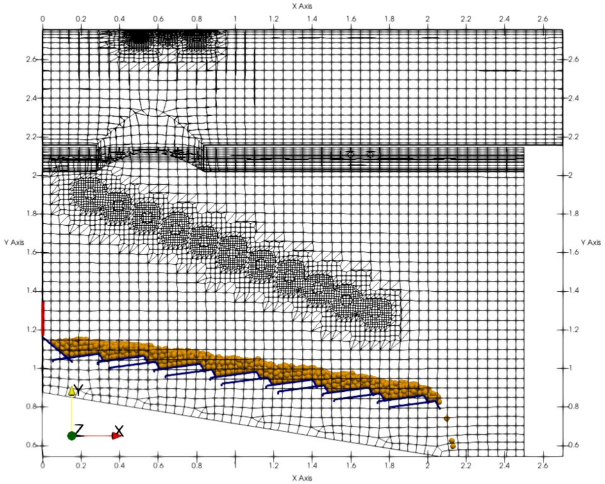
- Designing and implementing a web interface was out of scope

Spreadsheet Input File



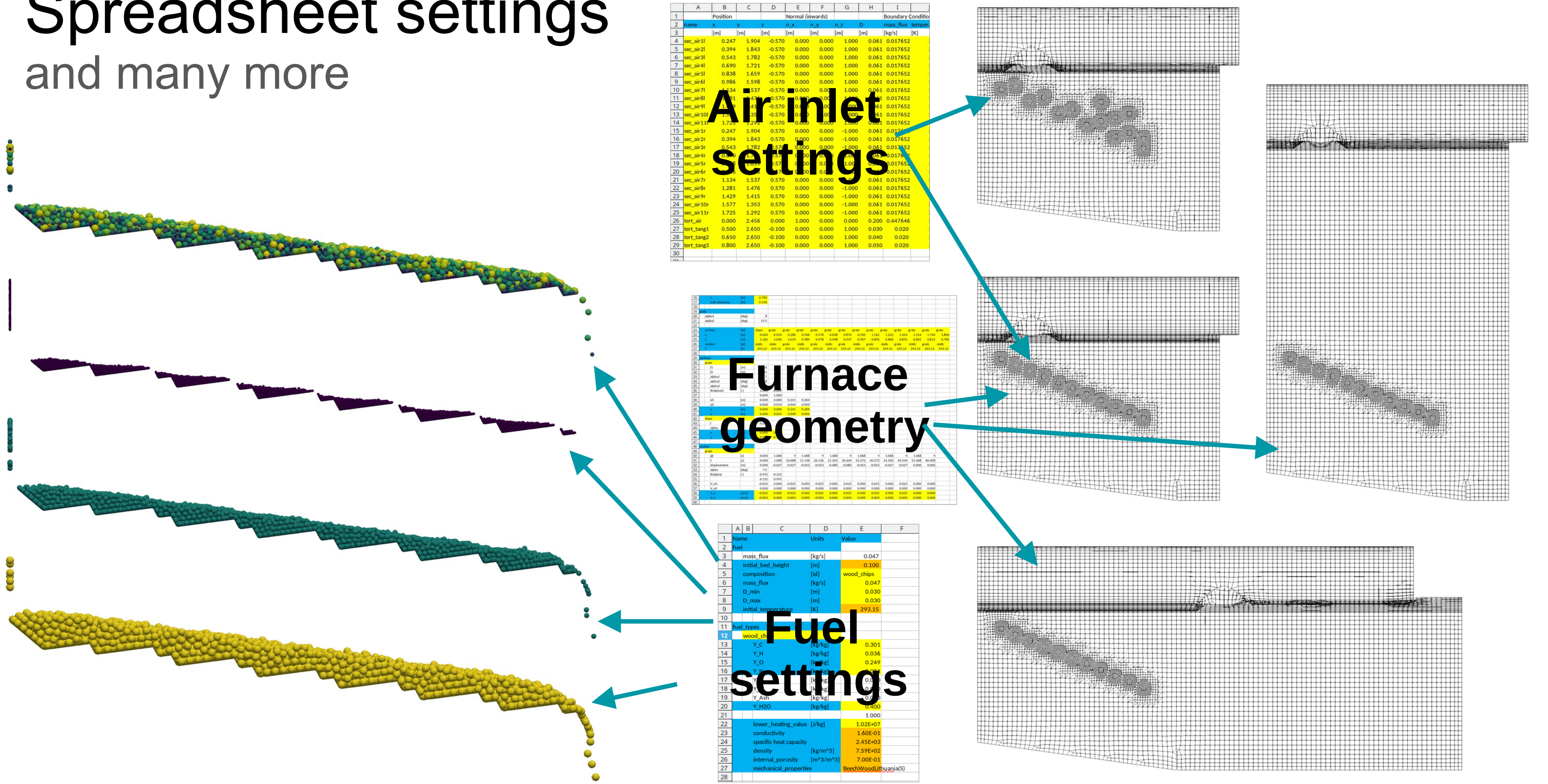
Automatic generation of the CFD+DEM case





Spreadsheet settings

and many more



Job submission

HPC Simulation
with Singularity
on IT4T HPC cluster

IT4Innovations
national01$#&0
supercomputing
center@#01%101

Biomass Furnace Simulation Workflow

Welcome! This workflow takes an Excel file that contains the input parameters of a bio mass furnace simulation. The simulation uses XDEM (discrete particles) and foam-extend (computational fluid dynamics). It automatically generates all necessary inputs (geometry, mesh, input files) and returns a report for download.

