Parallel Multi-Physics Simulation of Biomass Furnace and Cloud-based Workflow for SMEs

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In collaboration with

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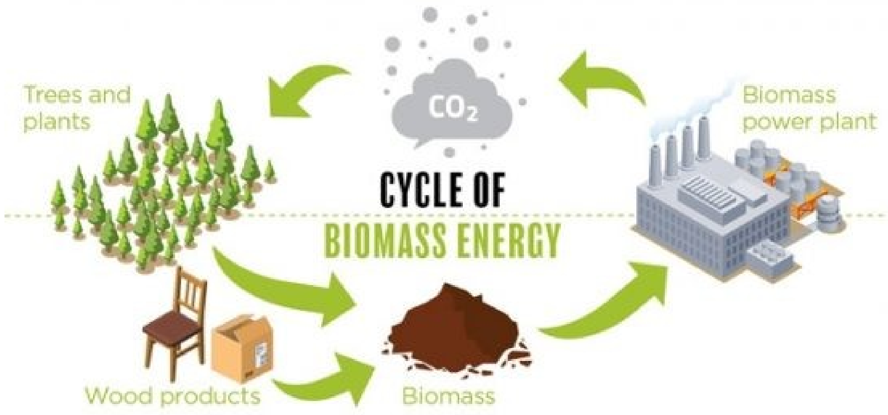
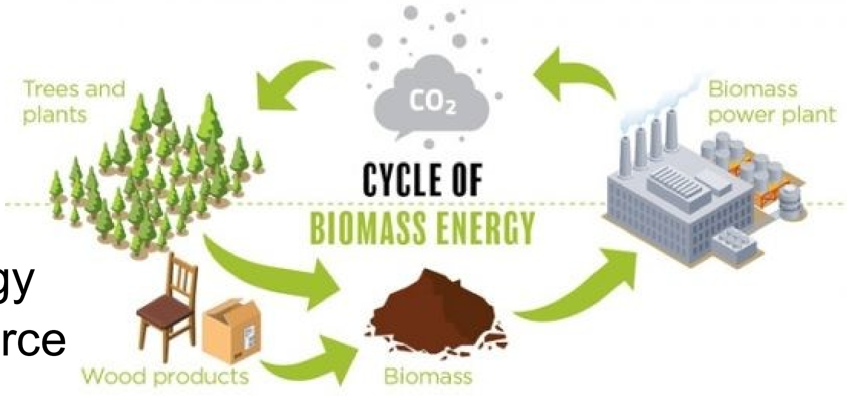
Introduction to Biomass Combustion



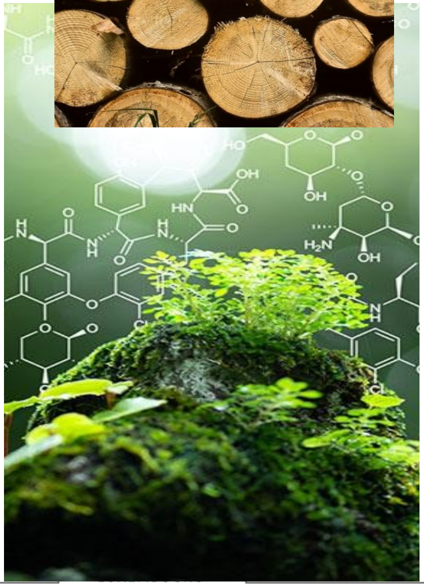
Biomass Combustion



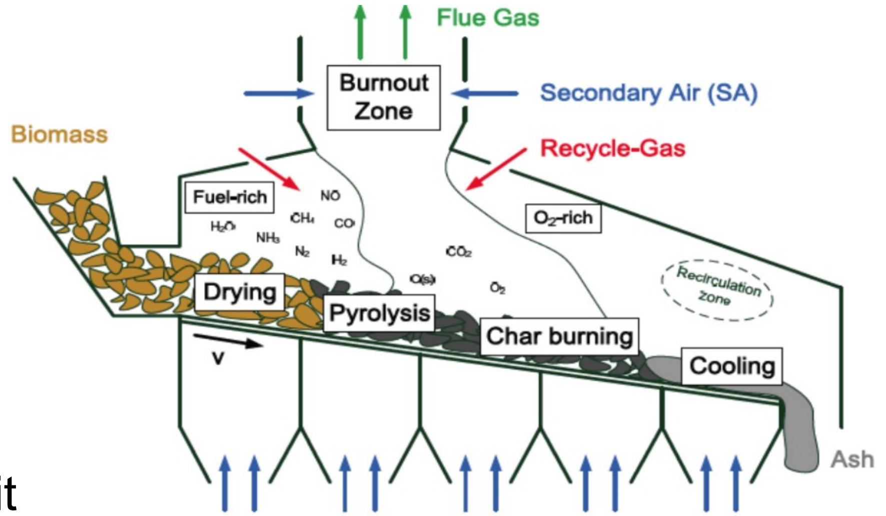
Biomass combustion (e.g. wood chips)
- widely used for generating electric and thermal energy
- renewable and potentially carbon-neutral energy source

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



[Paces and Kozek, 2011]

Combustion chamber of a biomass furnace

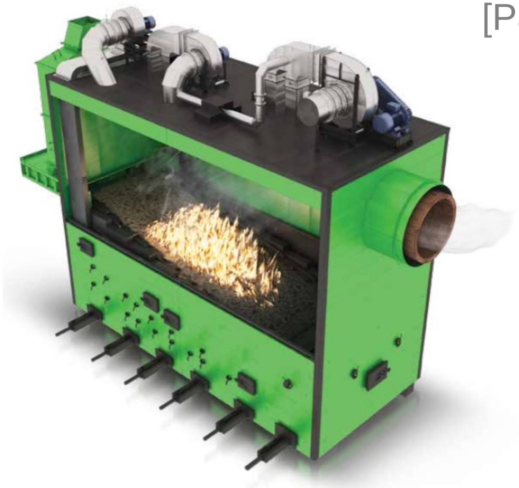
- forward acting grate
- transports the fuel through the furnace

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



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Research & Work Objectives

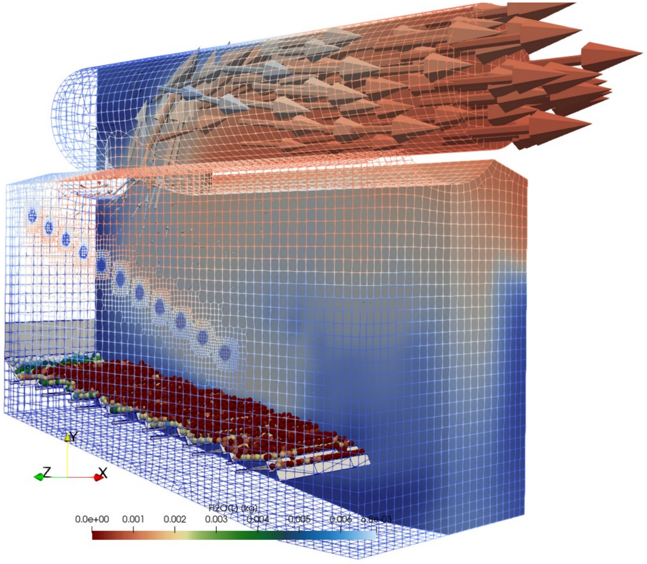
Multi-Physics Simulation of a Biomass Furnace

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

Seamless Cloud-based Workflow for SMEs

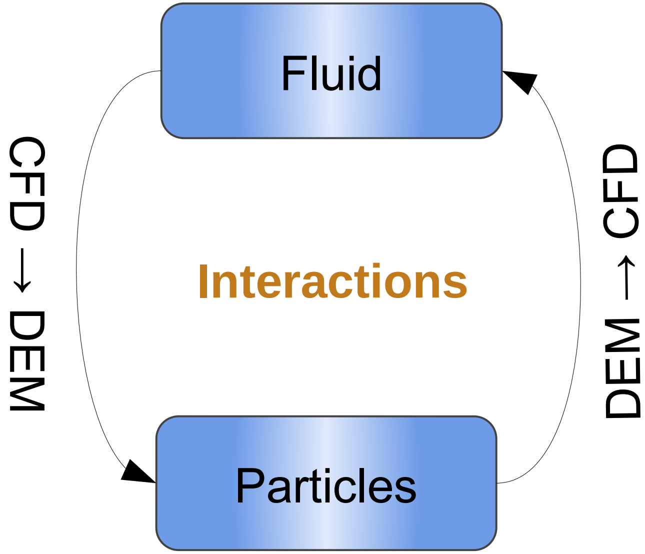
- Configurable Furnace Setup
  → specified by our industrial partner Enerstena UAB
  → results expected in less than 48h
- Fully automatic, from furnace specifications to simulation report

Parallel Multi-Physics Biomass Furnace Simulation



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

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



XDEM (Lagrangian) for:

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

OpenFOAM (Eulerian) for:

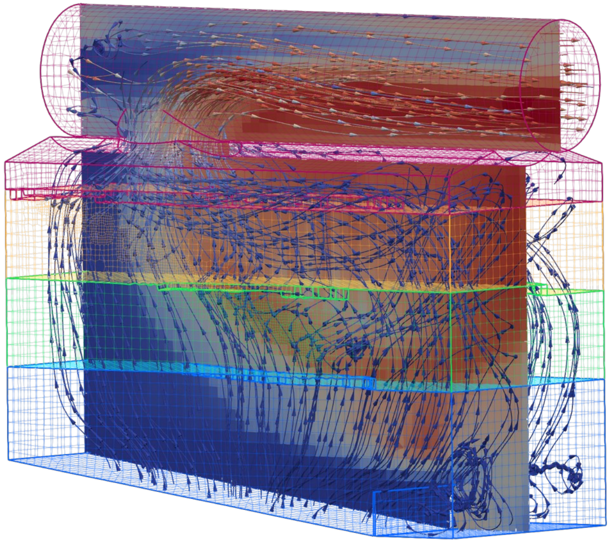
- Flow of gas phase
- Reactions in the gas phase

