Toward High-Performance Multi-Physics Coupled Simulations for the Industry with XDEM

Xavier Besseron, Prasad Adhav, Daniel L. Louw, Bernhard Peters

University of Luxembourg
LuXDEM Research Centre
https://luxdem.uni.lu

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IS26b - High performance computing in research and industry

Outline

High-Performance Biomass Furnace Simulation

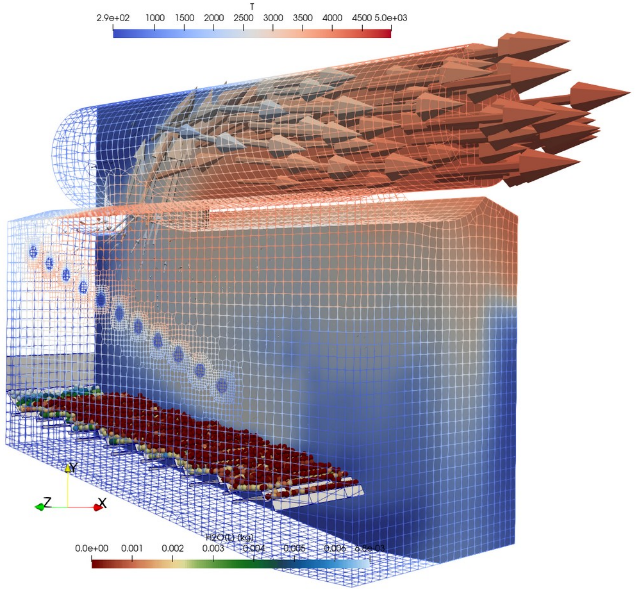
- CFD-DEM volume coupling
- Co-located partitioning
- Simulation approach and results

Cloud-based Workflow for the Industry

- Seamless integration in HPC

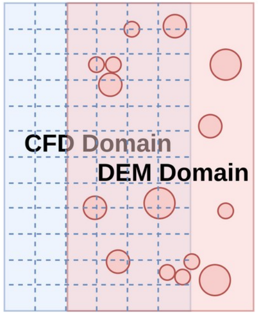
Coupling with more Flexibility

- Using the preCICE coupling library

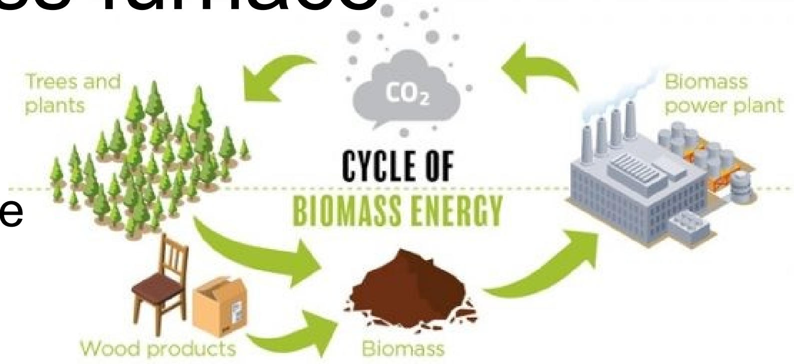


Parallel Coupling for Biomass Furnace Simulation

- CFD-DEM Volume Coupling
- Co-located Partitioning



Combustion process in a biomass furnace



Biomass combustion (e.g. wood chips)

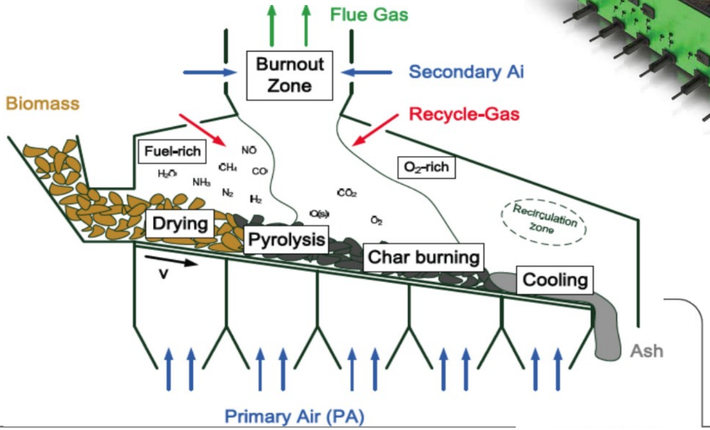
- widely used for generating electric and thermal energy
- renewable and potentially carbon-neutral energy source

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

Numerical Approach for Biomass Furnace:
Multi-Physics Simulation

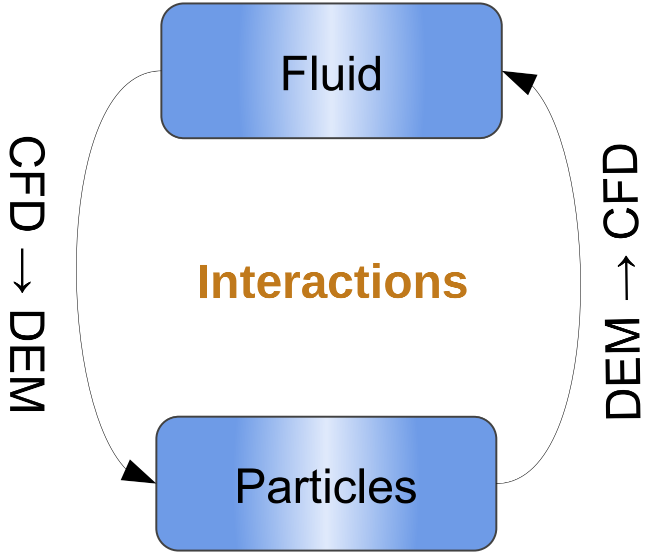
Two-way coupling between Discrete Element Method (DEM) and Computational Fluid Dynamics (CFD)

XDEM (Lagrangian) for:

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

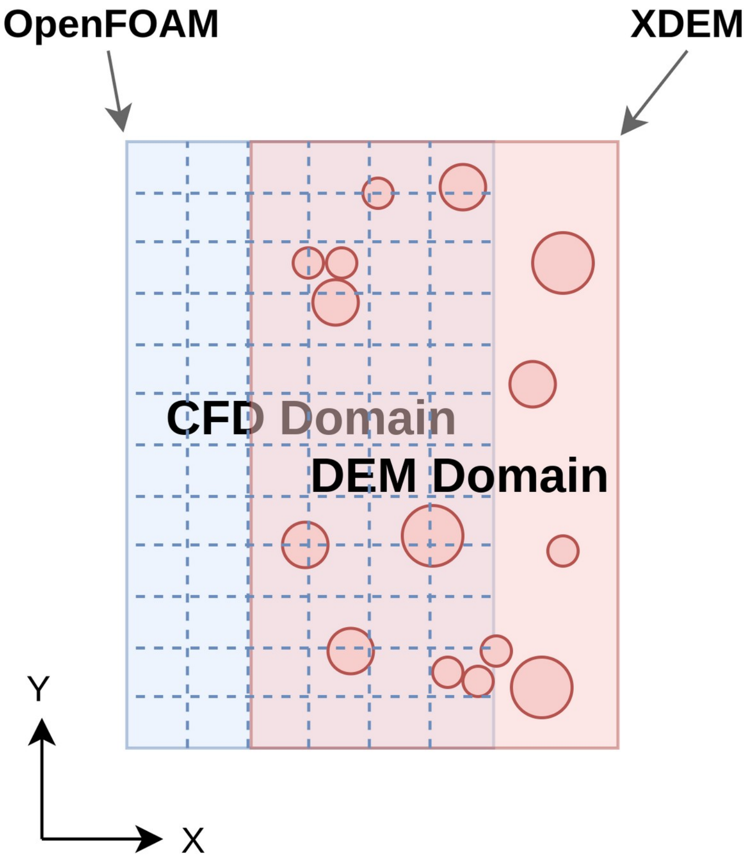
OpenFOAM (Eulerian) for:

- 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



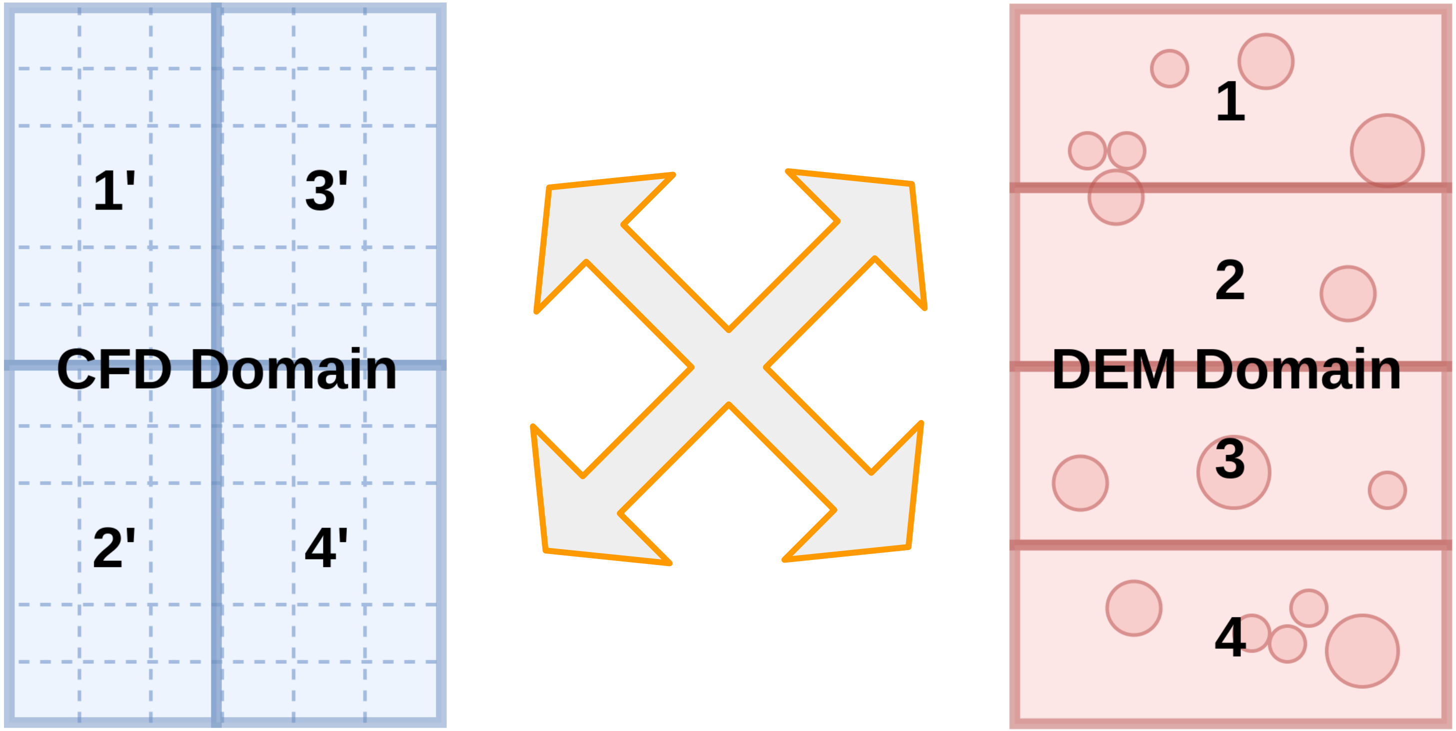
The domains overlap in space

Challenges in CFD-XDEM parallel coupling

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

CFD-DEM Parallel Coupling: Challenges

Classical Approach: the domains are partitioned independently



Complex pattern and large volume of communication

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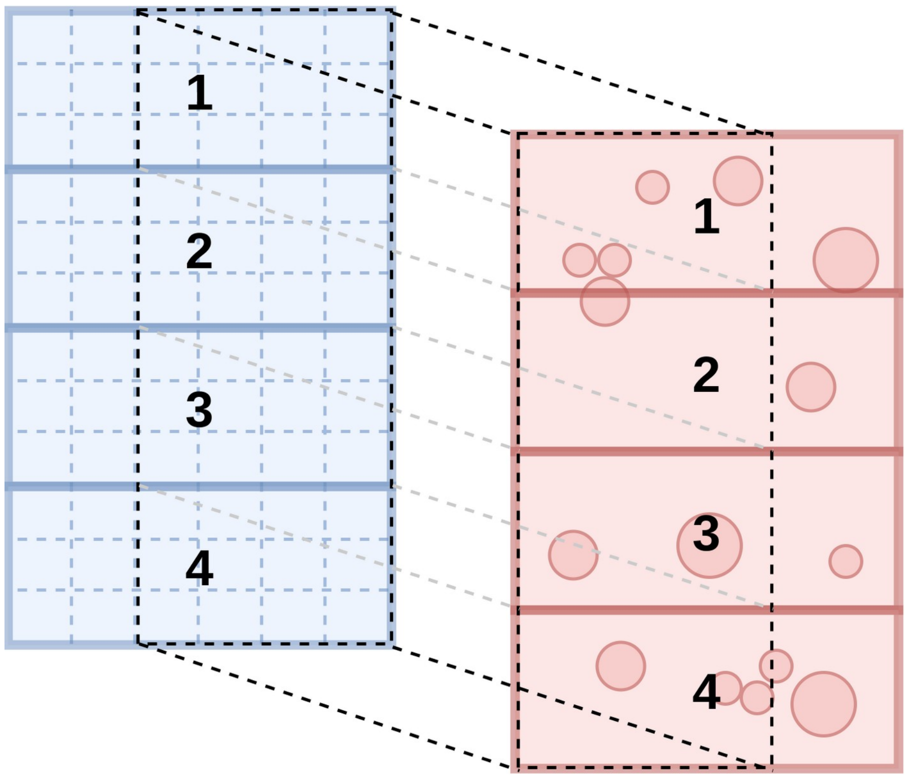
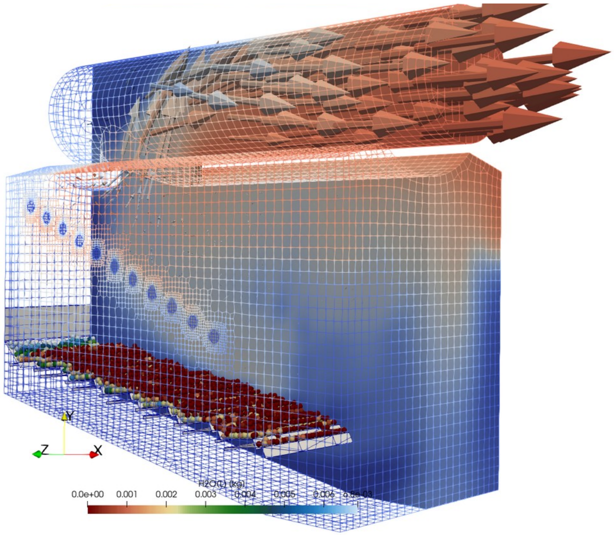
Co-located Partitioning Strategy



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

High Performance
Biomass Furnace Simulation

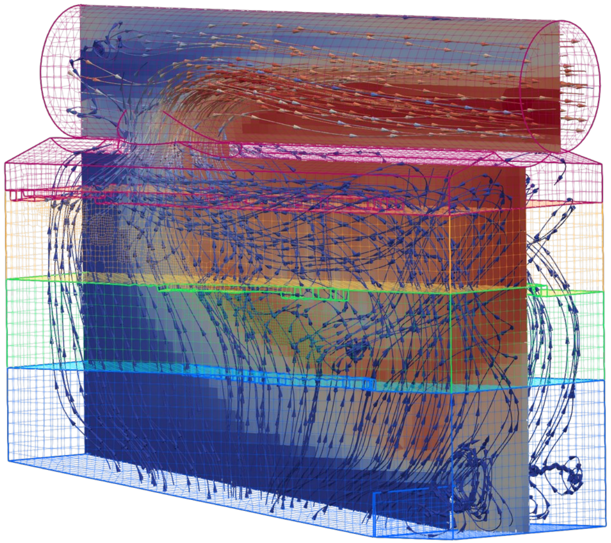
Simulation approach and results



Volume Coupling for Biomass Furnace Simulation
Momentum, Heat and Mass transfer

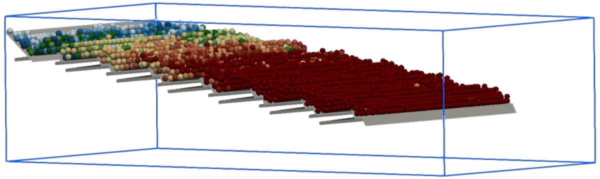
CFD to DEM

- Fluid velocity, density, dynamic viscosity
- Pressure Gradient
- Temperature
- Thermal conductivity
- Specific heat
- Diffusivity
- Species mass fraction (CH4, CO2, CO, H2, H2O, N2, O2, Tar)



Fluid phase in OpenFOAM

- Porosity
- Momentum source (acceleration, omega)
- Heat source
- Mass sources (CH4, CO2, CO, H2, H2O, N2, O2, Tar)



Particles in XDEM

DEM to CFD

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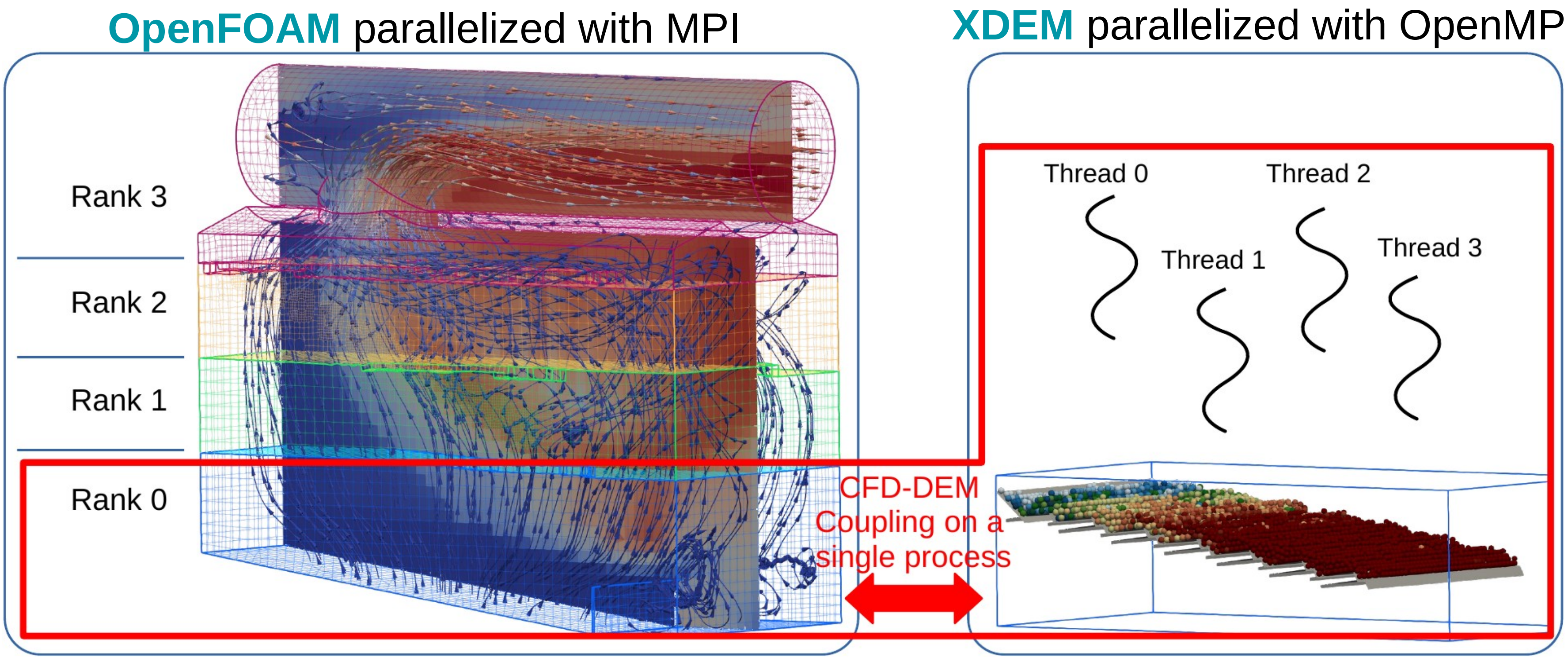
Parallelization approach for Biomass Furnace Simulation