Workflow steps

1. **Select input Excel file**
2. Perform simulation
3. Download results

Step 1: Excel-file selection

Select the Excel file that contains the inputs for the furnace simulation.

Choose selected file | Reset tree

- IT4I storage (Anselm cluster)
  - scratch
  - home
    - cfg-bioopt-input
      - FurnaceInputs.xlsx
    - hrus
    - dd-18-13-01
    - hpc_logs
    - .config
    - exp15testapp.simg
    - xdem
    - cfg-xdem-bioopt.simg
    - openfoam5.simg
    - .fltk

Submission Web Portal

Execution of the workflow is delegated to the SemWES engine

SemWES

HPC job running

The job is running but didn't set its own status yet. Please wait ...

```
eXtended Discrete Element Method (XDEM)
http://luxdem.uni.lu/

Versions
  XDEM version:    heads/cfg-bioopt-NEW-0-g7a10073
  BioOpt version:  heads/master_WR30000-0-g11299e4

Input File
  File path: /scratch/FurnaceInputs.xlsx
  ... 2836cf5a7c0fe25
```

```
Execution Progress
  Step: 1/3 Pre-processing started at Sat Oct  9 23:57:14 CEST 2021
    - parse -> done
    - render_controlDict -> done
    - grateGeometry -> done
    - prepareFuel -> done
    - mappingRegion -> done
    - geometry -> done
    - renderMeshDict -> done
    - surfaceFeatureEdges -> done
    - cartesianMesh -> done
    - prepareFoam -> done
    - cellSet -> done
    - adjustFurnaceGeometry -> done
    - prepareXDEMPackedBed -> done
    - BedPackingInput -> done
    - runXDEMBedPacking -> done
    - prepareXDEM -> done
    - BioOptInput -> done
    - checkBioOptInput -> done
    - renderDecomposeParDict -> done
    - decomposePar -> done
  Step: 2/3 Simulation started at Sun Oct 10 00:02:44 CEST 2021
    - runXDEM -> done
```