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

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

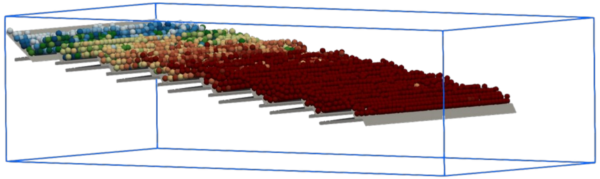
CFD to DEM

- 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

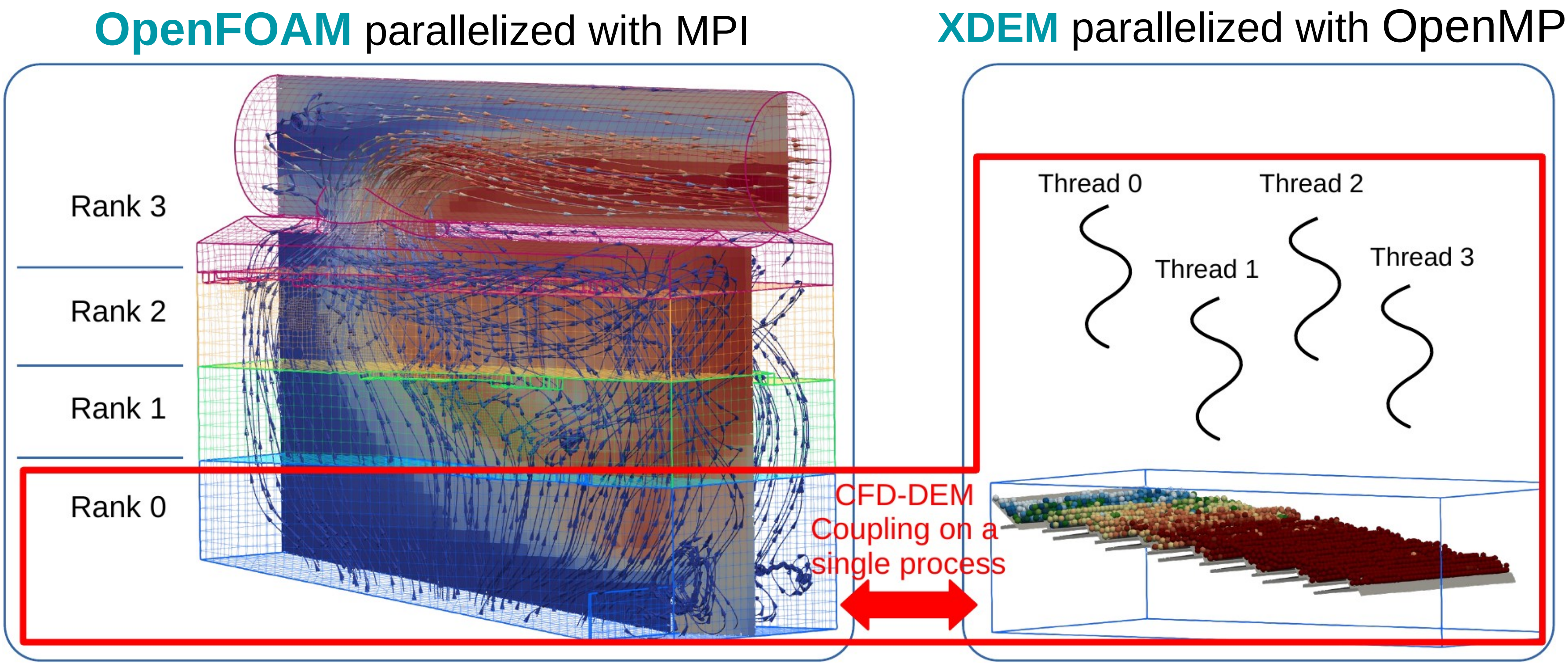
- Porosity
- Momentum source (*acceleration*, omega)
- Heat source
- Mass sources (CH_4, CO_2, CO, H_2, H_2O, N_2, O_2, Tar)



Particles in XDEM

DEM to CFD

Parallelization approach for Biomass Furnace Simulation

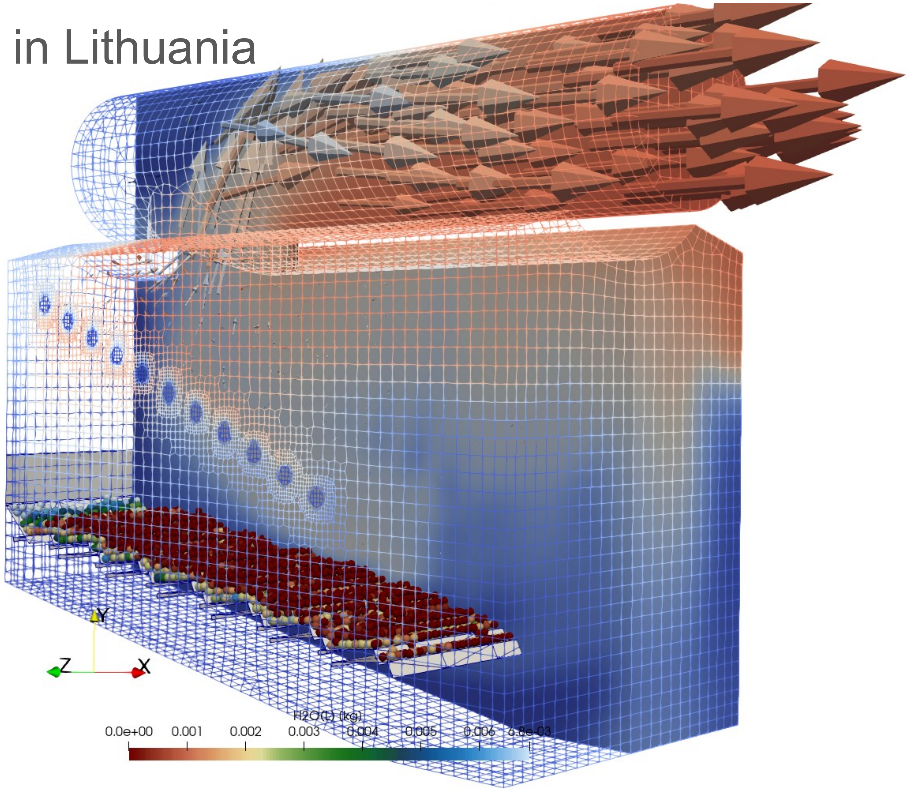


Co-located partitioning → Account for the spatial-locality of the data between the two solvers

