# HPC Multi-physics Biomass Furnace simulations as a Service


Xavier Besseron[1]
Henrik Rusche[2], Bernhard Peters[1], Alban Rousset[1]
Ralfas Lukoševičius[3], Linas Paukštaitis[3], Laimonas Narbutas[3]

1: University of Luxembourg
2: Wikki GmbH, Germany
3: Enerstena UAB, Lithuania


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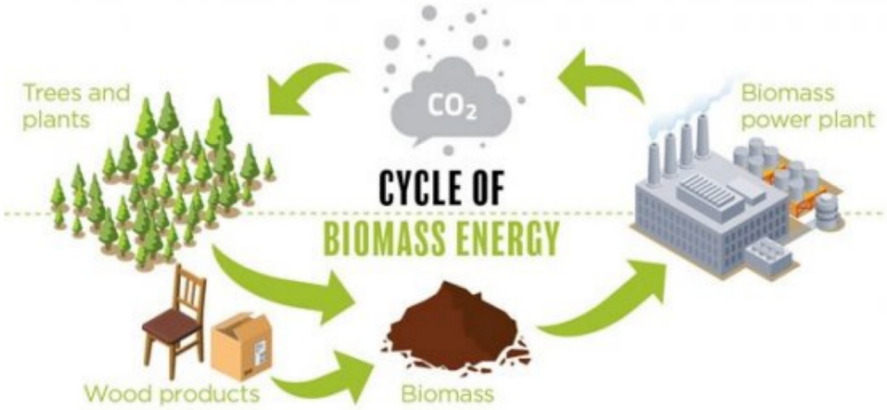
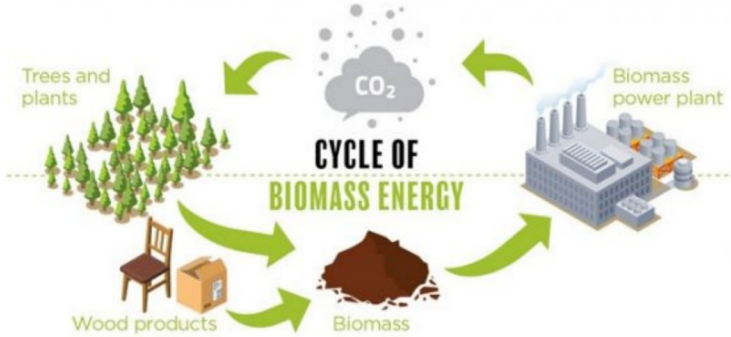
# Challenges in the simulation of biomass combustion



# Introduction




## Biomass combustion (e.g. wood chips)

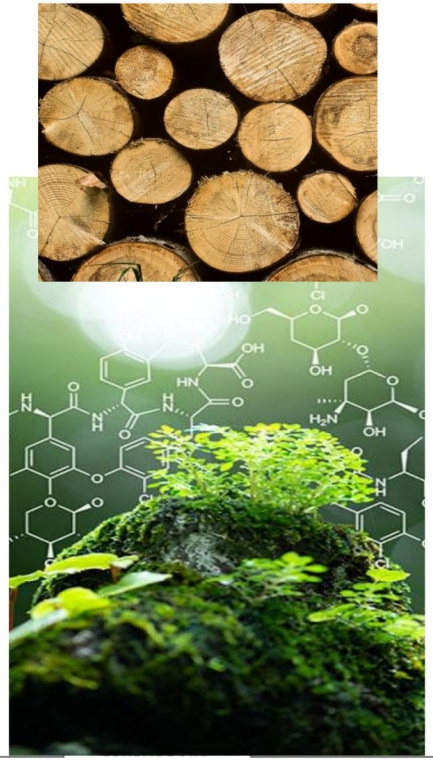
- widely used for generating electric and thermal energy
- renewable and potentially carbon-neutral energy source