Real-time progress report

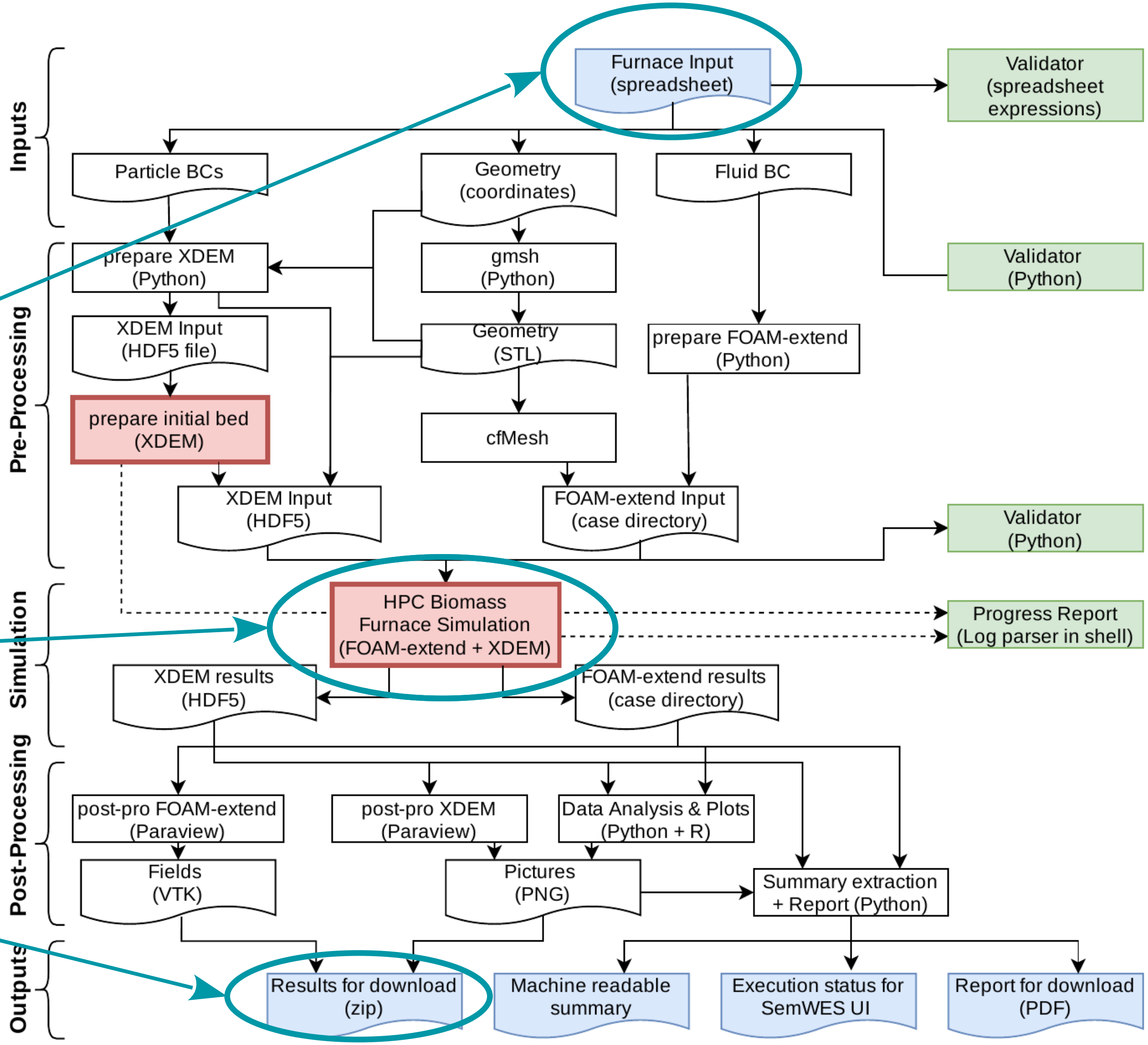
Internal workflow

running on HPC in a Singularity container

User Input

HPC Furnace Simulation

Simulation Output



Simulation Results

SemWES

This workflow has finished

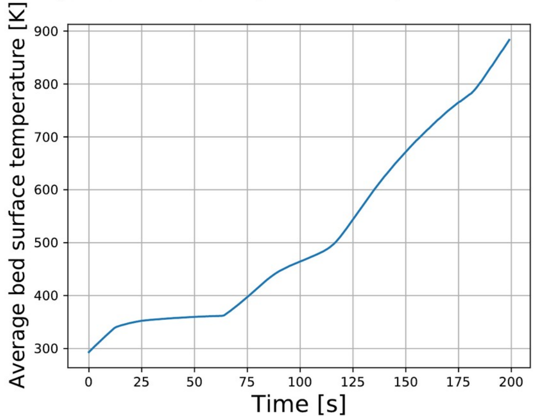
The execution of this workflow is done. You may now inspect the results.

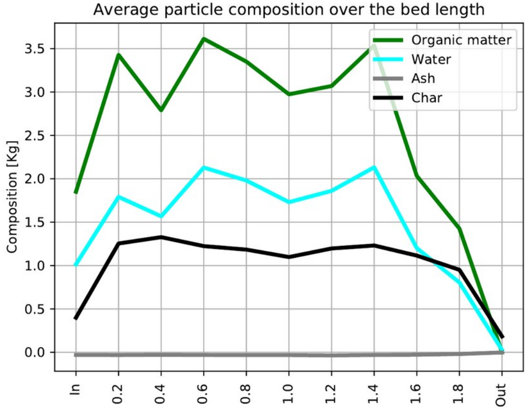
Results

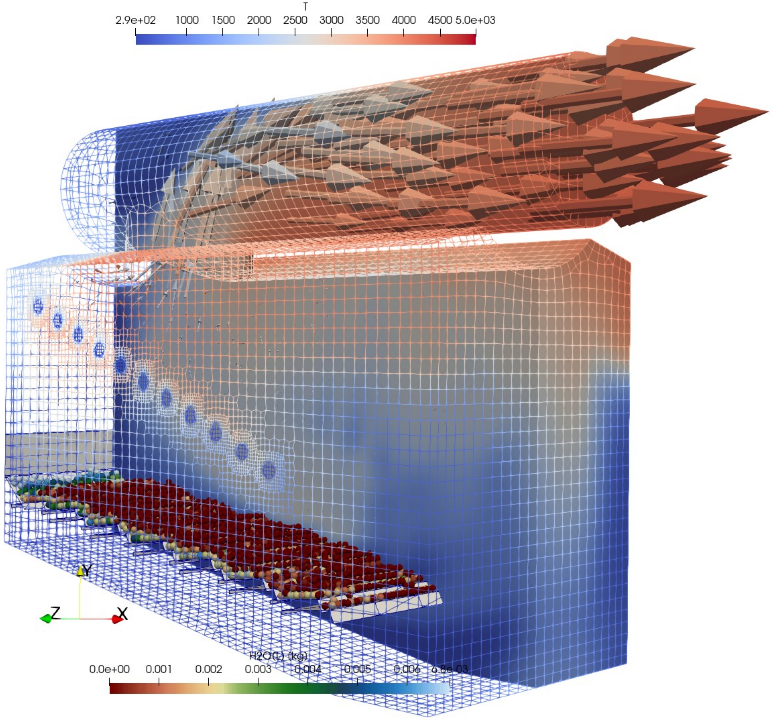
OUTPUT it4i_anselm://scratch/CFG-XDEM-BioOpt_2020-09-15_16-03-18/XDEM_output_2020-09-15_16-03-18.zip