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

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

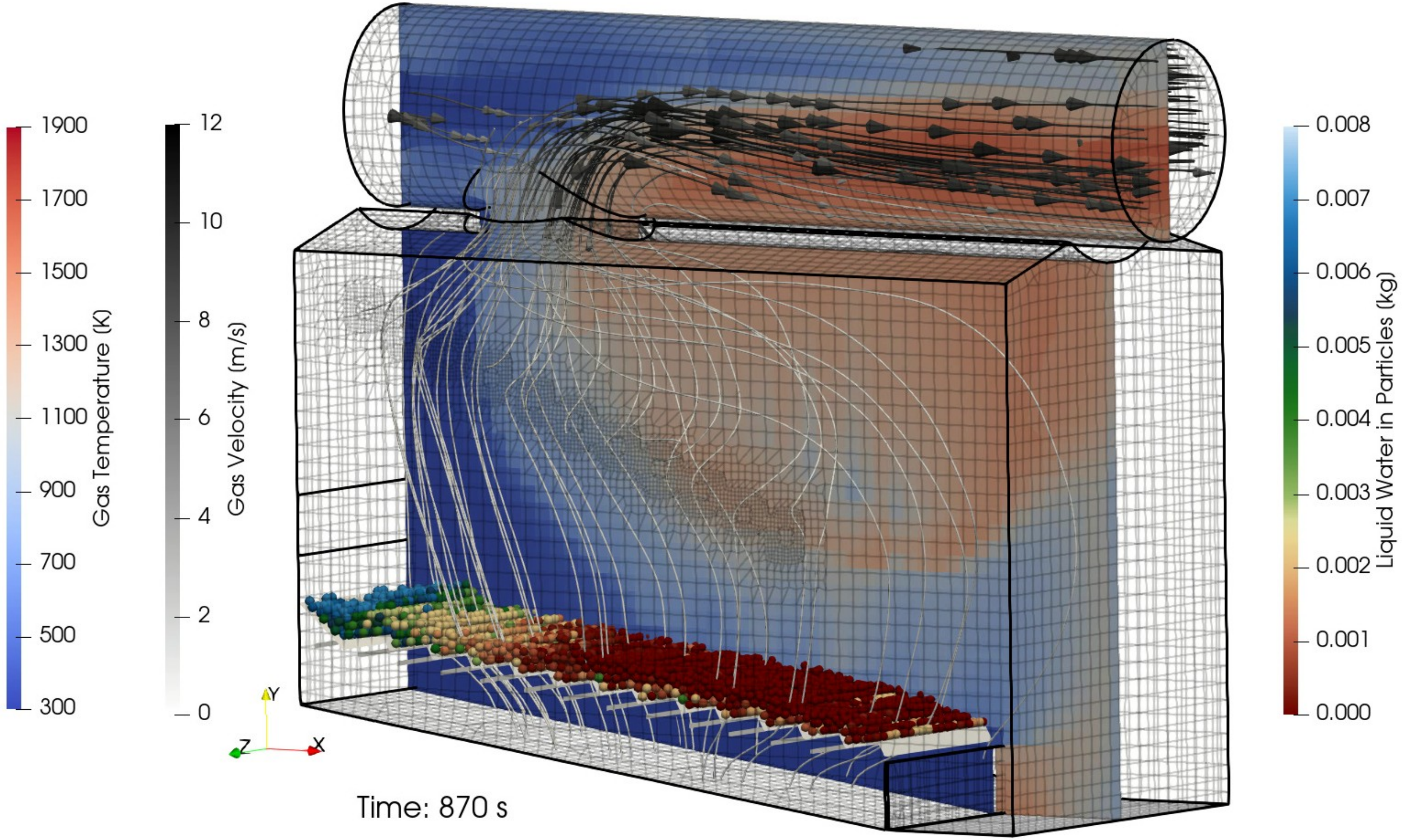
Fuel bed

- Initial fuel bed height 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

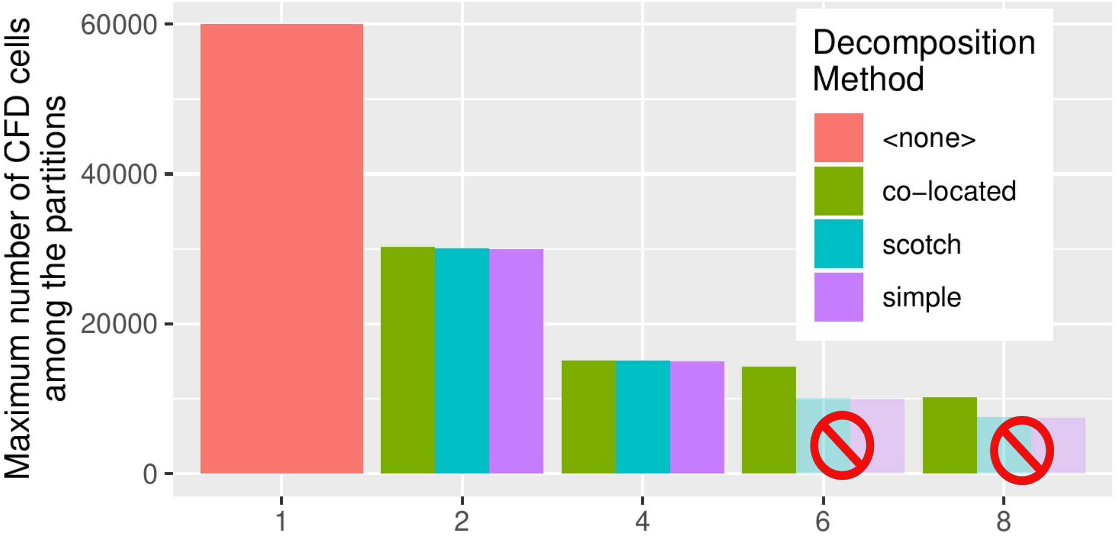
Following performance measurements were carried out on the *Barbora* cluster of the IT4Innovations HPC platform.

Biomass Furnace simulation using XDEM+OpenFOAM



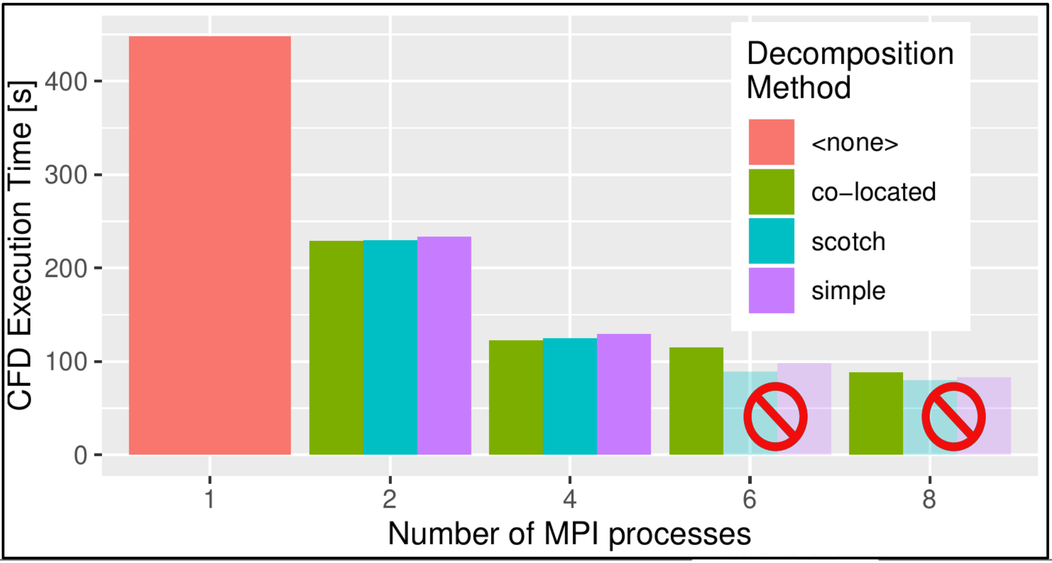
Decomposition and scalability of OpenFOAM

- Execution of the coupled problem, but looking at the **CFD part only**
- Execution time for the first 10s of simulation
- OpenFOAM mesh is relatively small: only 60k cells



Co-located compared to SCOTCH on 8 processes

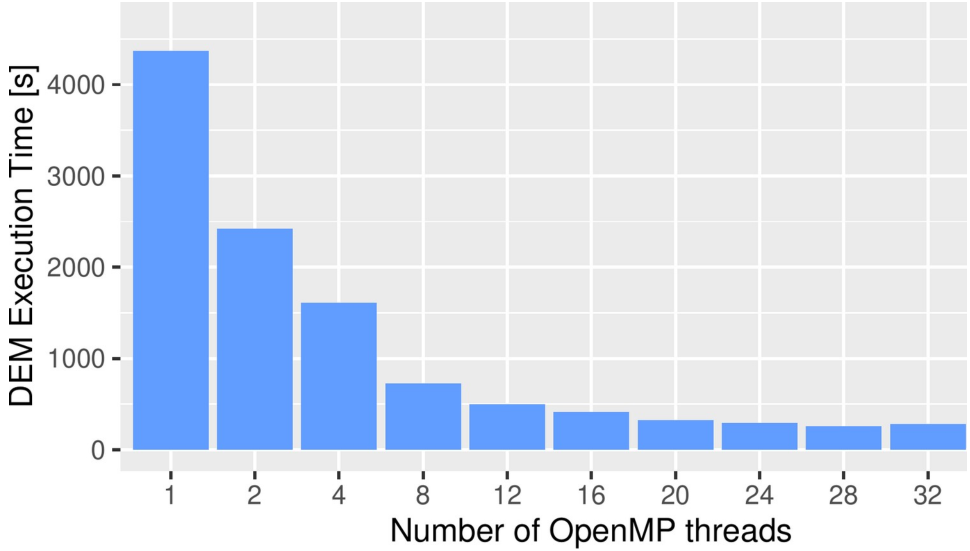
- Load-balancing → +37%
- CFD Execution time → +11% only