## 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.

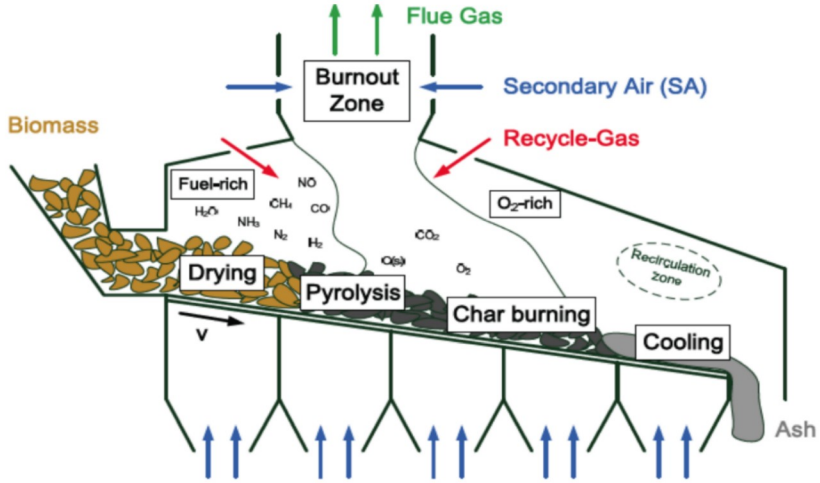


# Combustion process in a biomass furnace

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




# Numerical Approach: **Multi-Physics Simulation**

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

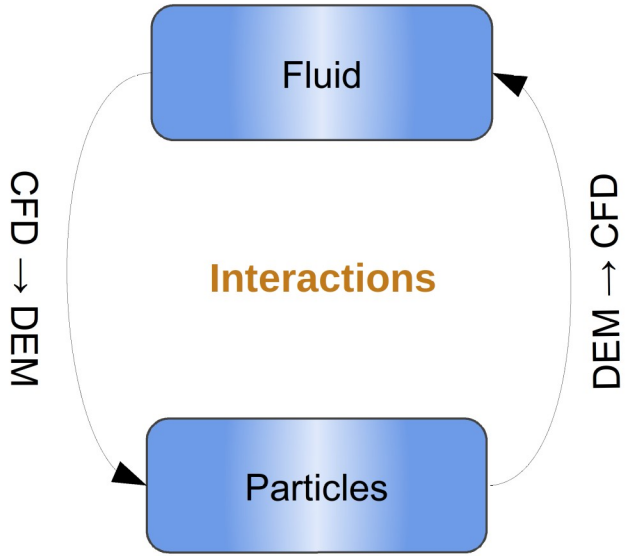
**XDEM** (Lagrangian) for:

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

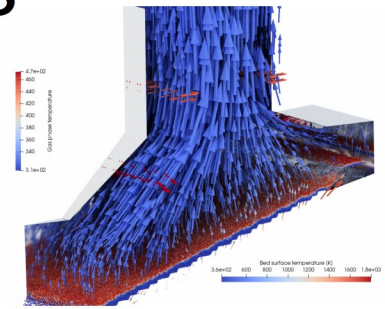
**OpenFOAM** (Eulerian) for:

- 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.



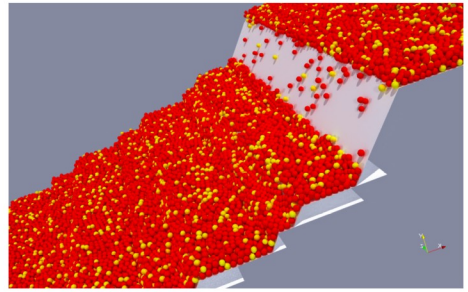
# Complexity of biomass furnace simulations



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

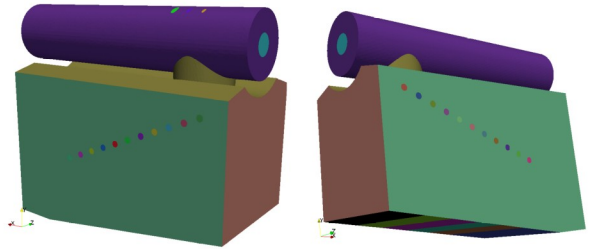
The necessary steps include:

- 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.



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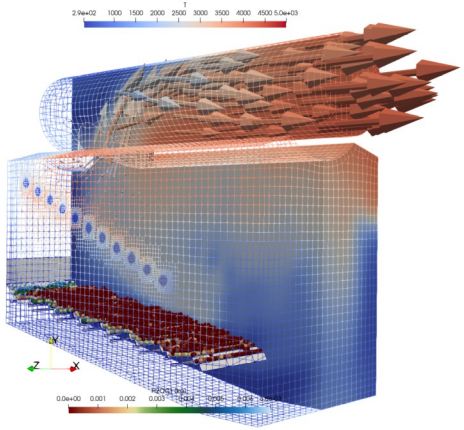
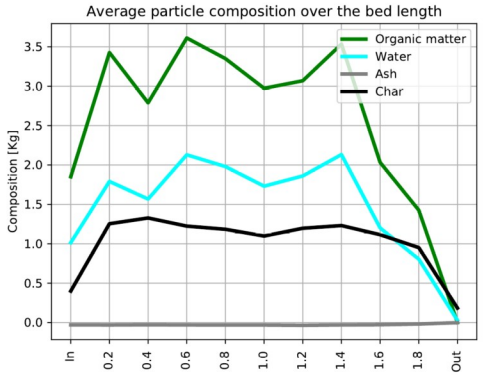
# HPC Multi-physics Biomass Furnace simulations as a Service