Download link

Average bed surface temperature temperature over time







Report

Extracts of the Simulation Reports

```
//*************************************************************************//
//      _           _   _  _  _  _      _  _  _  _  _   _           _      //
//     (_)_       _(_) (_)(_)(_)(_)    (_)(_)(_)(_)(_) (_) _     _ (_)     //
//       (_)_   _(_)    (_)      (_)_  (_)             (_)(_)   (_)(_)     //
//         (_)_(_)      (_)        (_) (_) _  _        (_) (_)_(_) (_)     //
//          _(_)_       (_)        (_) (_)(_)(_)       (_)   (_)   (_)     //
//        _(_) (_)_     (_)       _(_) (_)             (_)         (_)     //
//      _(_)     (_)_   (_)_  _  (_)   (_) _  _  _  _  (_)         (_)     //
//     (_)         (_) (_)(_)(_)(_)    (_)(_)(_)(_)(_) (_)         (_)     //
//                                                                         //
//                 eXtended Discrete Element Method (XDEM)                 //
//                          http://luxdem.uni.lu/                          //
//                                                                         //
//*************************************************************************//

Versions
  XDEM version:   heads/cfg-bioopt-NEW-0-gfbec735
  BioOpt version: heads/master-0-g91cd409

Input File
  File path: /scratch/FurnaceInputs.xlsx
  sha256sum: c27d9bc300b2eb8e333884a1724cda00c444399f9a0d693b46d27992bbbcd0bd

Output Files
  Results report: /scratch/CFG-XDEM-BioOpt/526544.isrv1/CFG-XDEM-BioOpt_Report_2021-09-27_09-00-04.zip
  Execution Log file: /scratch/CFG-XDEM-BioOpt/526544.isrv1/XDEM_output_RANK0.log
```

Header of the report with software versions and checksum of the input file

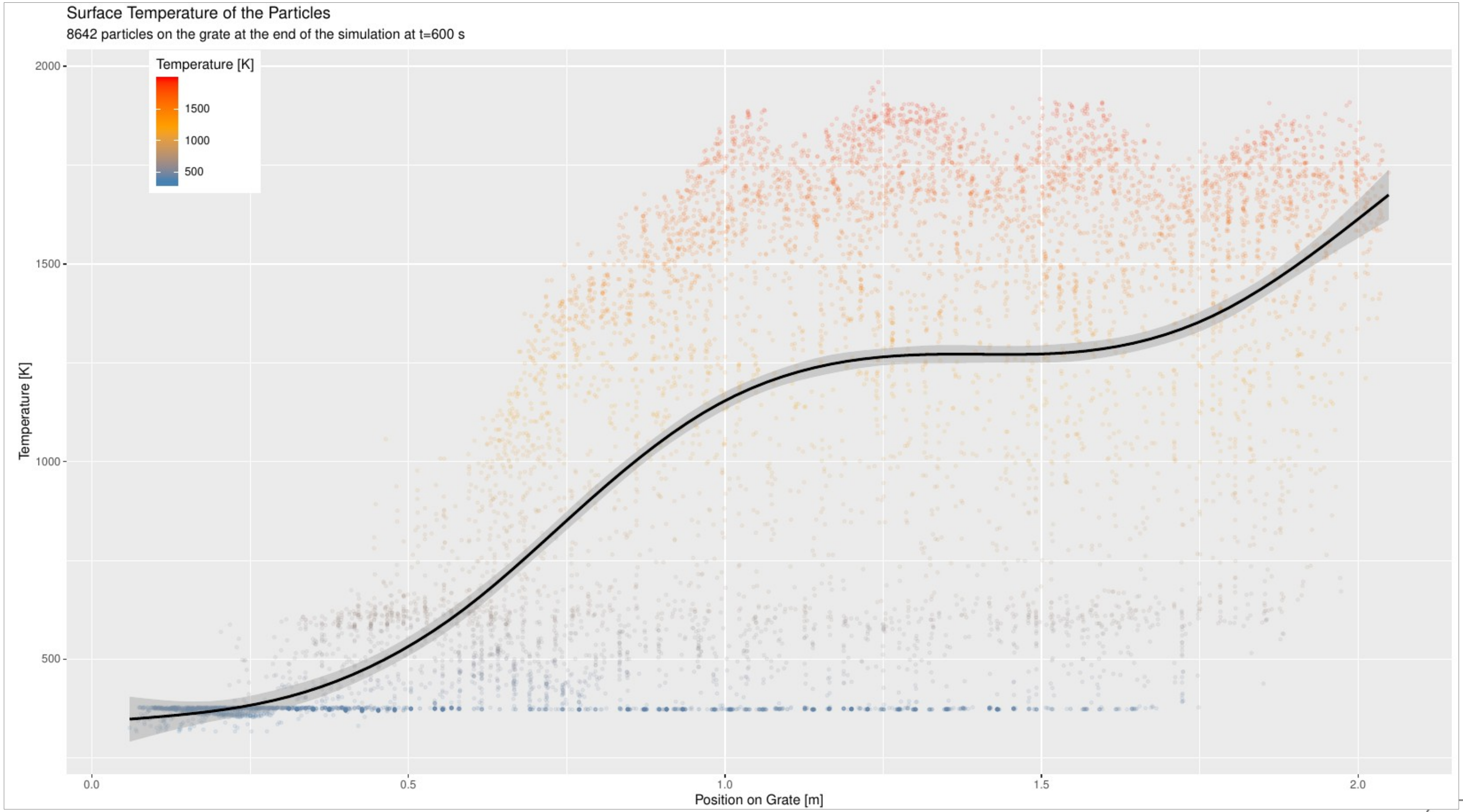
Extracts of the Simulation Reports

```
Average properties at the outlet

    Average of T over patch outlet[3] = 1422.4505
    Average of rho over patch outlet[3] = 0.23866349
    Average of CH4 over patch outlet[3] = 0.0002149707
    Average of CO over patch outlet[3] = 0.023597323
    Average of CO2 over patch outlet[3] = 0.12360054
    Average of H2 over patch outlet[3] = 0.00014842204
    Average of H2O over patch outlet[3] = 0.18191674
    Average of O2 over patch outlet[3] = 0.078764601
    Average of TarLithuania_1 over patch outlet[3] = 0.029753928
```