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

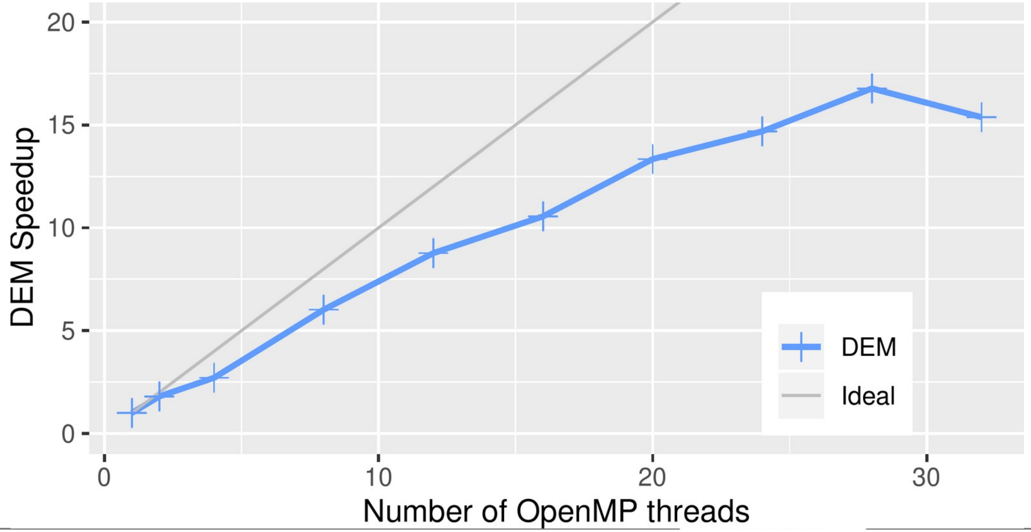
Scalability of XDEM

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



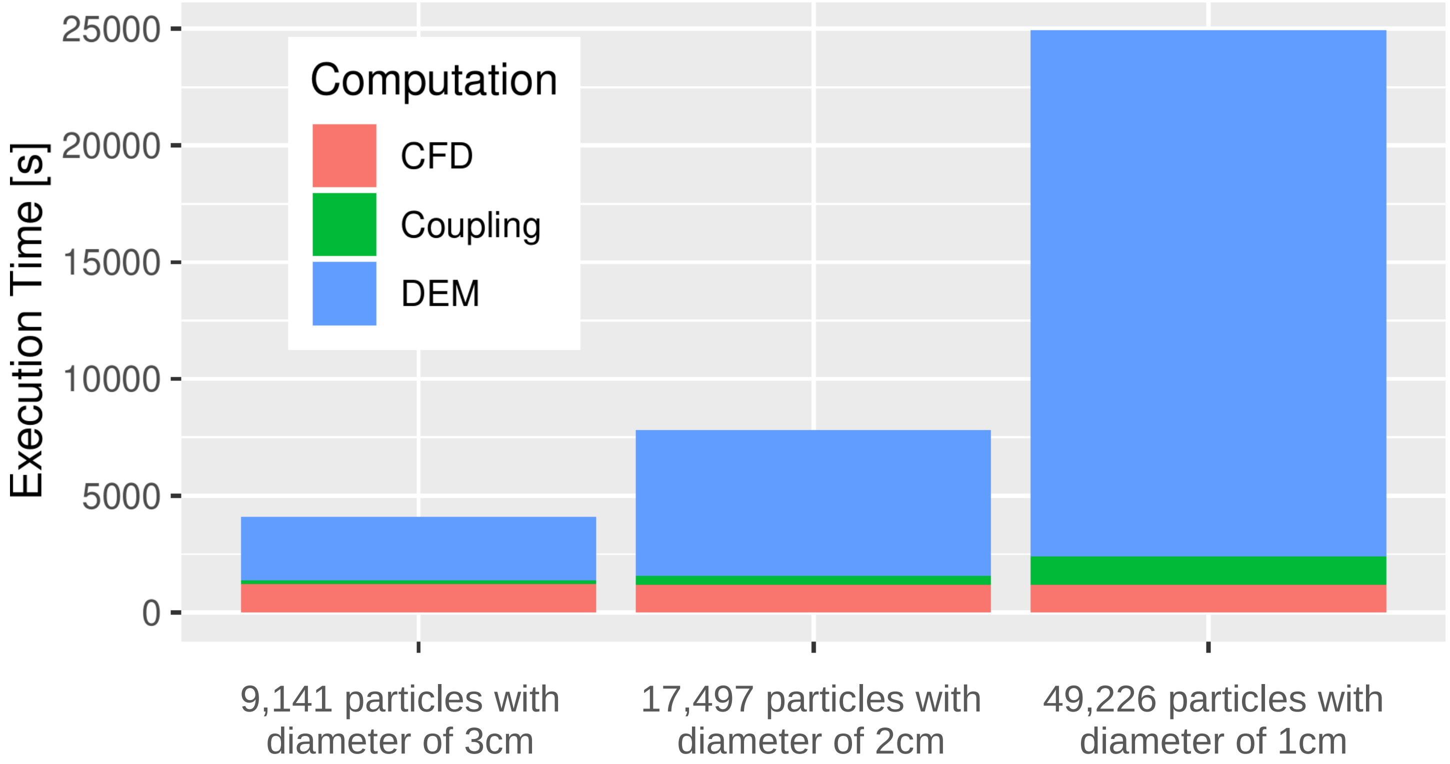
XDEM speedup of 16.8 with 28 threads

- 60% efficiency for 9k particles



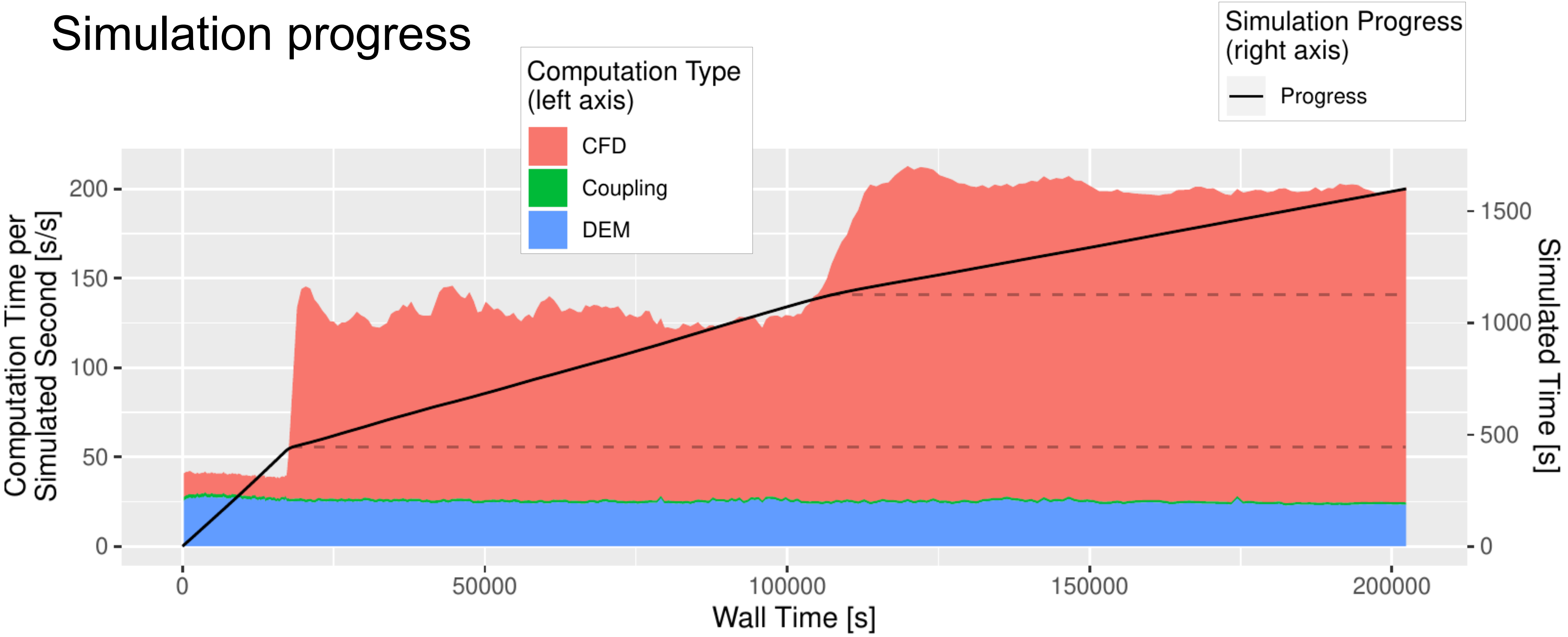
Influence of the number of particles

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



⇒ Workload between CFD and DEM changes with the furnace setup

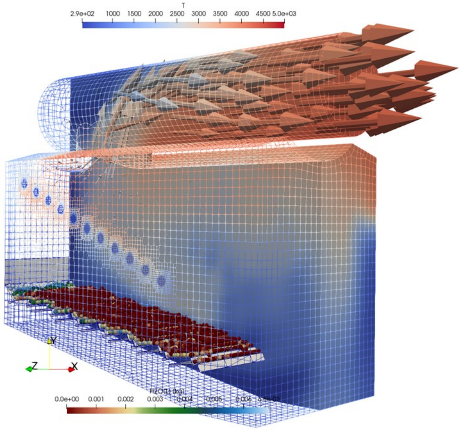
Simulation progress

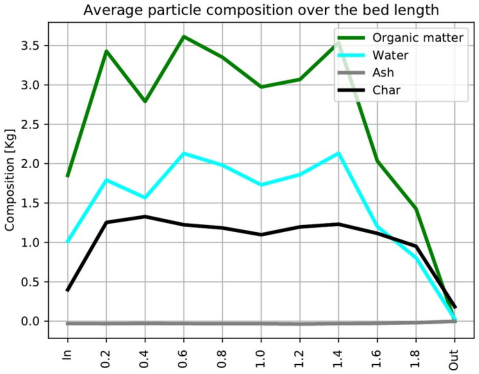


- At 445s of simulated time, lighting-up of the furnace
- Around 1125s, furnace reaches the steady state (all hot gases are burning)