a simplified workflow for end user



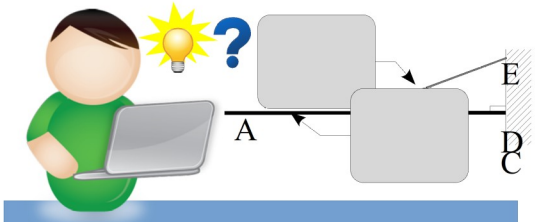


# CloudiFacturing Overview


- The CloudiFacturing solution is designed to support manufacturing SMEs and their needs for advanced cloud- or HPC-based ICT solutions.
- The CloudiFacturing solution will be open, empowering different stakeholders to become members of the community.
- All the services offered in the CloudiFacturing Solution will be 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

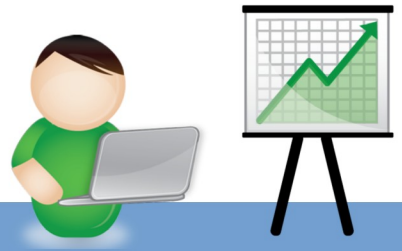
- define the geometry and the settings of the furnace
- based on a Spreadsheet

### Submit Input File

- via the CloudiFacturing web portal

### Run the Simulation

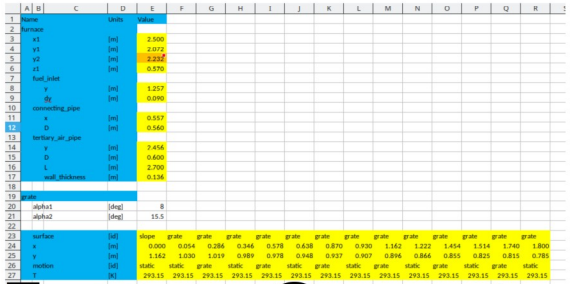
- on the HPC platform
- no interaction needed from the user