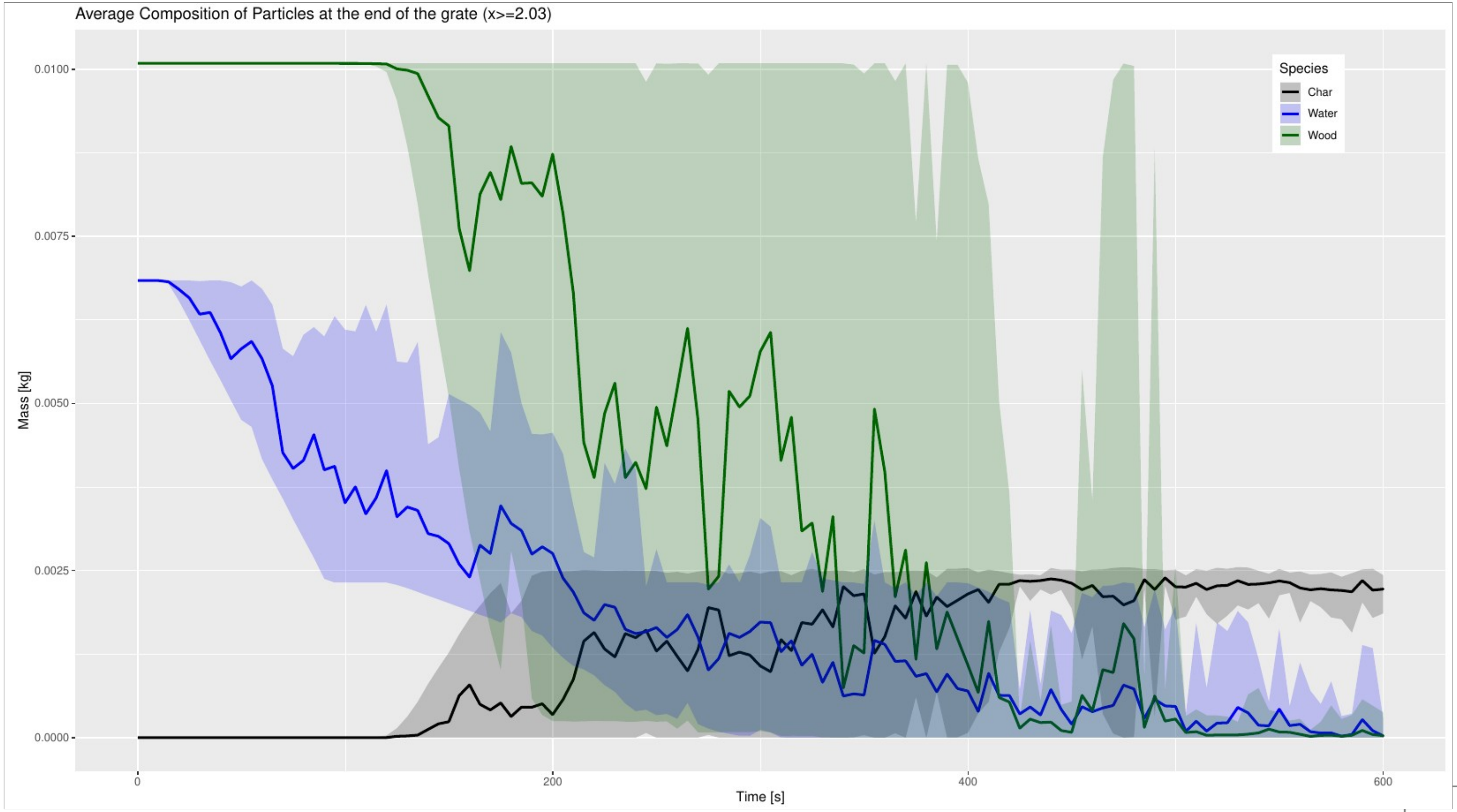
Average properties at exit of the exhaust pipe