⇒ Workload between CFD and DEM changes with the simulation progress

Cloud-based Workflow for Biomass Furnace Simulation





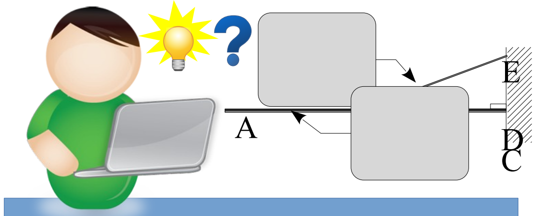
Part of CloudiFacturing initiative

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 workflow for SMEs

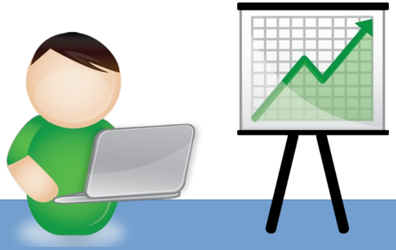
From the spreadsheet to the report



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

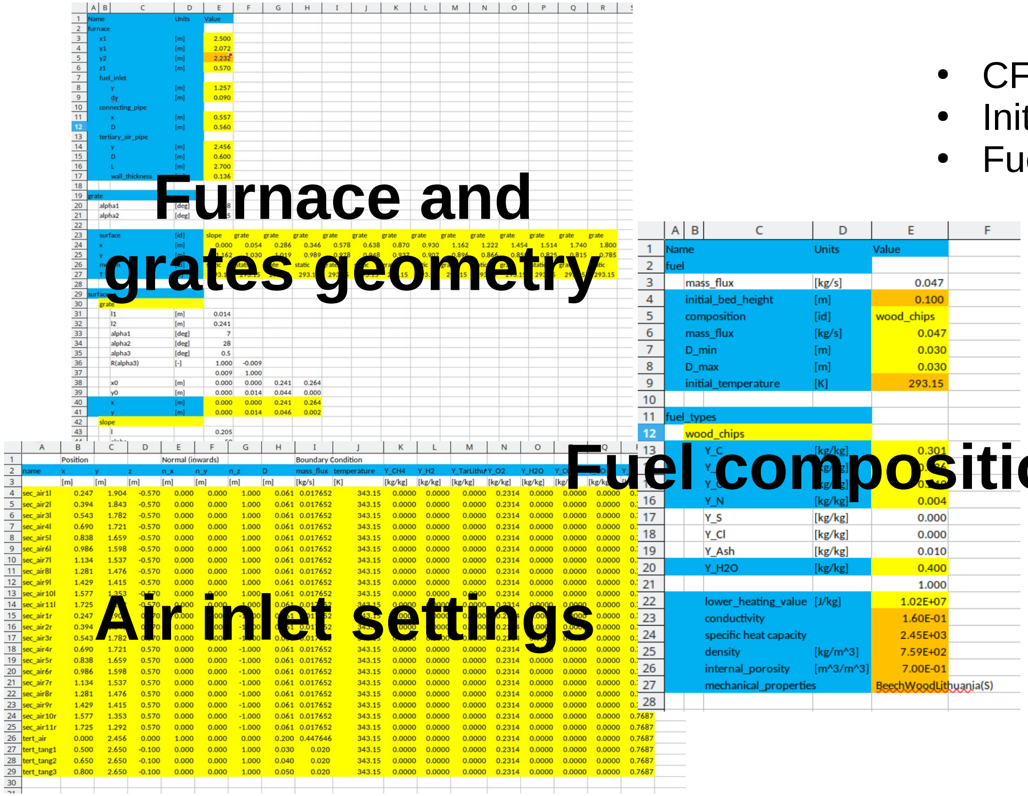
Submit Input File
- via the CloudiFacturing web portal

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

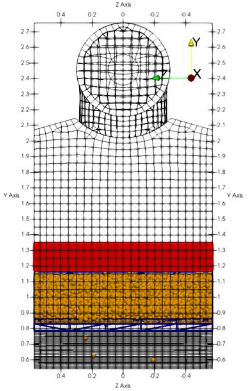
Spreadsheet Input File

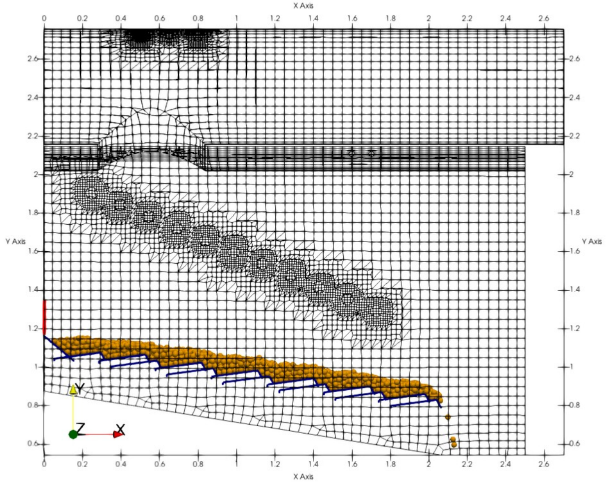


	Name	Units	Value
1	Name	Units	Value
2	fuel		
3	mass_flux	[kg/s]	0.047
4	initial_bed_height	[m]	0.100
5	composition	[id]	wood_chips
6	mass_flux	[kg/s]	0.047
7	D_min	[m]	0.030
8	D_max	[m]	0.030
9	initial_temperature	[K]	293.15
10			
11	fuel_types		
12	wood_chips		
13	Y_C	[kg/kg]	0.301
14	Y_[illegible]	[kg/kg]	[illegible]
15	Y_[illegible]	[kg/kg]	[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)

Automatic generation of the CFD+DEM case

- CFD mesh
- Initial particle bed
- Fuel characterization with ultimate analysis



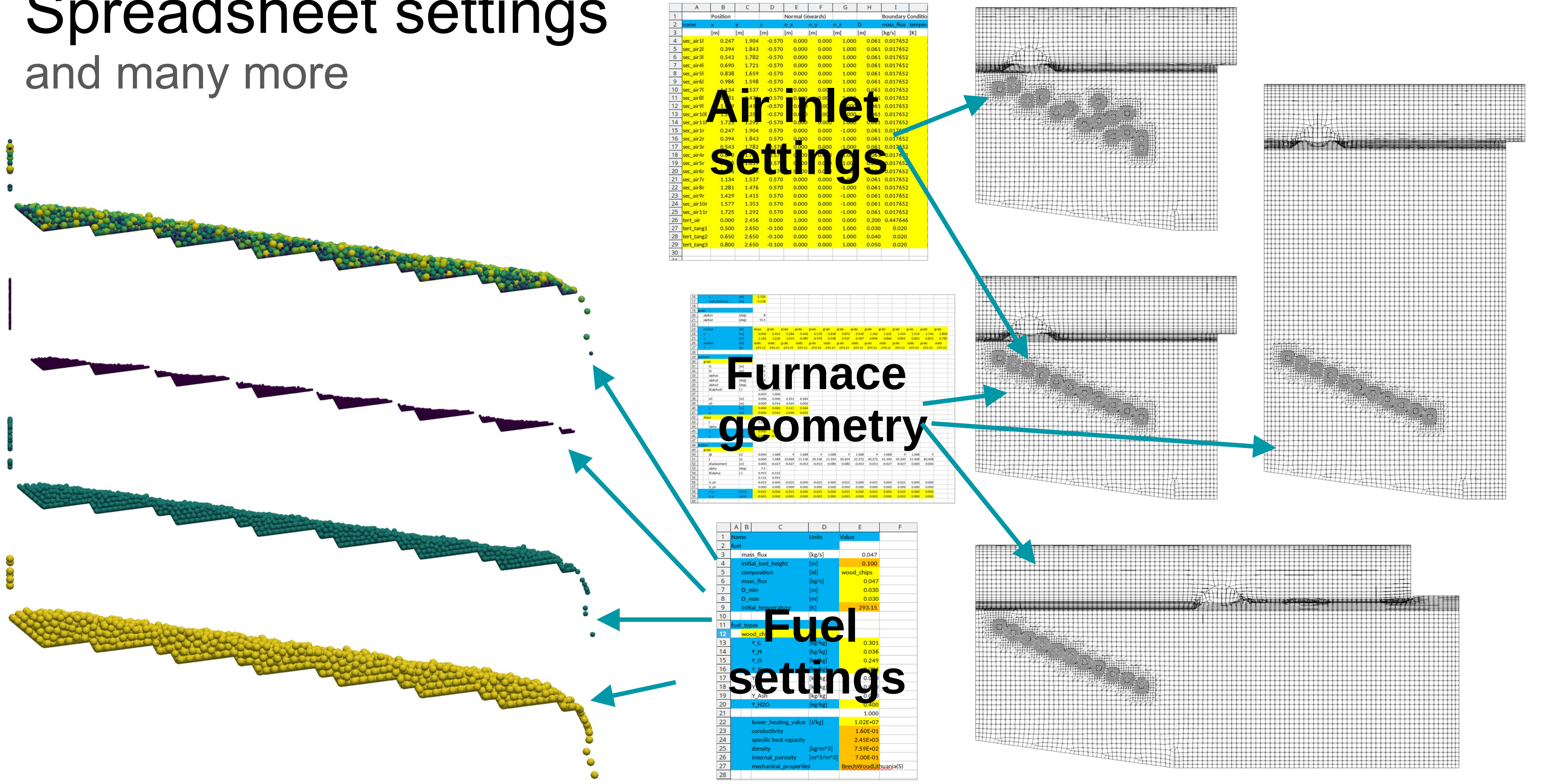


→ A few hundred degrees of freedom!