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

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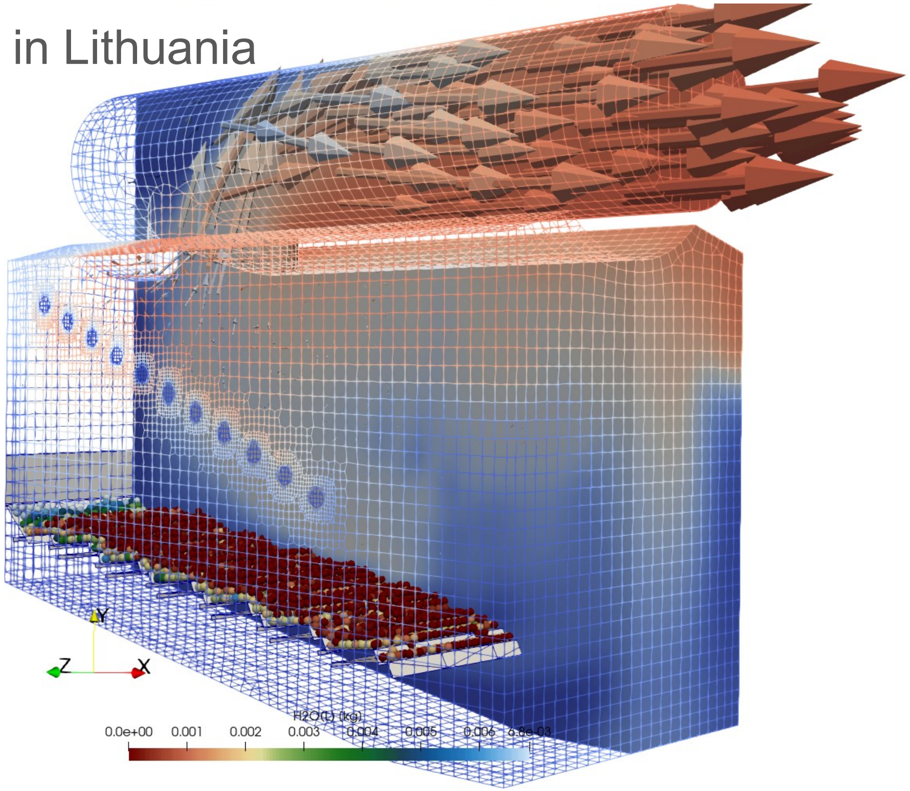
Biomass Furnace Setup

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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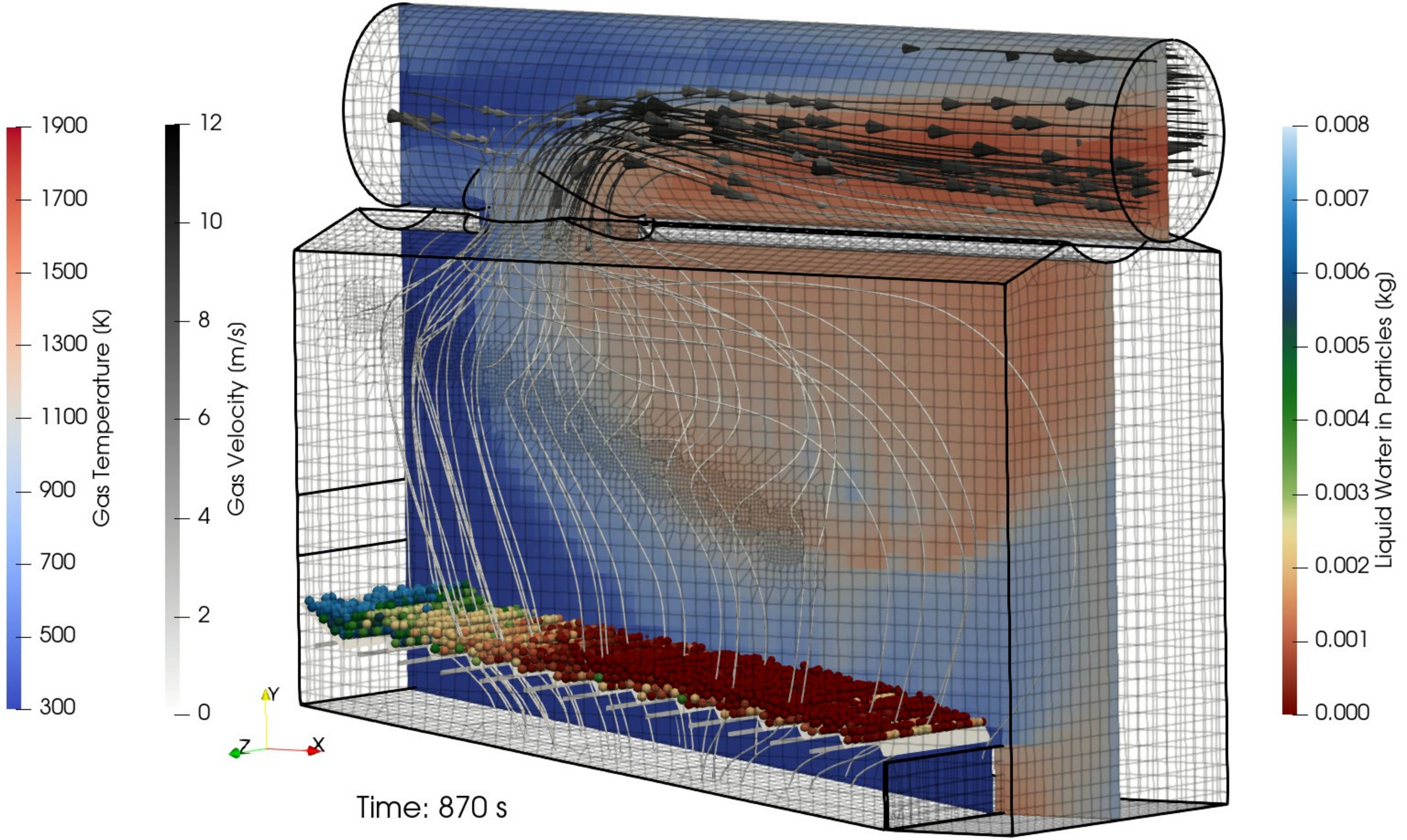
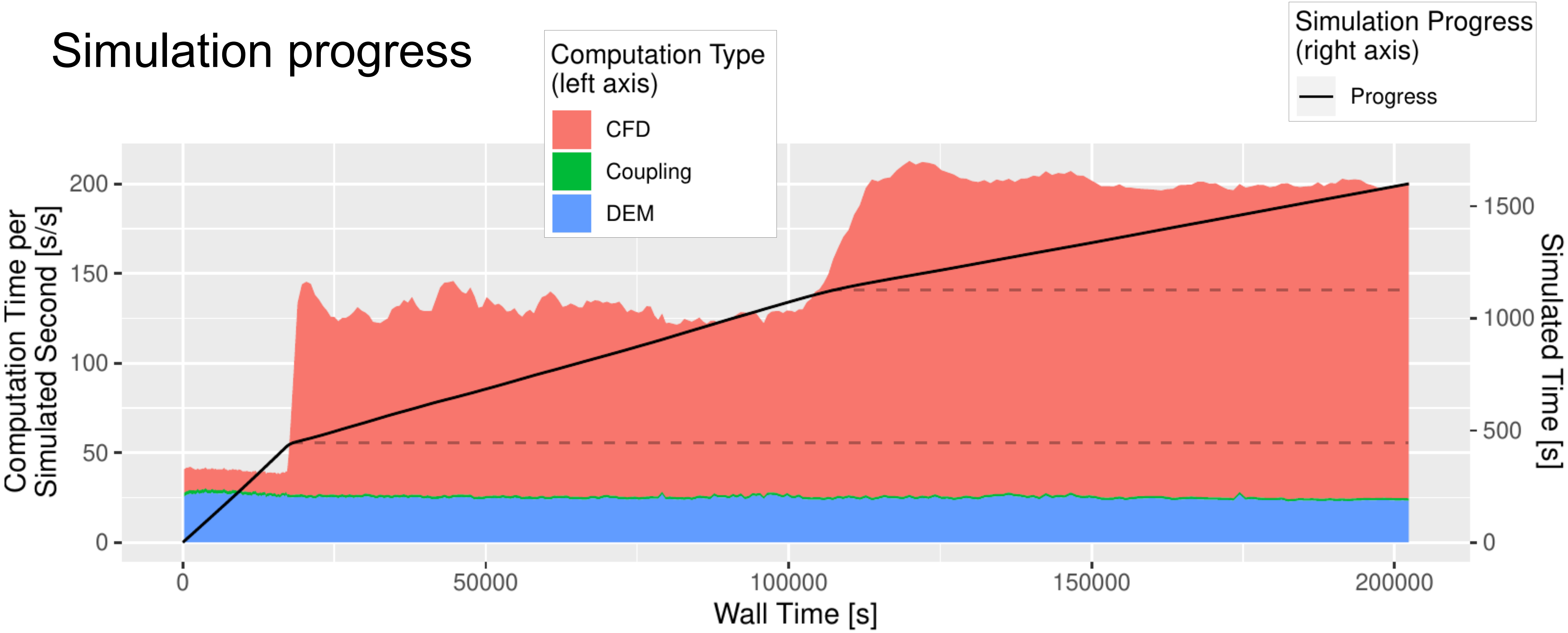
Biomass Furnace simulation using XDEM+OpenFOAM



Simulation progress

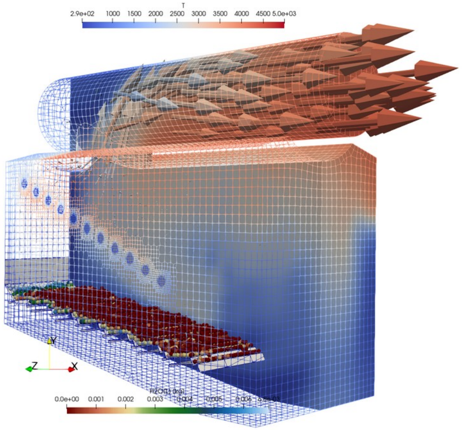


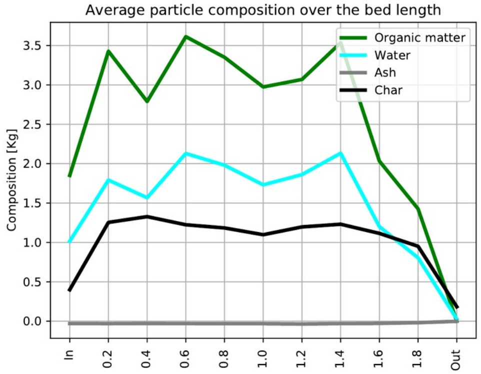
- At 445s of simulated time, lighting-up of the furnace
- Around 1125s, furnace reaches the steady state (all hot gases are burning)

⇒ **Dynamics** and **coupling-aware** load-balancing approaches required

Cloud-based Workflow for the Industry

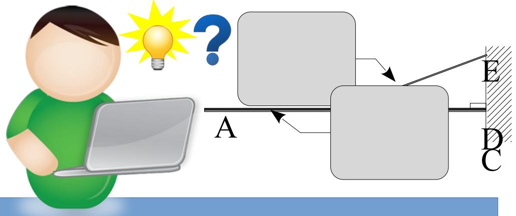
Seamless integration in HPC





Objective: a simple user workflow

Cloudi Facturing
https://www.cloudifacturing.eu

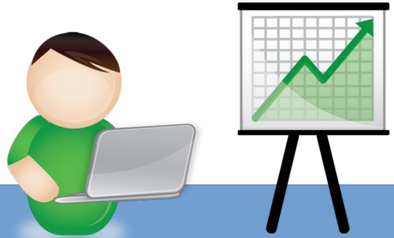


From the spreadsheet to the report

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

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How to much input is required?