Extracts of the Simulation Reports



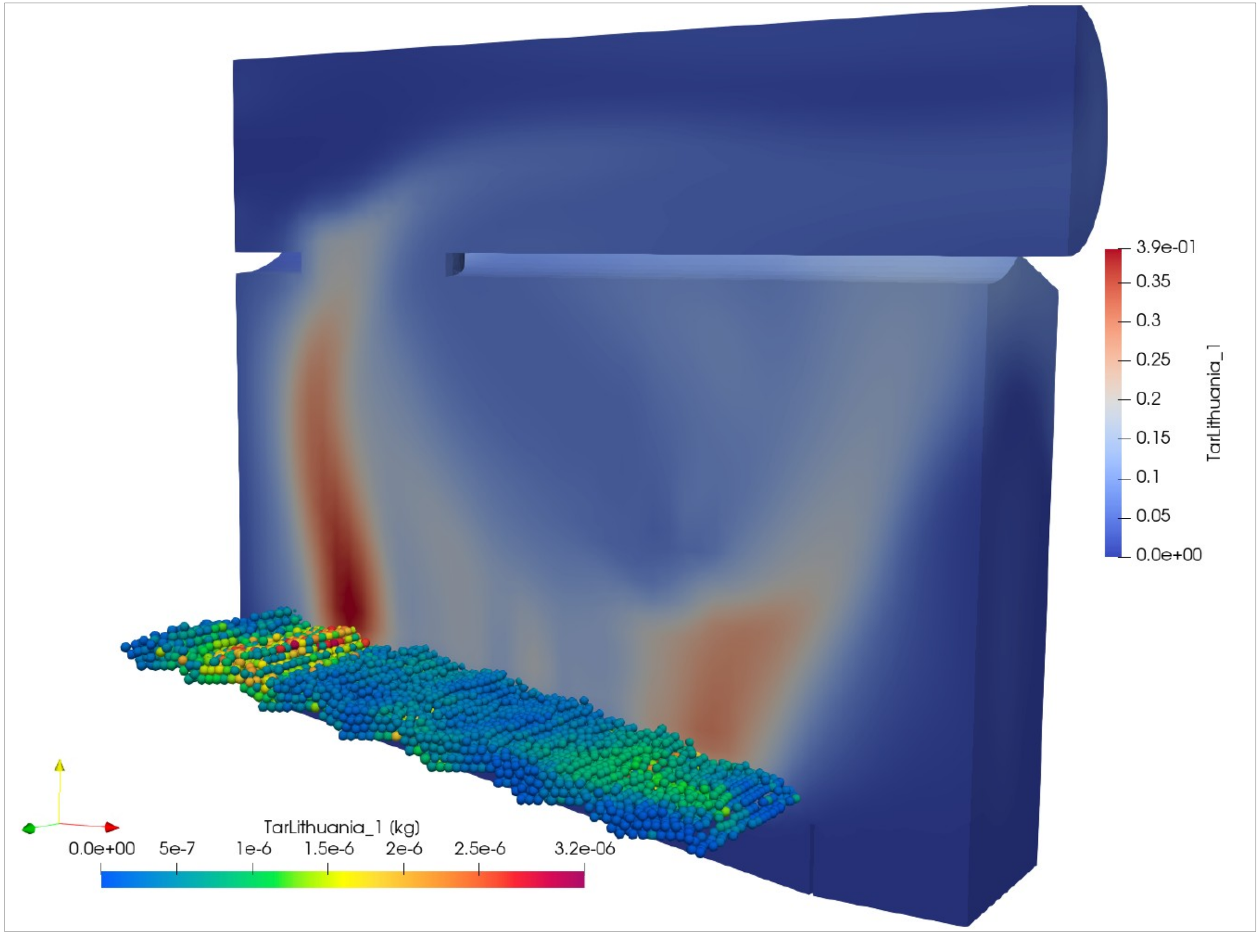
Surface temperature along the grate

Extracts of the Simulation Reports



Evolution of particle composition at the exit of the grate

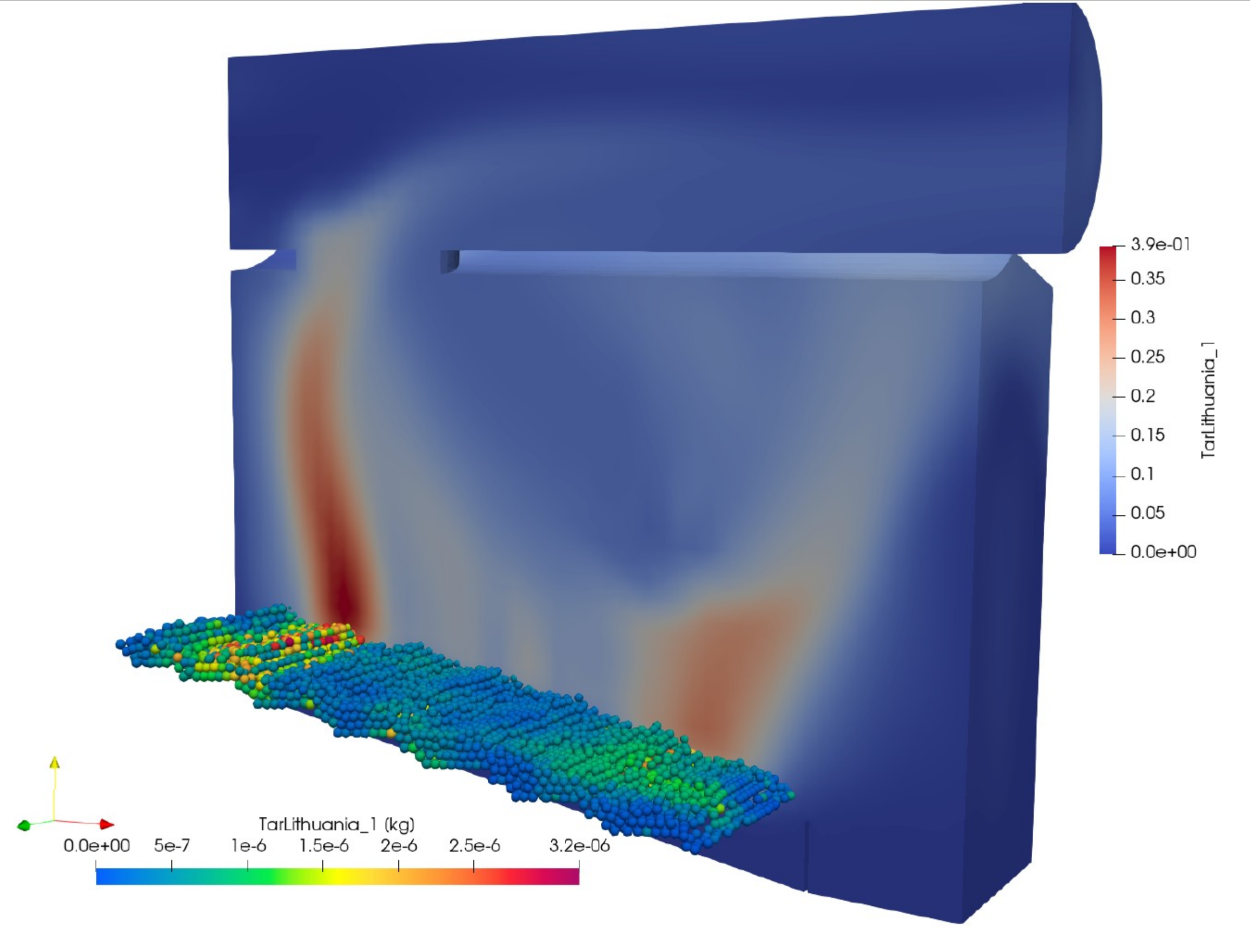
Extracts of the Simulation Reports



Tar content of the particles and in the gas

Extracts of the Simulation Reports

and many more...



Tar content of the particles and in the gas

Breakdown of the workflow execution time

Same setup as before, for 1200s of simulated time

Pre-processing	**5min 30s**	
- in XDEM bed packing	5min 10s	32 OpenMP threads
Simulation	**34h 10min 30s**	
- in FOAM-extend code	31h 51min 2s	4 MPI processes
- in XDEM code	2h 19min 28s	28 OpenMP threads
Post-processing	**29min 33s**	
- in FOAM-extend reconstructPar	25min 21s	

The CFD-DEM simulation represents the main part of the computation.

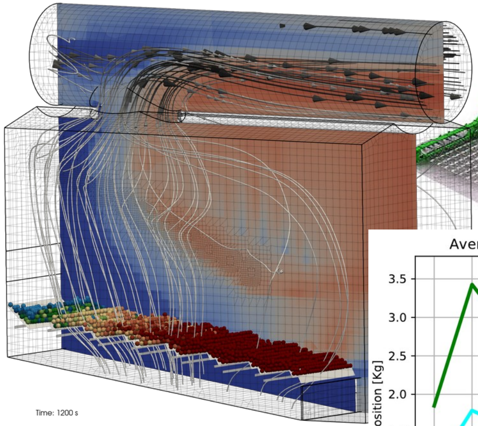
Summary: Biomass Furnace Simulation as a Service