- Designing and implementing a web interface was out of scope

Spreadsheet settings

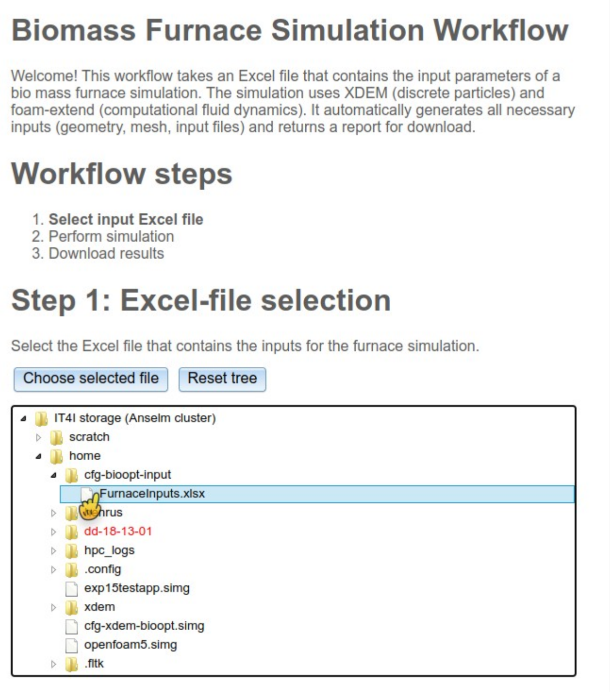
and many more



Job submission

via the CloudiFacturing / emGORA marketplace

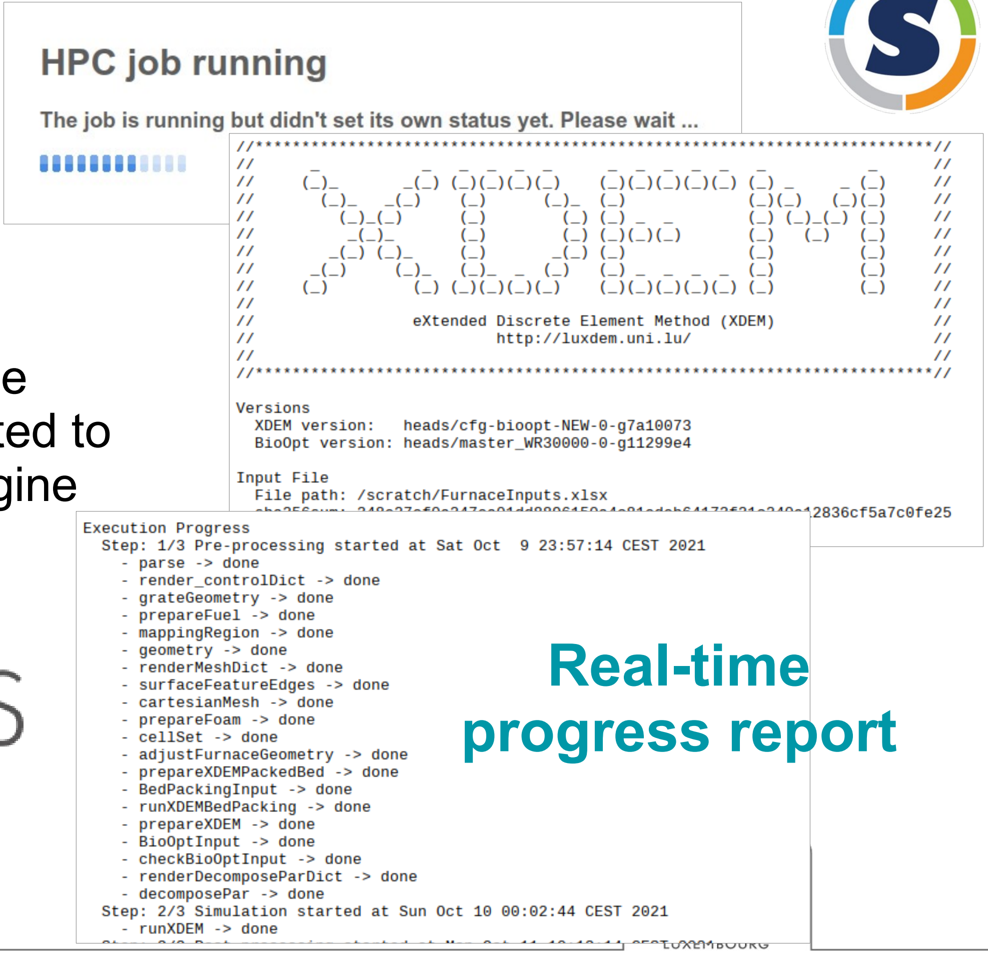
https://www.emgora.eu/



Execution of the workflow is delegated to the SemWES engine

HPC Simulation

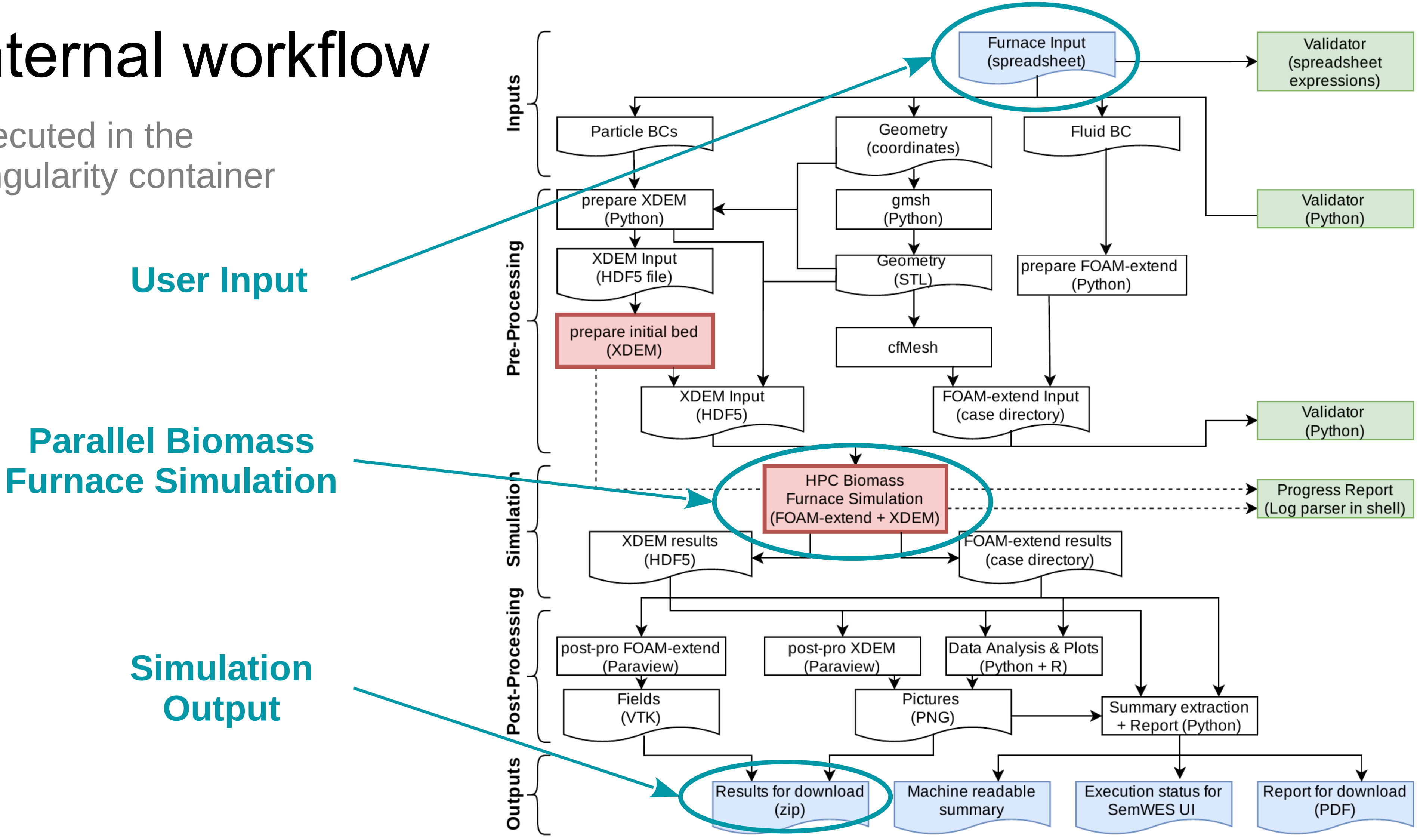
with Singularity on IT4T HPC cluster



Real-time progress report

Internal workflow

executed in the
Singularity container



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

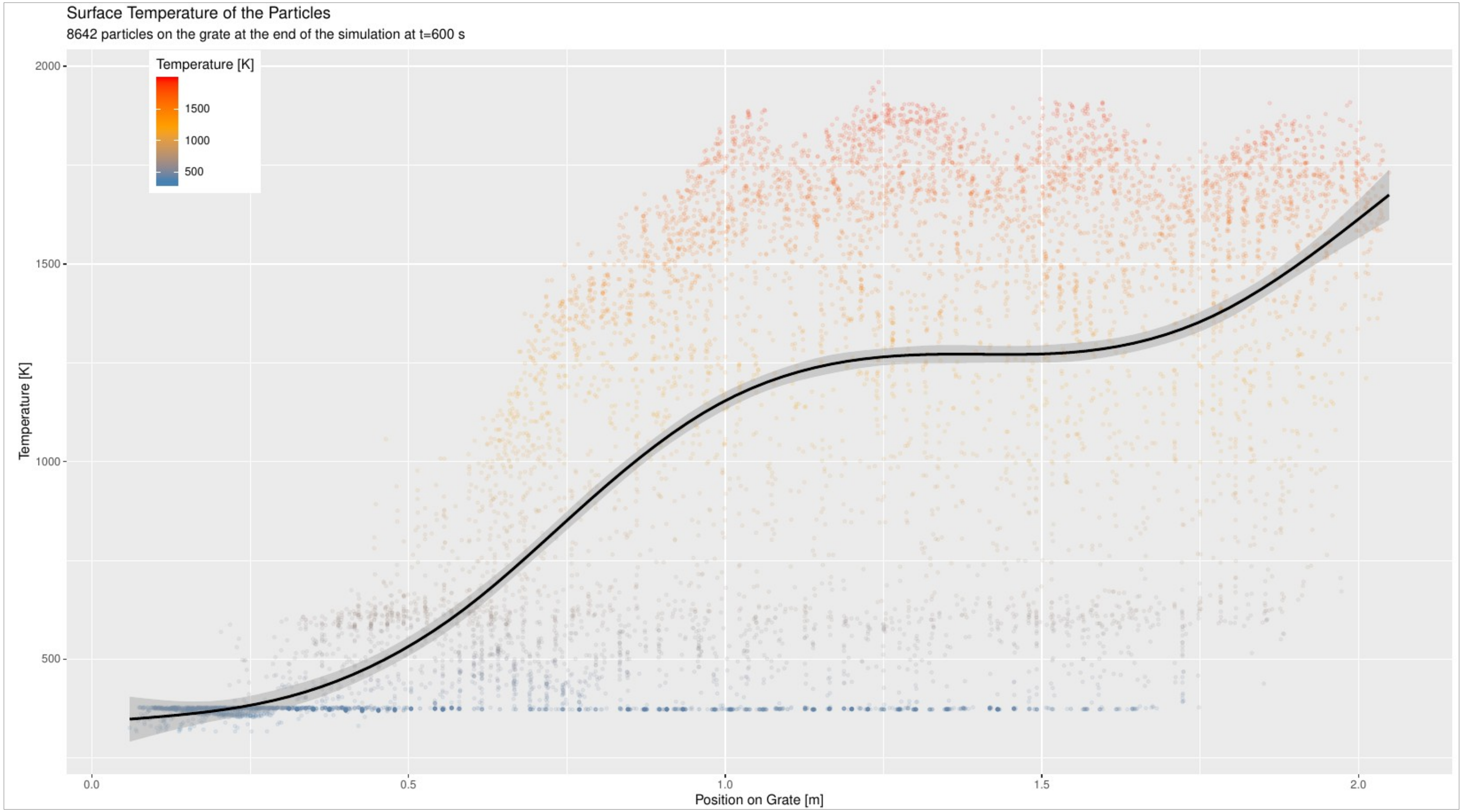
Extracts of the Simulation Reports

```
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
```