Furnace and grate design

- parametrised with a few numbers
- geometry is generated automatically

Fuel / Wood chip

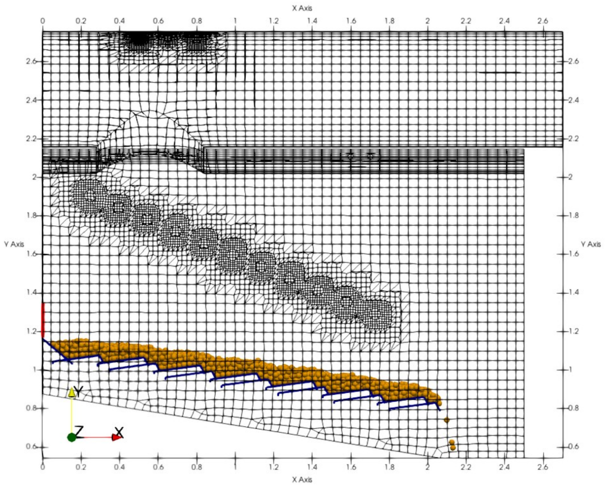
- characterised by ultimate analysis
- thermo-physical values obtained from standard experiments

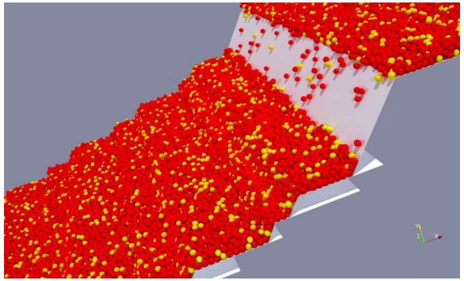
Air inlets

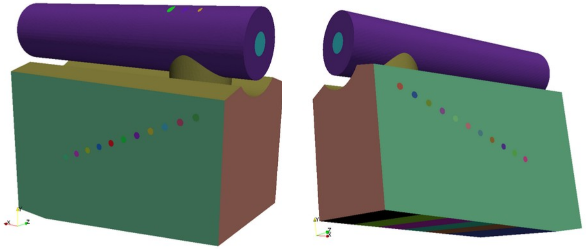
- can be placed at any position
- require the full composition when recirculation is used

→ A few hundred degrees of freedom!

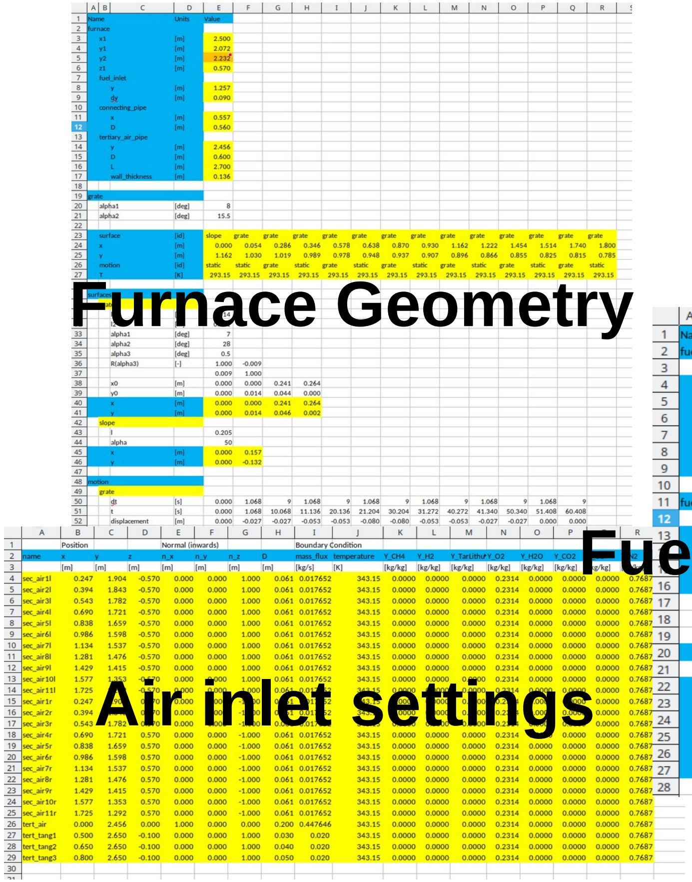
- Designing and implementing a web interface was out of scope







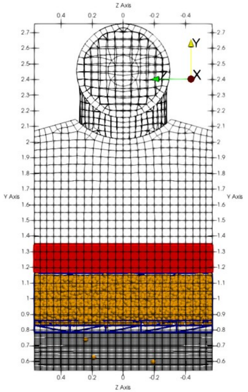
Spreadsheet Input File

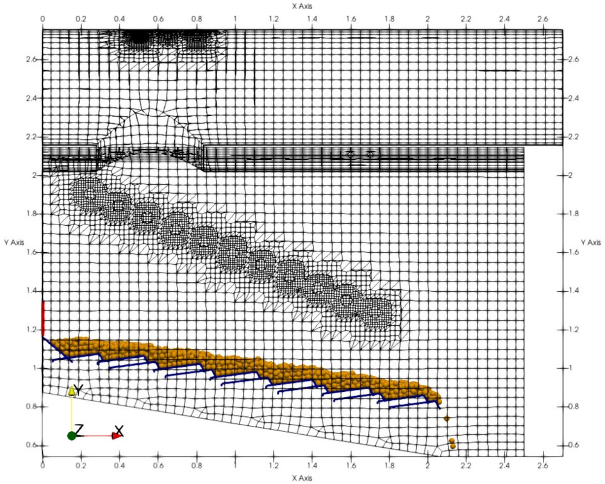


Fuel composition

	A	B	C	D	E
1	Name			Units	Value
2	fuel				
3			mass_flux	[kg/s]	0.047
4			initial_bed_height	[m]	0.100
5			composition	[id]	wood_chips
6			mass_flux	[kg/s]	0.047
7			D_min	[m]	0.030
8			D_max	[m]	0.030
9			initial_temperature	[K]	293.15
10					
11	fuel_types				
12			wood_chips		
13			Y_C	[kg/kg]	0.301
14			Y_[illegible]	[illegible]	[illegible]
15			Y_[illegible]	[illegible]	[illegible]
16			Y_N	[kg/kg]	0.004
17			Y_S	[kg/kg]	0.000
18			Y_Cl	[kg/kg]	0.000
19			Y_Ash	[kg/kg]	0.010
20			Y_H2O	[kg/kg]	0.400
21					1.000
22			lower_heating_value	[J/kg]	1.02E+07
23			conductivity		1.60E-01
24			specific heat capacity		2.45E+03
25			density	[kg/m^3]	7.59E+02
26			internal_porosity	[m^3/m^3]	7.00E-01
27			mechanical_properties		BeechWoodLithuania(S)
28					

Automatic generation of the CFD+DEM case





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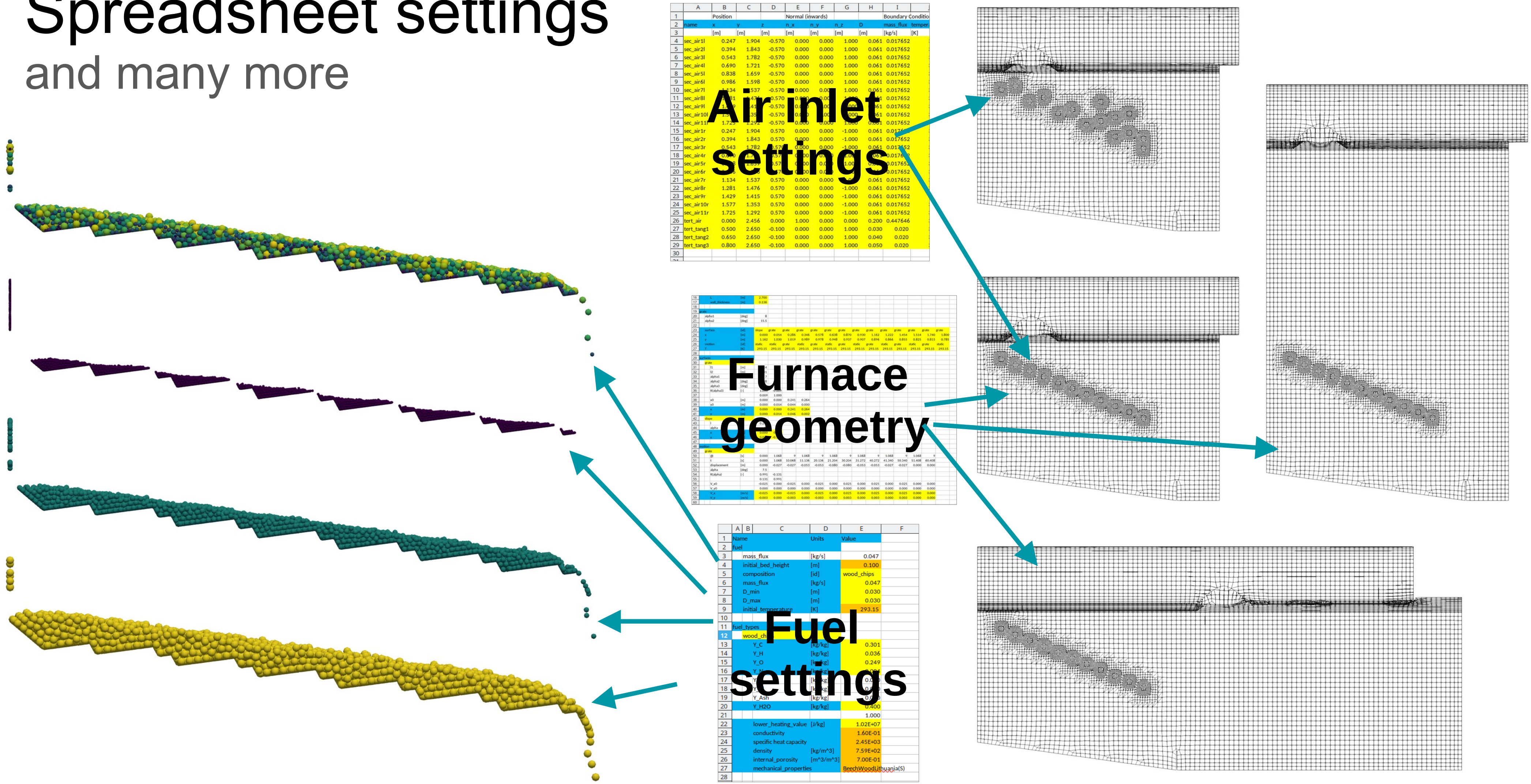
Spreadsheet settings