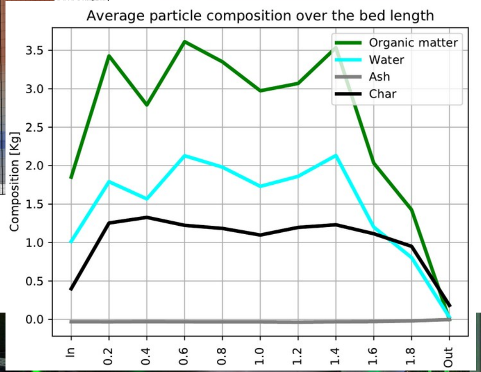
Multi-Physics Biomass Furnace Simulation
- Two-way 'in-memory' coupling CFD ↔ DEM
- Hybrid parallelization scheme: MPI + OpenMP

Cloud-based interface and submission portal
- Portable execution using Singularity
- HPC Job submission using SemWES
- Execution on IT4Innovations HPC platform

Simplified Workflow for end user
- All input settings provided in a spreadsheet
- Automatic generation of the case
- Automatic execution on HPC platform
- Generation of a report with the results

→ Application as a Service (AaaS)





Difficulties & Future Work

Technical difficulties & constraints

- Application portability with Singularity
- Flexibility of the workflow with SemWES
- Numerous configuration options
  - Specifications given by industrial partner
  - Verification of user input is hard but necessary
  - Need robust code, regular checks, an clear error messages
  - Best configuration/parallelization for all cases is nearly impossible
    → Conservative choices in the implementation and optimization
- Fast results required
    → Small biomass furnace

Next Steps

- Remove coupling-related constraints
  → preCICE coupling library to handle the communication
- Develop coupling-aware partitioning techniques
- Tackle larger biomass furnaces in a shorter time

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References

Xavier Besseron, Henrik Rusche, and Bernhard Peters. **Parallel Multi-Physics Simulation of Biomass Furnace and Cloud-based Workflow for SMEs**. In *Practice and Experience in Advanced Research Computing (PEARC ’22)*, July 10–14, 2022, Boston, MA, USA.

https://doi.org/10.1145/3491418.3530294

Gabriele Pozzetti, Xavier Besseron, Alban Rousset, Bernhard Peters. **A co-located partitions strategy for parallel CFD–DEM couplings**. In *Advanced Powder Technology*, Volume 29, Issue 12, 2018.

https://doi.org/10.1016/j.apt.2018.08.025

More details about the CloudiFacturing BioOpt Experiment:

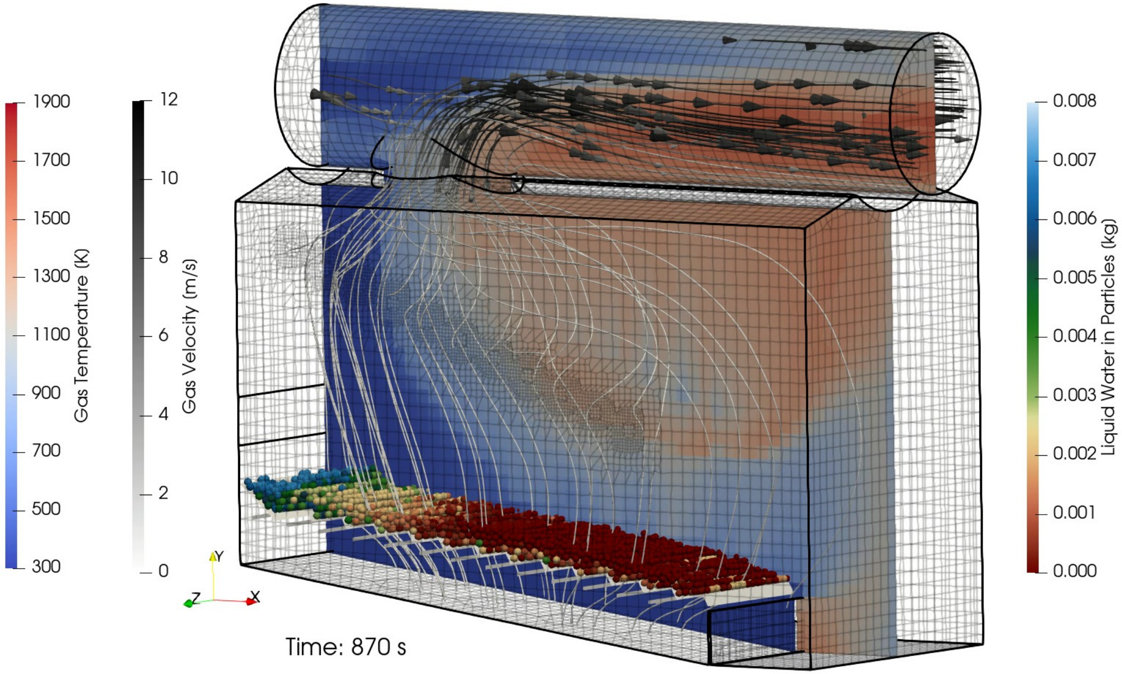
http://luxdem.uni.lu/projects/2020-CloudiFacturing_BioOpt/

CloudiFacturing project:

https://www.cloudifacturing.eu

Thank you for your attention!

Luxembourg XDEM Research Centre
http://luxdem.uni.lu/
University of Luxembourg



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