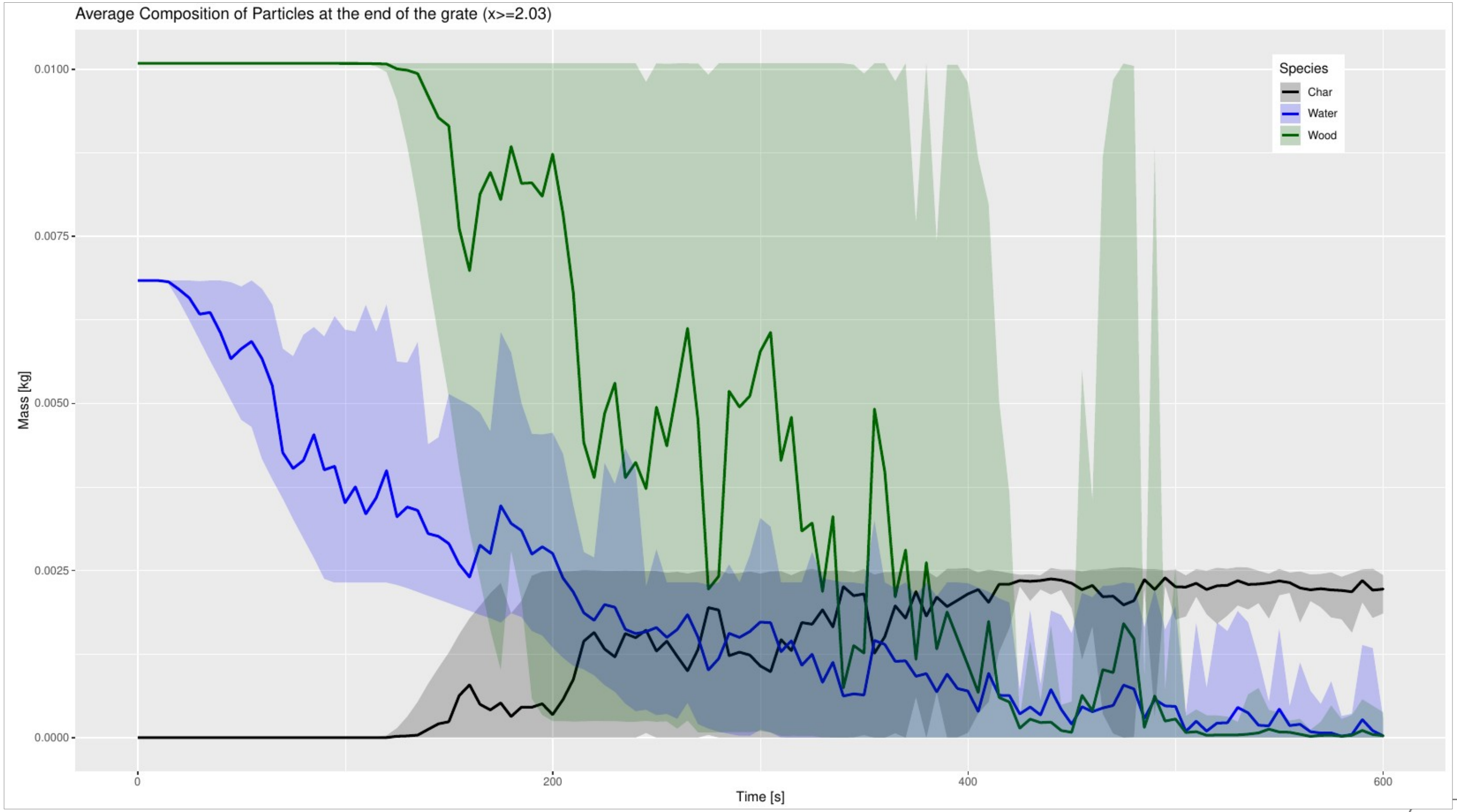
Average properties at exit of the exhaust pipe

Extracts of the Simulation Reports



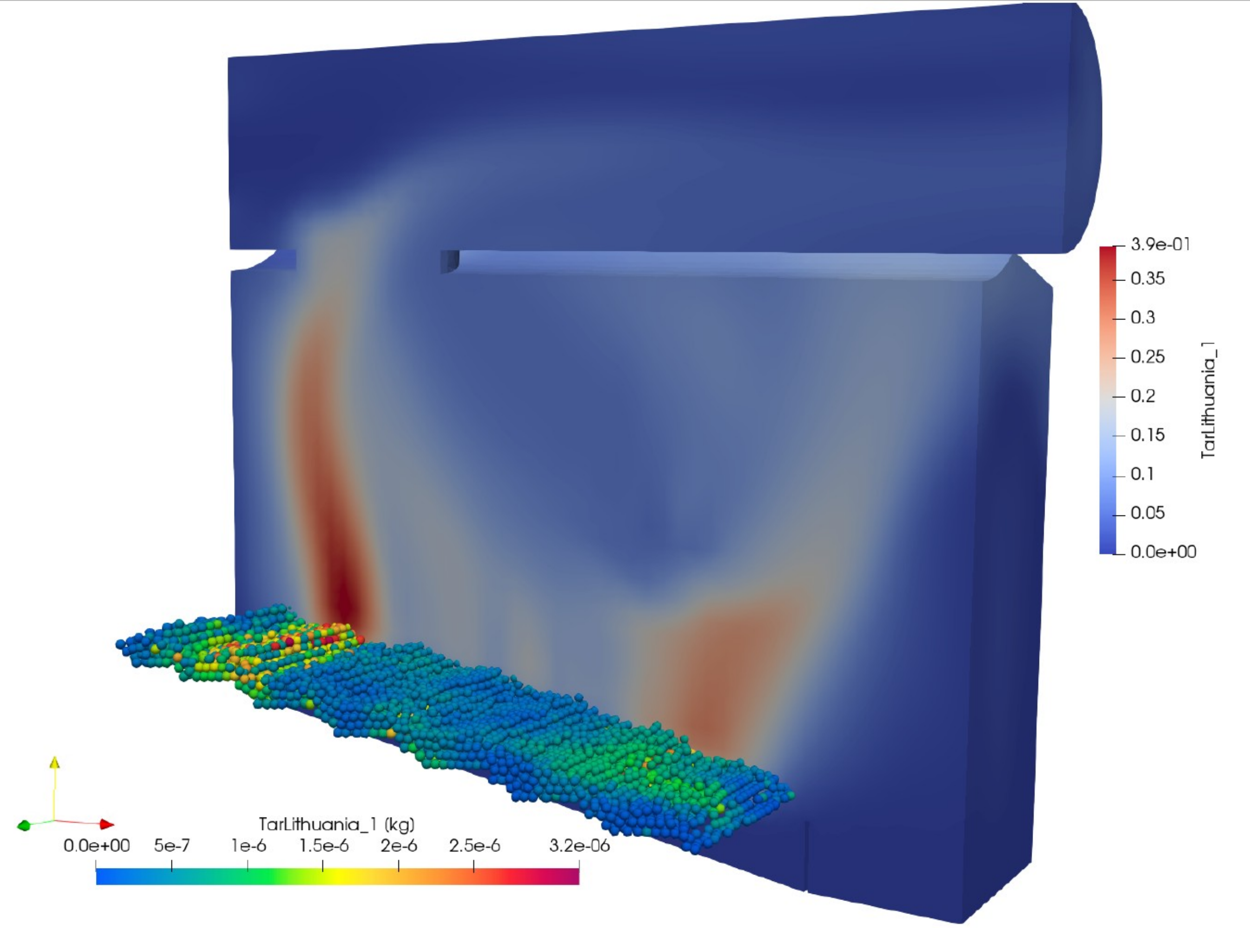
Surface temperature of the particles along the grate