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

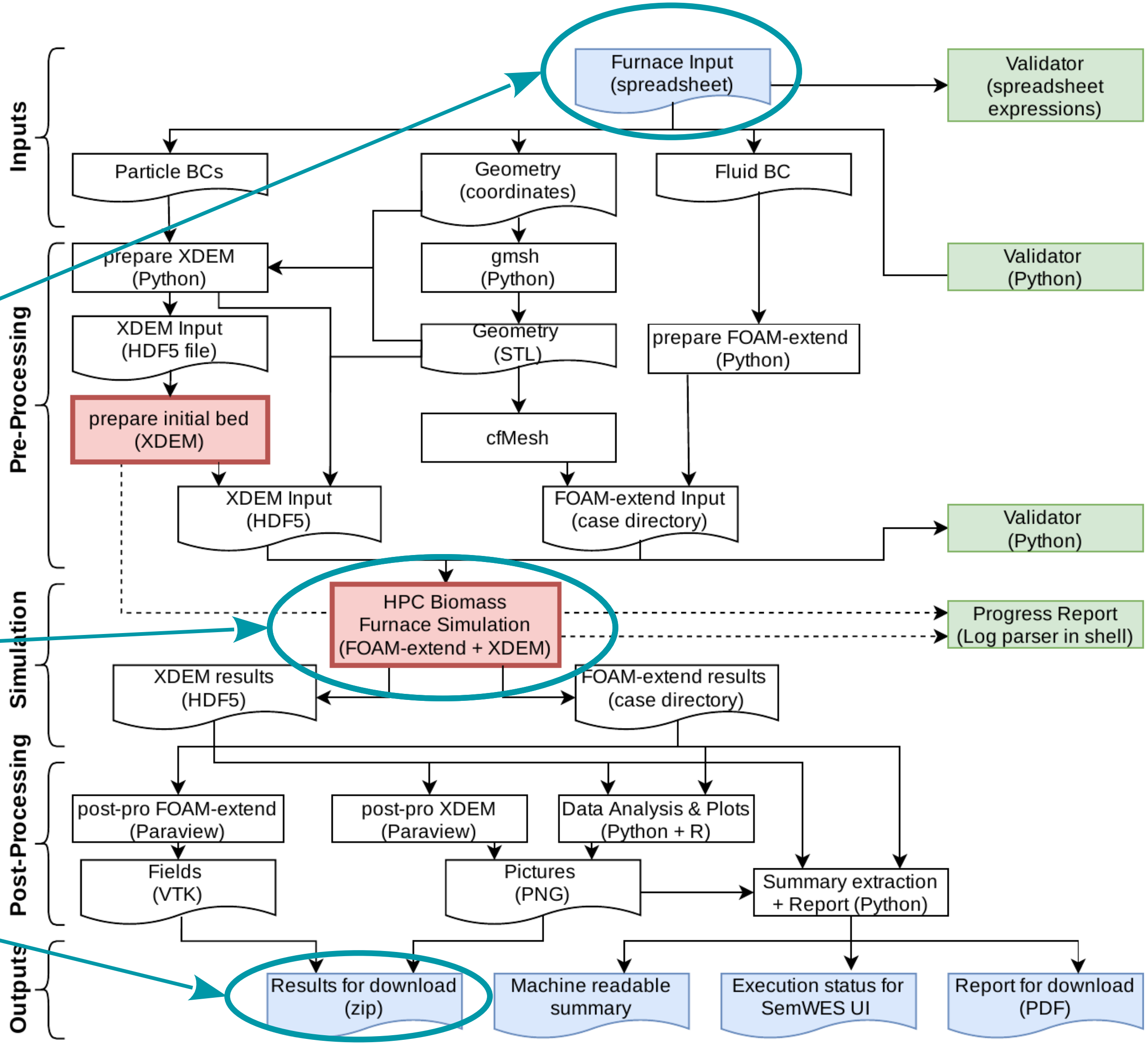
Internal workflow

running on HPC in a Singularity container

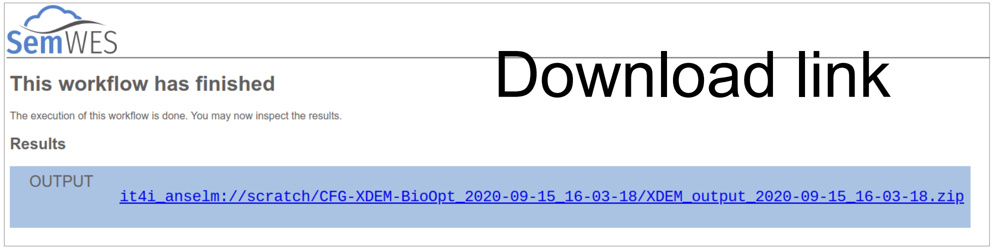
User Input

HPC Furnace Simulation

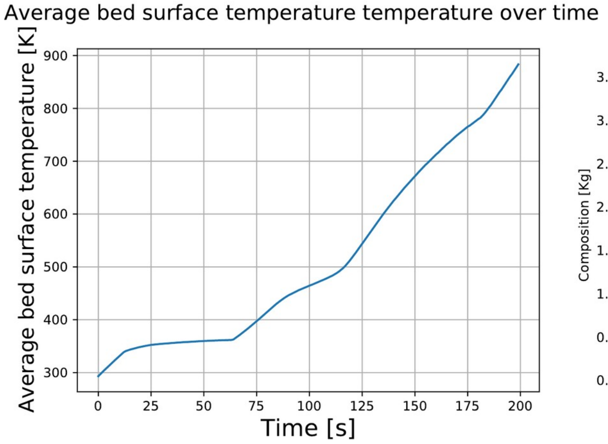
Simulation Output

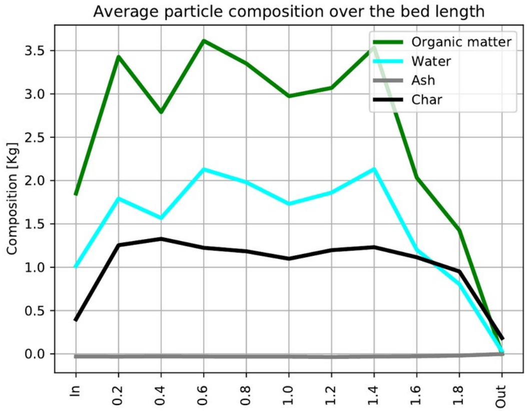


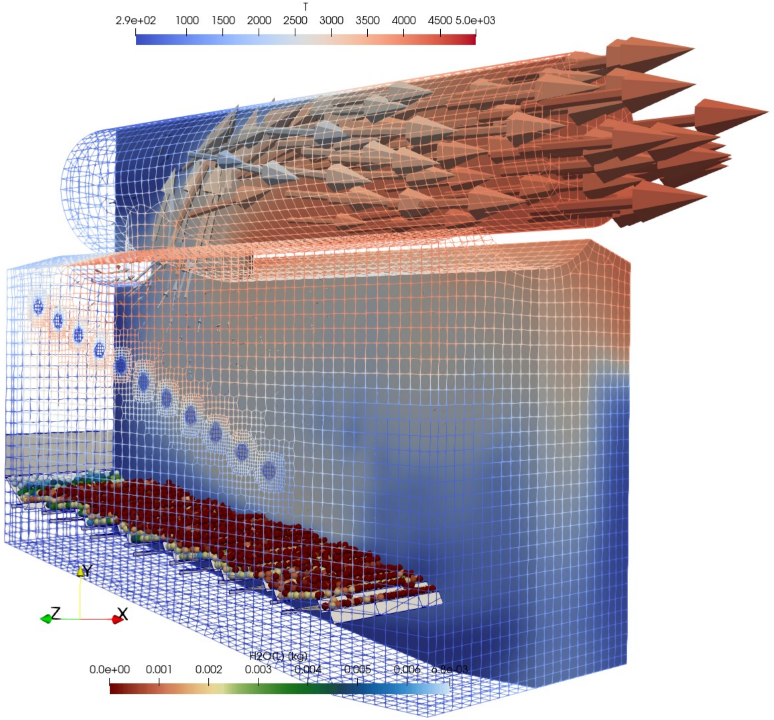
Simulation Results



Download link







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

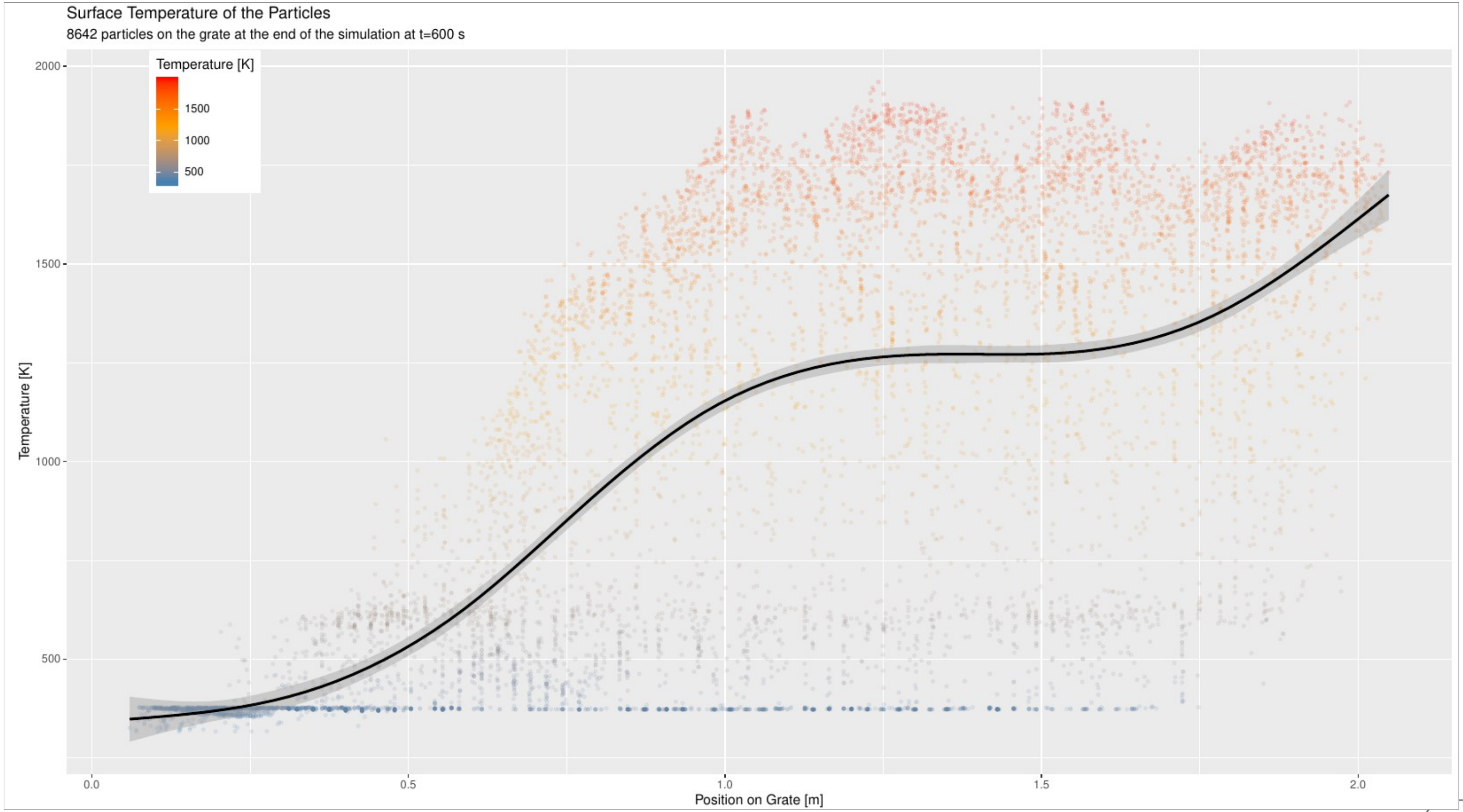
Extracts of the Simulation Reports

```
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
```