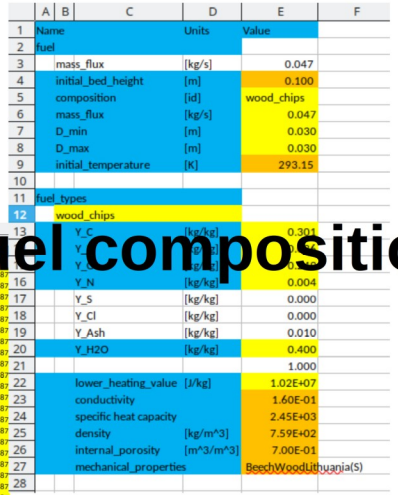
### Visualize the results

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

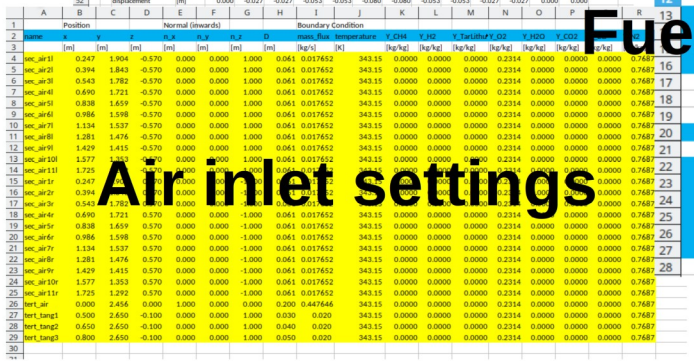
# Spreadsheet Input File



**Furnace Geometry**

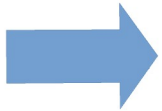


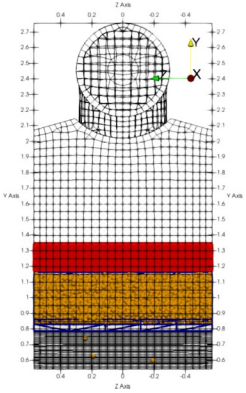
**Fuel composition**

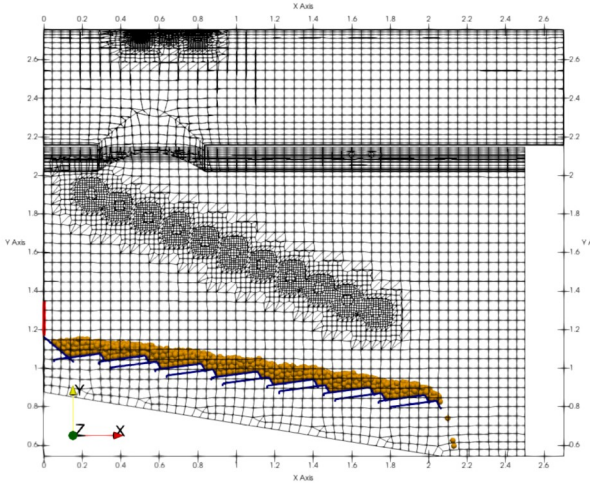


**Air inlet settings**

**Automatic generation of the CFD+DEM case**







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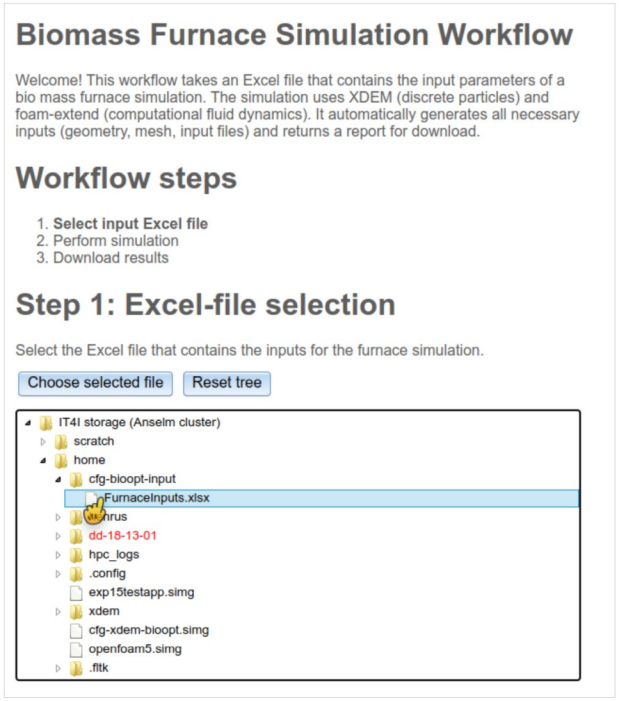
# Job submission

# HPC Simulation




Submission Web Portal


```
.  decomposePar
.  runXDEM
//*************************************************************************//
//                                                                         //
//                  DISCRETE PARTICLE METHOD (DPM)                         //
//                                                                         //
//*************************************************************************//
// XDEM Git Branch: master
// XDEM Git Hash: 673313e1b00bbf5dfbaf2f485706dd2a75abfb66
// XDEM Git Description: heads/master-0-g673313e
//*************************************************************************//

------------- 1.1)  I N I T I A L I Z I N G :            ----------

     DPM Input File : biomass_furnace_3D.h5
 DPM Input Directory : ./
DPM Output Directory : ./output_biomass_furnace_3D/
```

```
DILUPBiCG:  Solving for hs, Initial residual = 0.018986329, Final residual = 4.769367e-06, No Iterations 7
ExecutionTime = 422.58 s  ClockTime = 138 s

Step   1200      - t =      0.235400 s      - Elapsed Time =    0.04398 s/step      - Percentage completed =  11.77 %
Courant Number mean: 0.12451675 max: 228.82797
Time = 0.25
```

Progress Report

# Simulation Results

SemWES

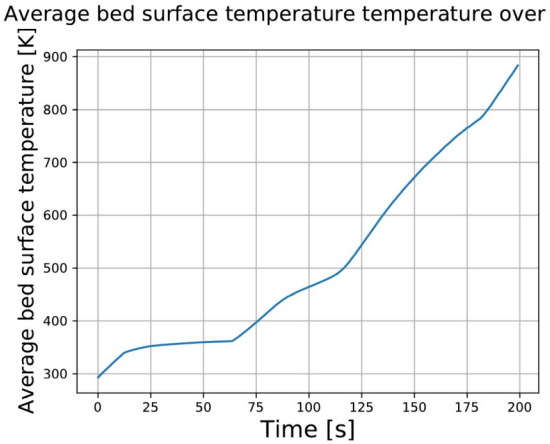
**This workflow has finished**

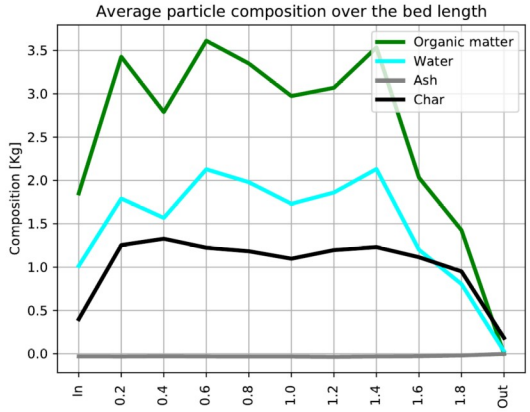
The execution of this workflow is done. You may now inspect the results.