Extracts of the Simulation Reports



Evolution of particle composition at the exit of the grate

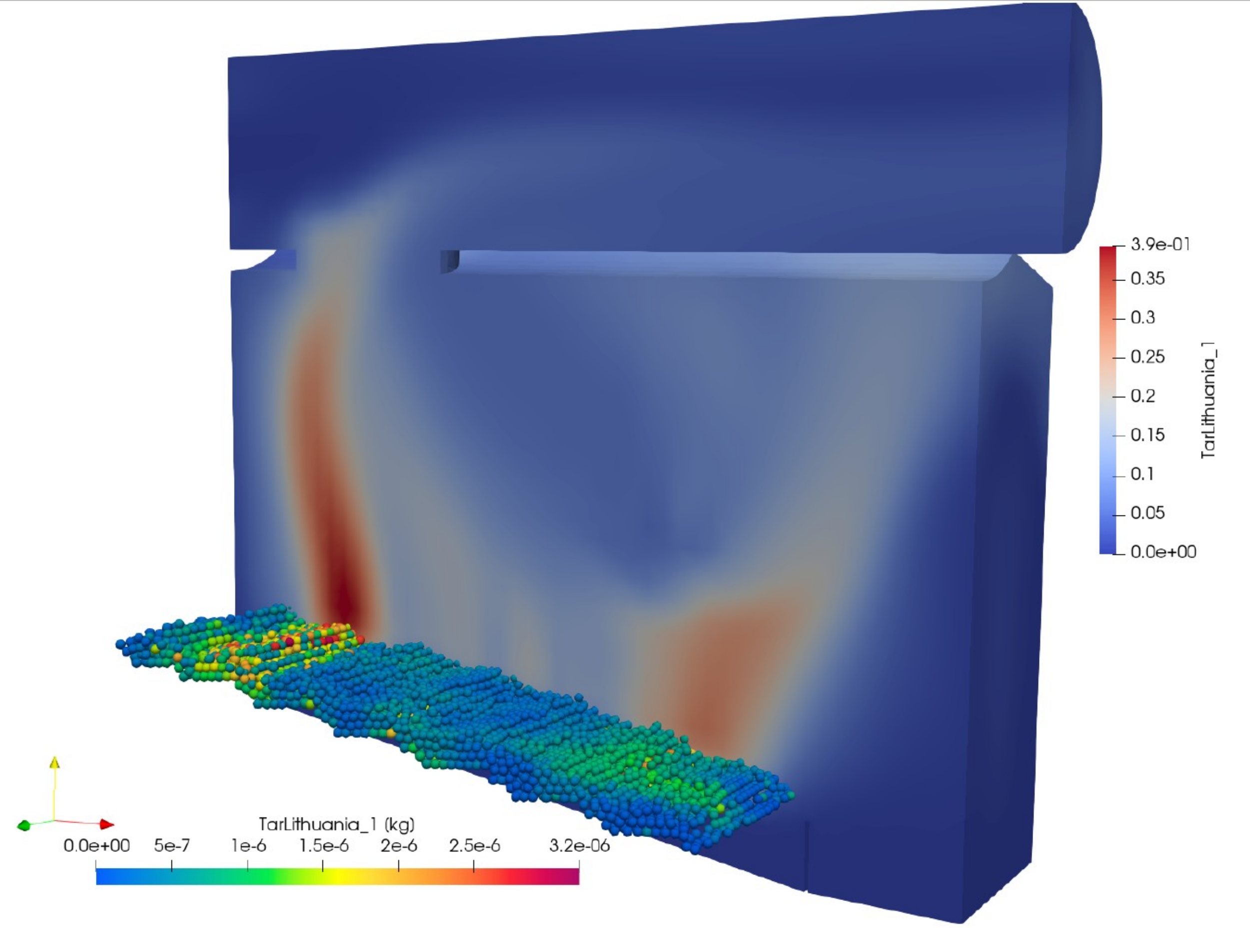
Extracts of the Simulation Reports



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.

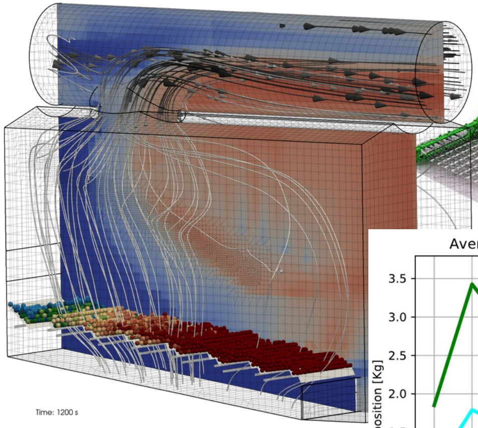
Summary: Biomass Furnace Simulation as a Service

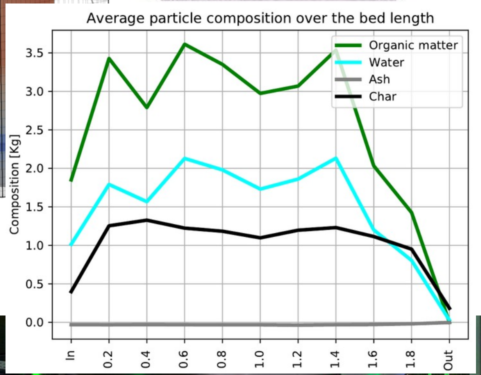
Multi-Physics Biomass Furnace Simulation
- Two-way ‘in-memory’ coupling CFD ↔ DEM
- Hybrid parallelization scheme: MPI + OpenMP

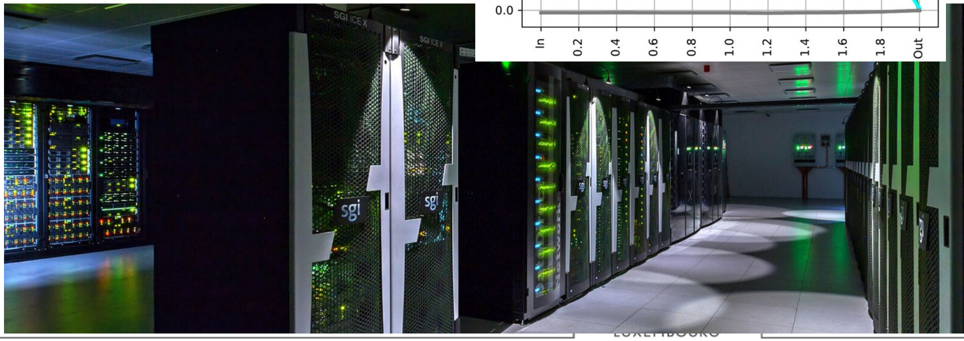
Cloud-based interface and submission portal
- Portable execution using Singularity
- HPC Job submission using SemWES
- Execution on IT4Innovations HPC platform

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

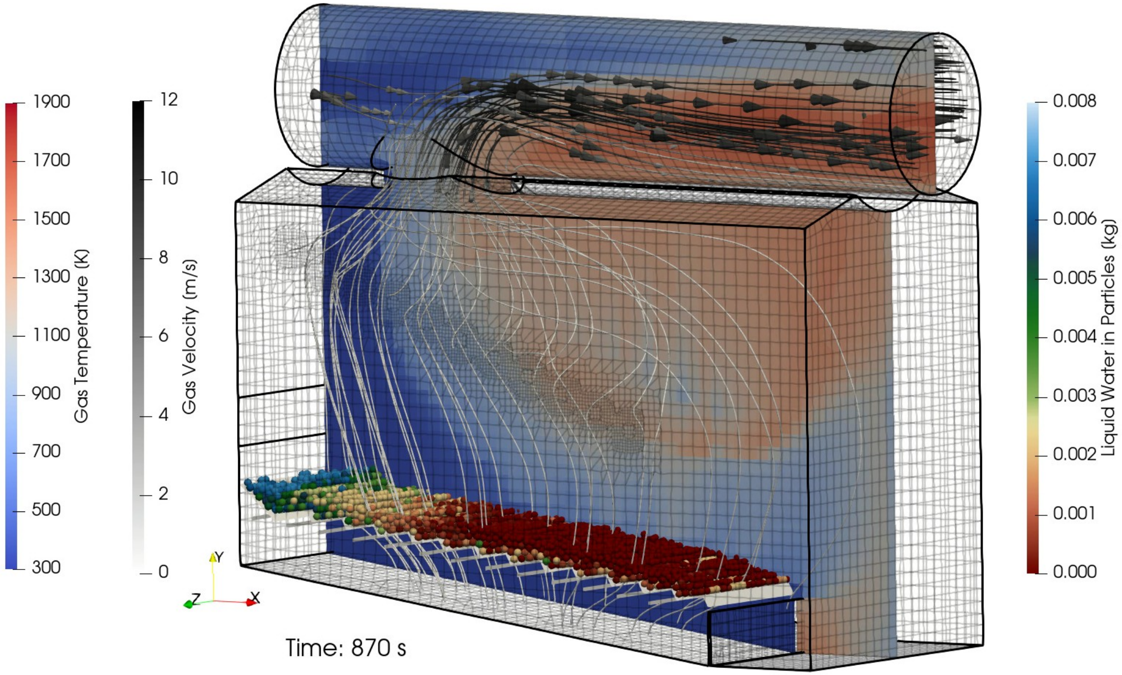
- Application portability issues with Singularity
- Lack of flexibility of the workflow with SemWES
- Numerous configuration options
  - Specifications given by industrial partner
  - Verification of user input is hard but necessary
  - Need robust code, regular checks, an clear error messages
  - Best 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

Thank you for your attention!

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



Acknowledgements

The EU initiative to digitalise the manufacturing industry

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