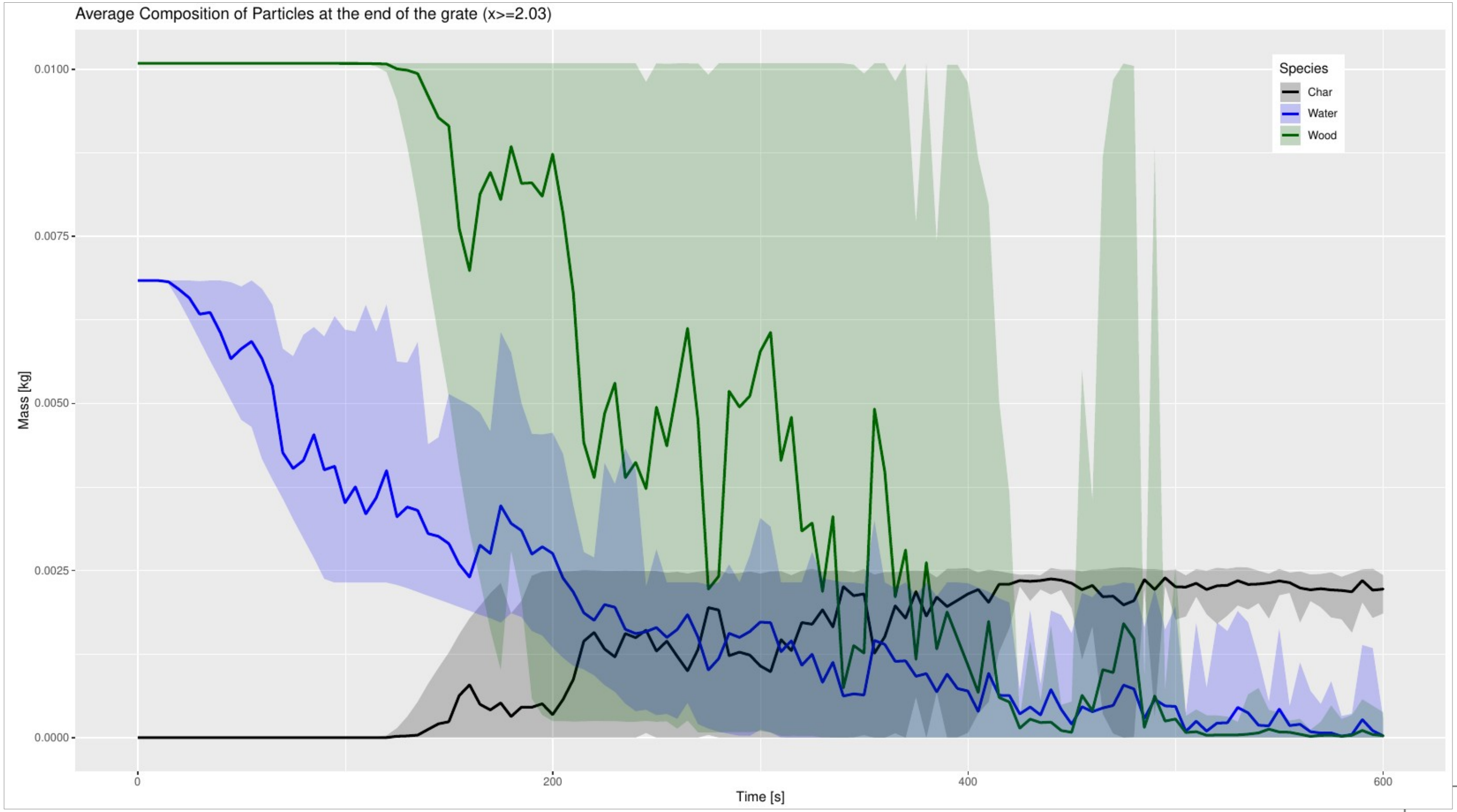
Average properties at exit of the exhaust pipe

Extracts of the Simulation Reports



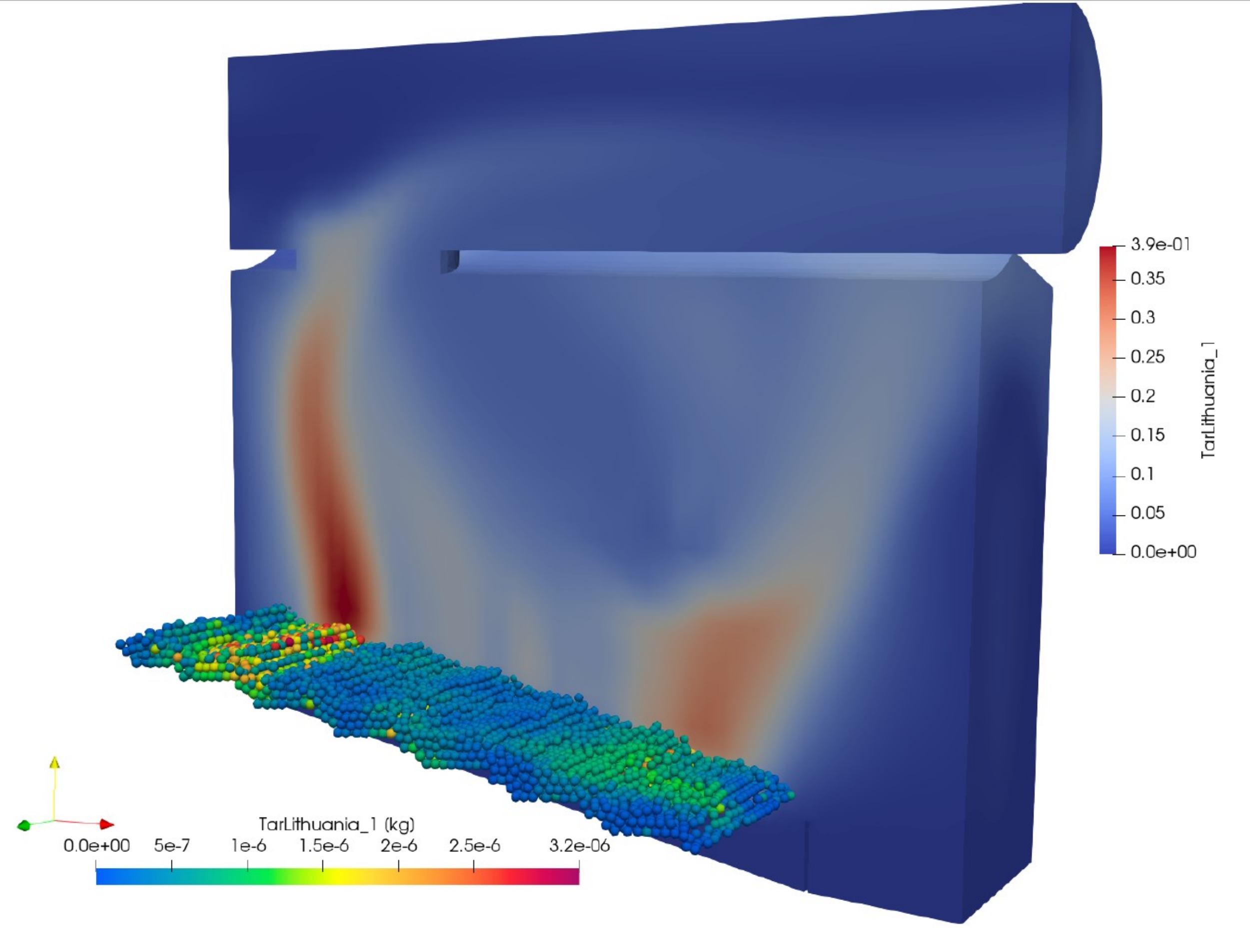
Surface temperature along the grate

Extracts of the Simulation Reports



Evolution of particle composition at the exit of the grate

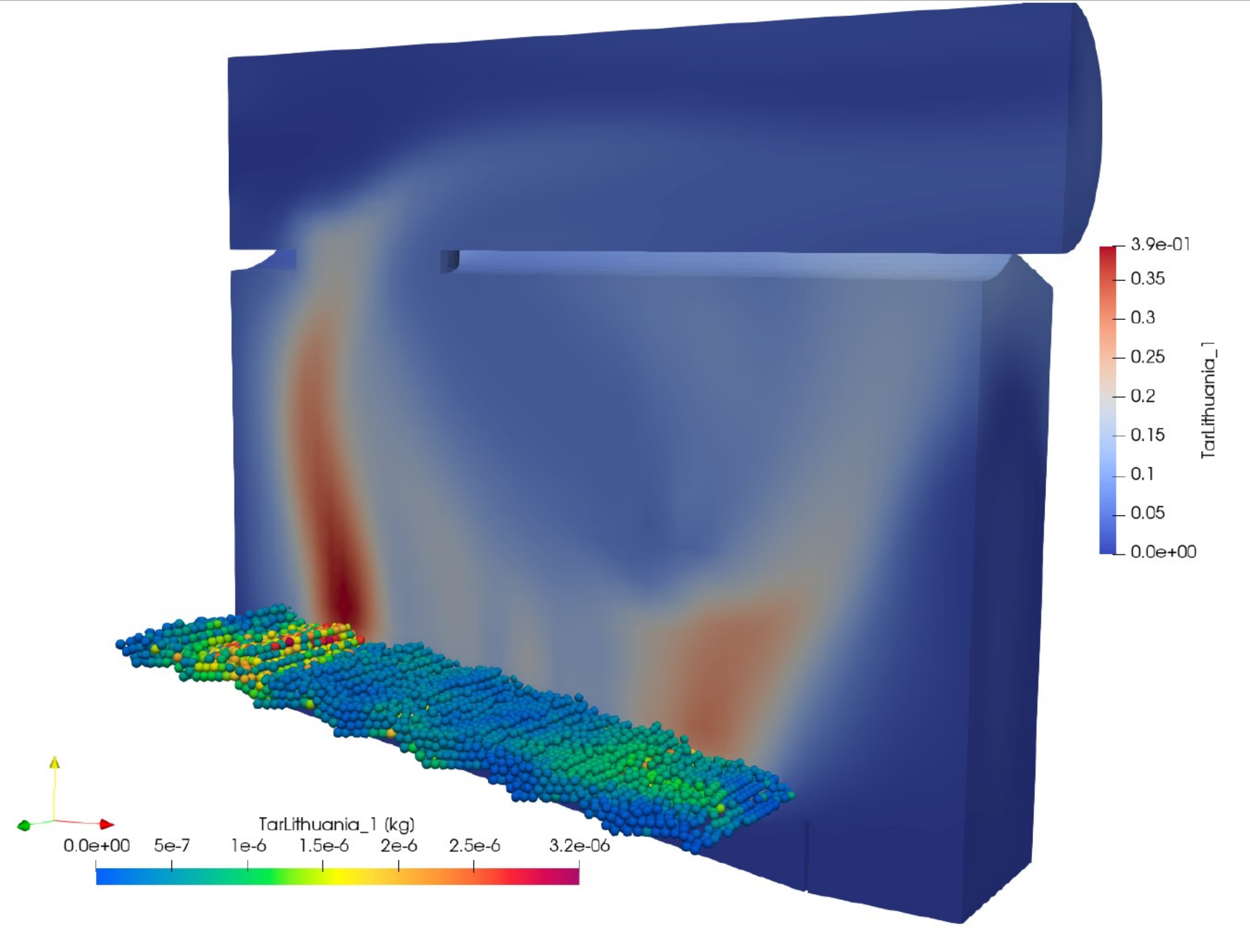
Extracts of the Simulation Reports



Tar content of the particles and in the gas

Extracts of the Simulation Reports

and many more...

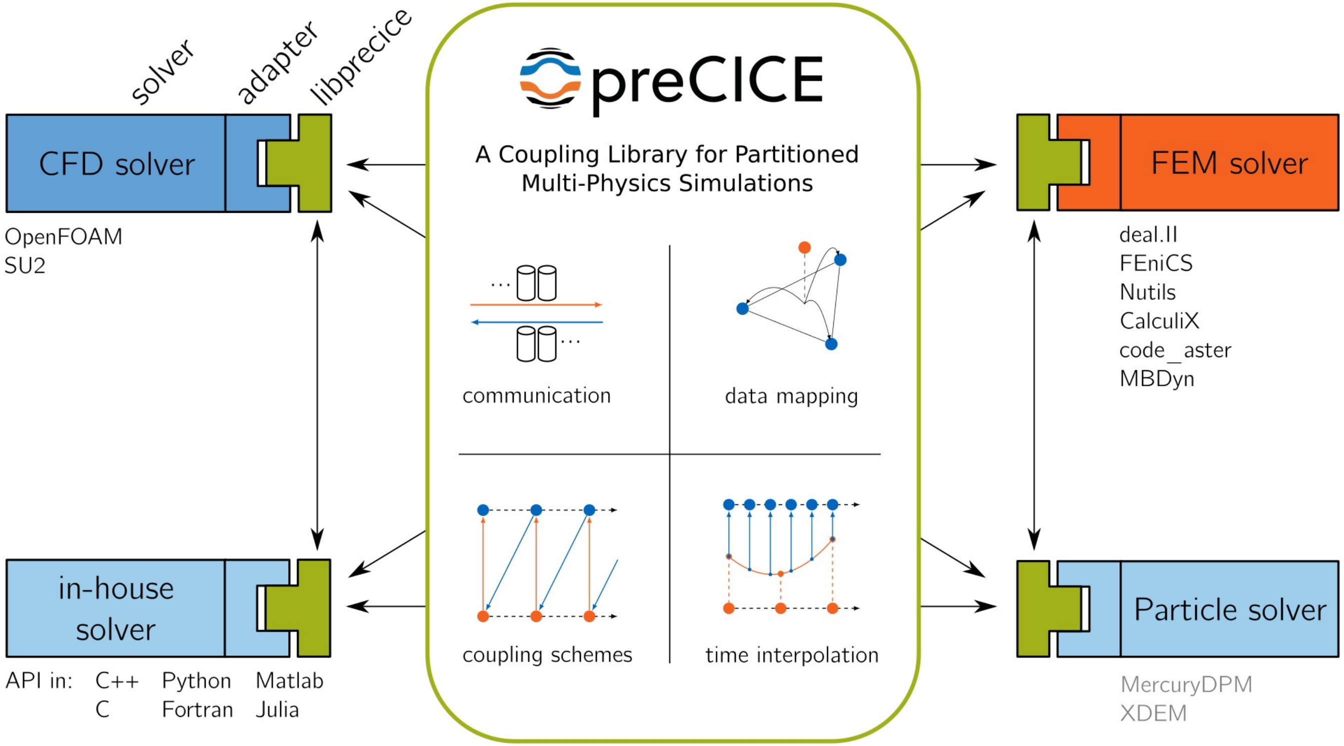


Tar content of the particles and in the gas

Toward more flexibility for the Industry

Coupling using the preCICE library

Replacing ad-hoc coupling in XDEM → Using preCICE coupling library



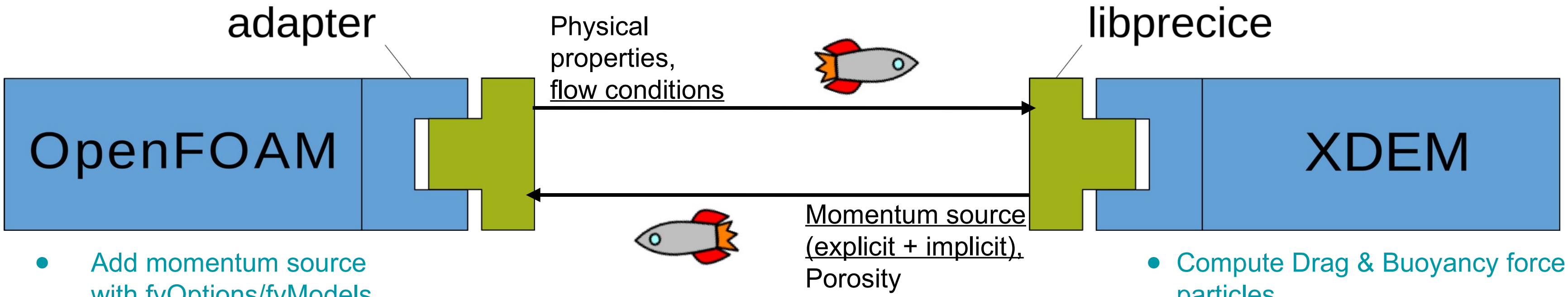
Black-box approach

- Solver can be replaced 'easily'
- Require an adapter
- Compatible with closed-source solvers

⇒ **more flexibility**

Homepage: https://precice.org/

XDEM-OpenFOAM coupling with preCICE



- Add momentum source with fvOptions/fvModels

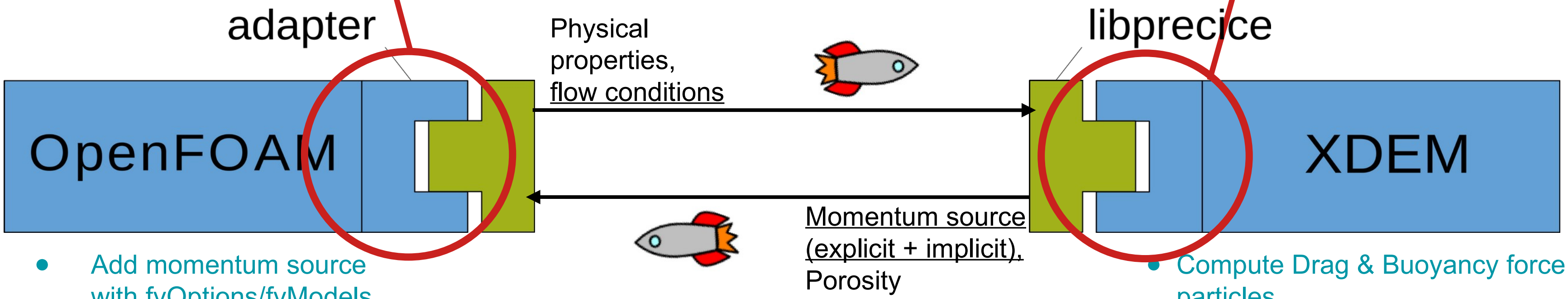
- Compute Drag & Buoyancy force on particles
- Compute momentum source terms [2]

[2] Xiao H, Sun J. Algorithms in a robust hybrid CFD-DEM solver for particle-laden flows. Communications in Computational Physics. 2011;9(2):297-323.
[-] preCICE 2021, Momentum coupling: https://youtu.be/7fpRsB55Oss

XDEM-OpenFOAM coupling with preCICE

Development OpenFOAM adapter
- Volume coupling
- Mass transfer (source terms, mass fractions, …)

New XDEM adapter



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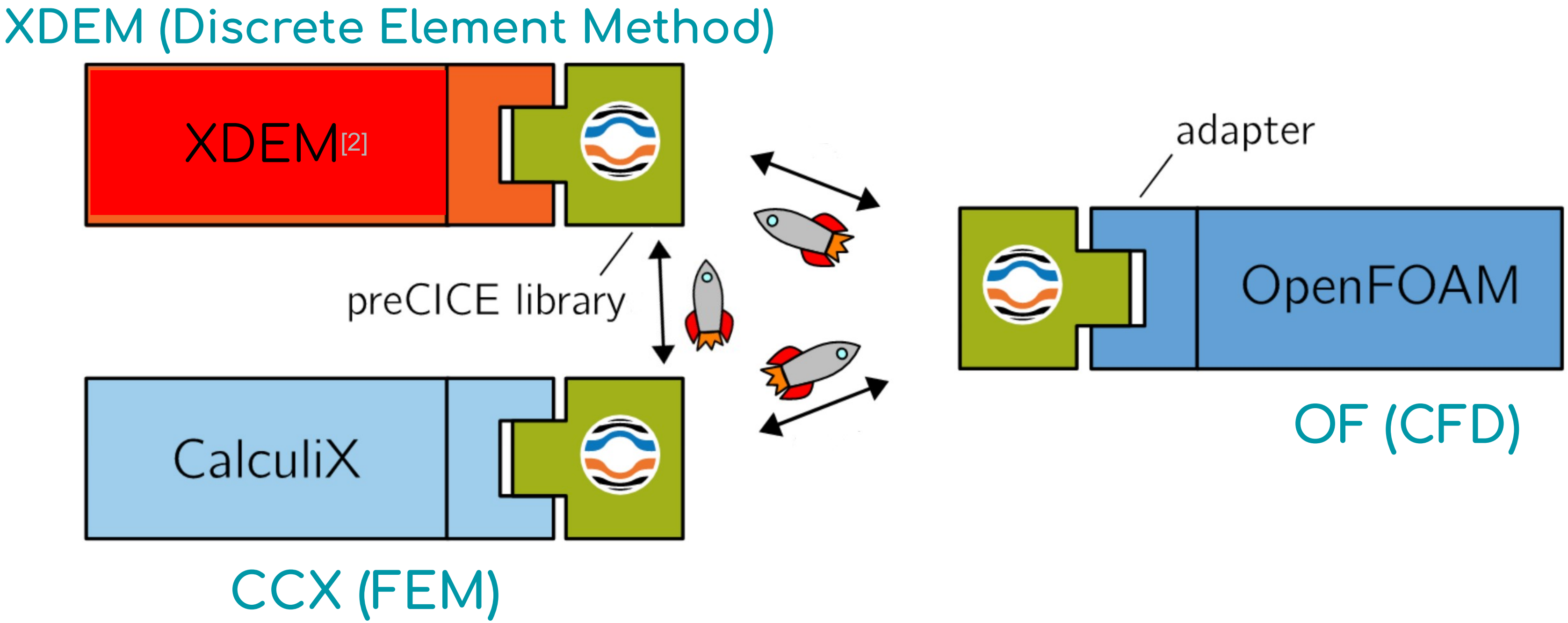
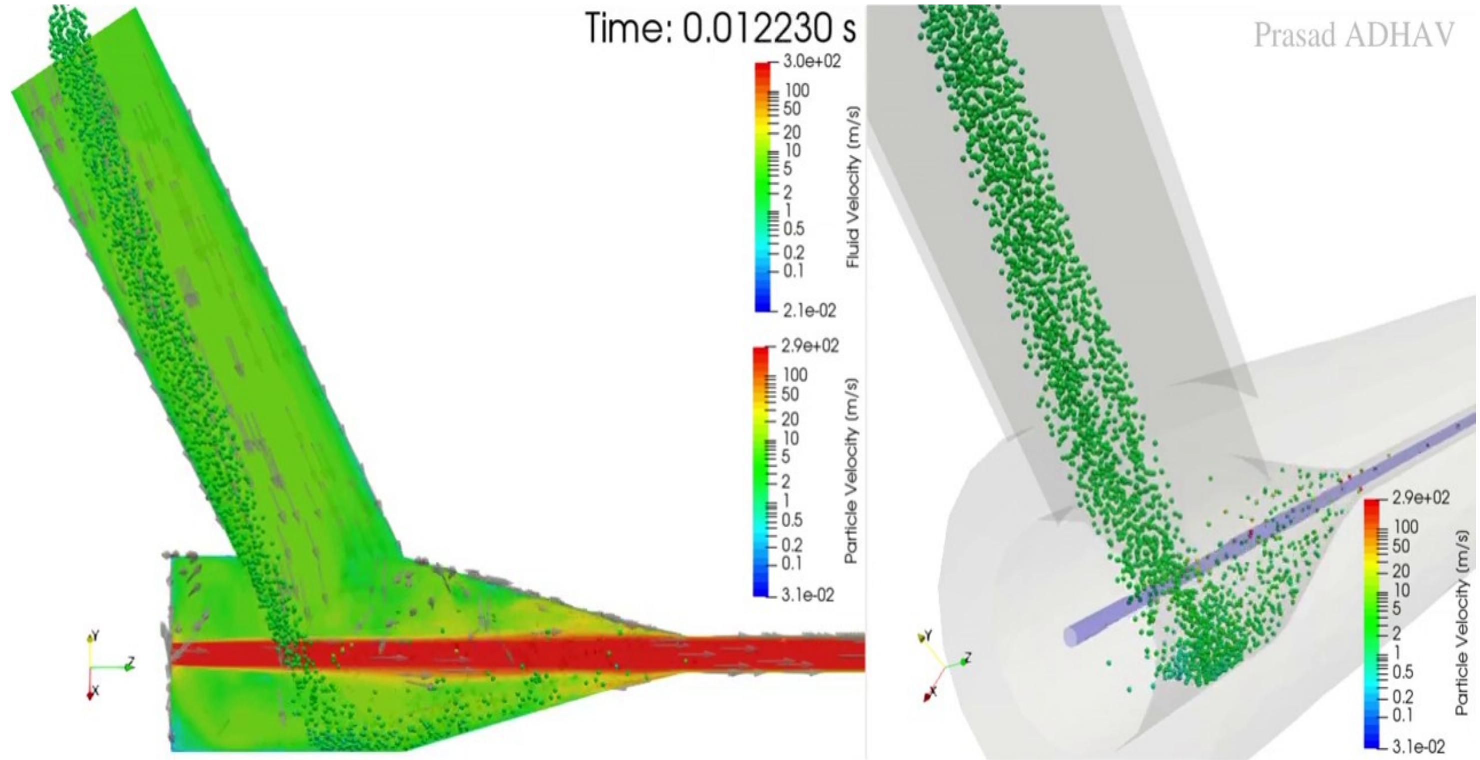
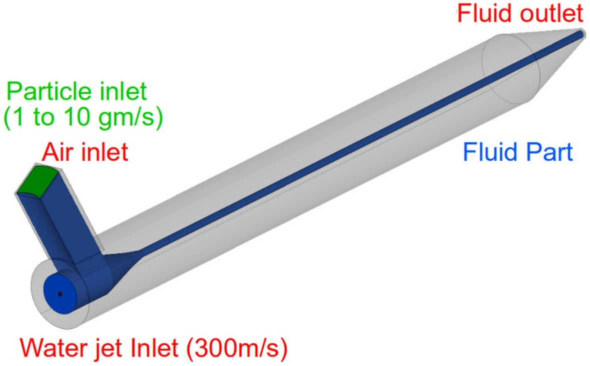
Going further: 6-way coupling DEM-CFD-FEM



Abrasive Water Jet Cutting Nozzle with preCICE coupling (work in progress)



AWJC Nozzle setup



Summary: HPC Multi-Physics Coupled Simulations for the Industry

Multi-Physics Biomass Furnace Simulation

- Two-way ‘in-memory’ coupling CFD ↔ DEM
- Hybrid parallelization scheme: MPI + OpenMP

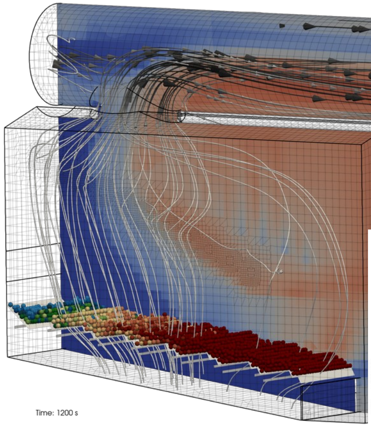
Cloud-based workflow

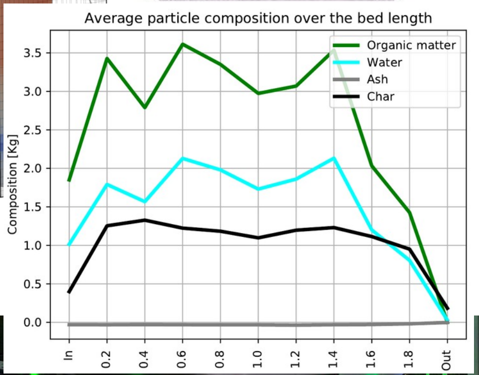
- From input to simulation report
- Portable execution using Singularity
- Job submission and execution on HPC platform

→ Application as a Service (AaaS)

Toward more flexibility

- preCICE coupling library
- coupling-aware load-balancing





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More details about the CloudiFacturing BioOpt Experiment:

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

CloudiFacturing project:

https://www.cloudifacturing.eu

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Thank you for your attention!

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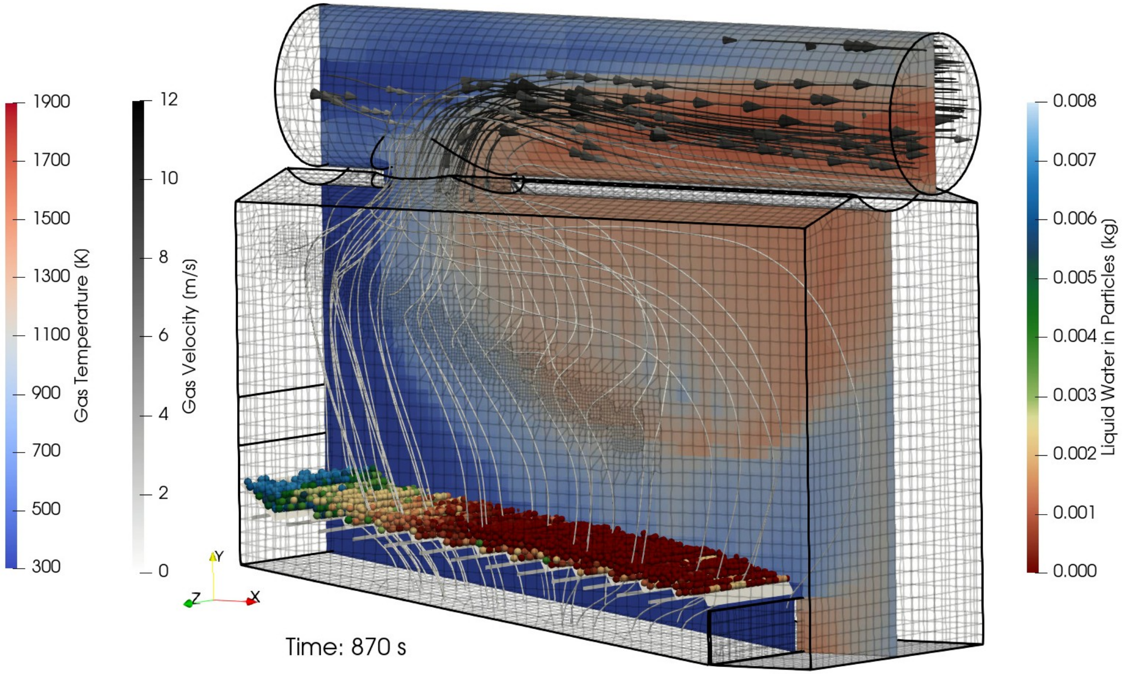

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