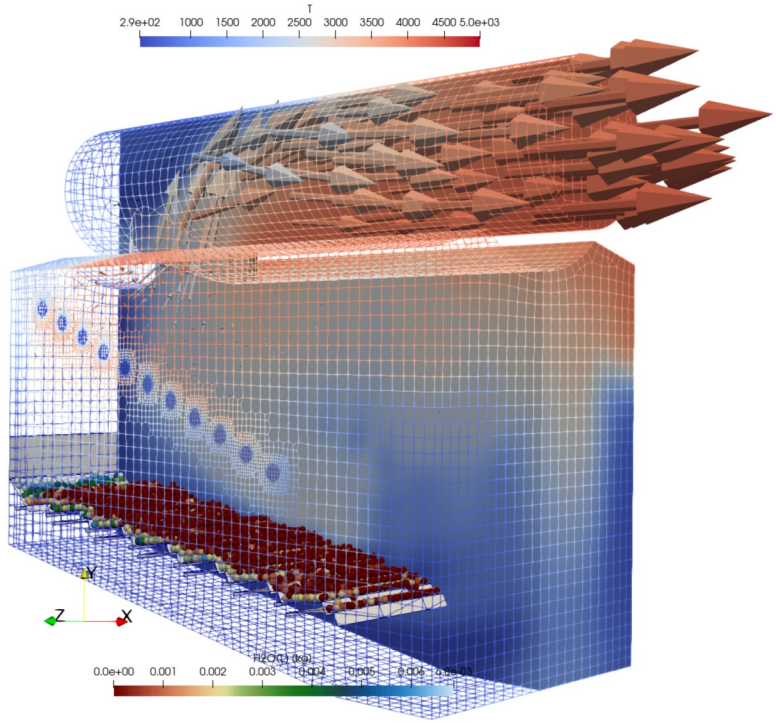
**Results**

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

Download link




Report

# 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

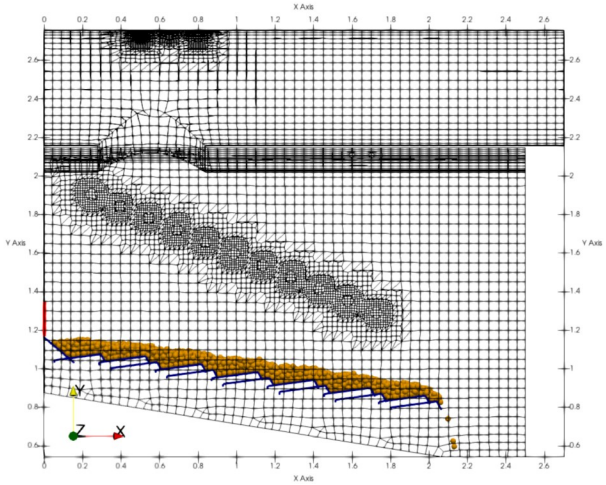
- characterised by ultimate analysis
- thermo-physical values obtained from standard experiments

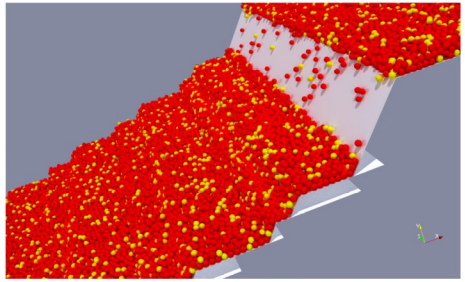
## Air inlets

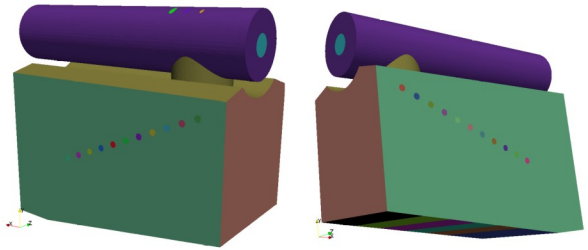
- can be placed at any position
- require the full composition when recirculation is used

**→ A few hundred degrees of freedom!**

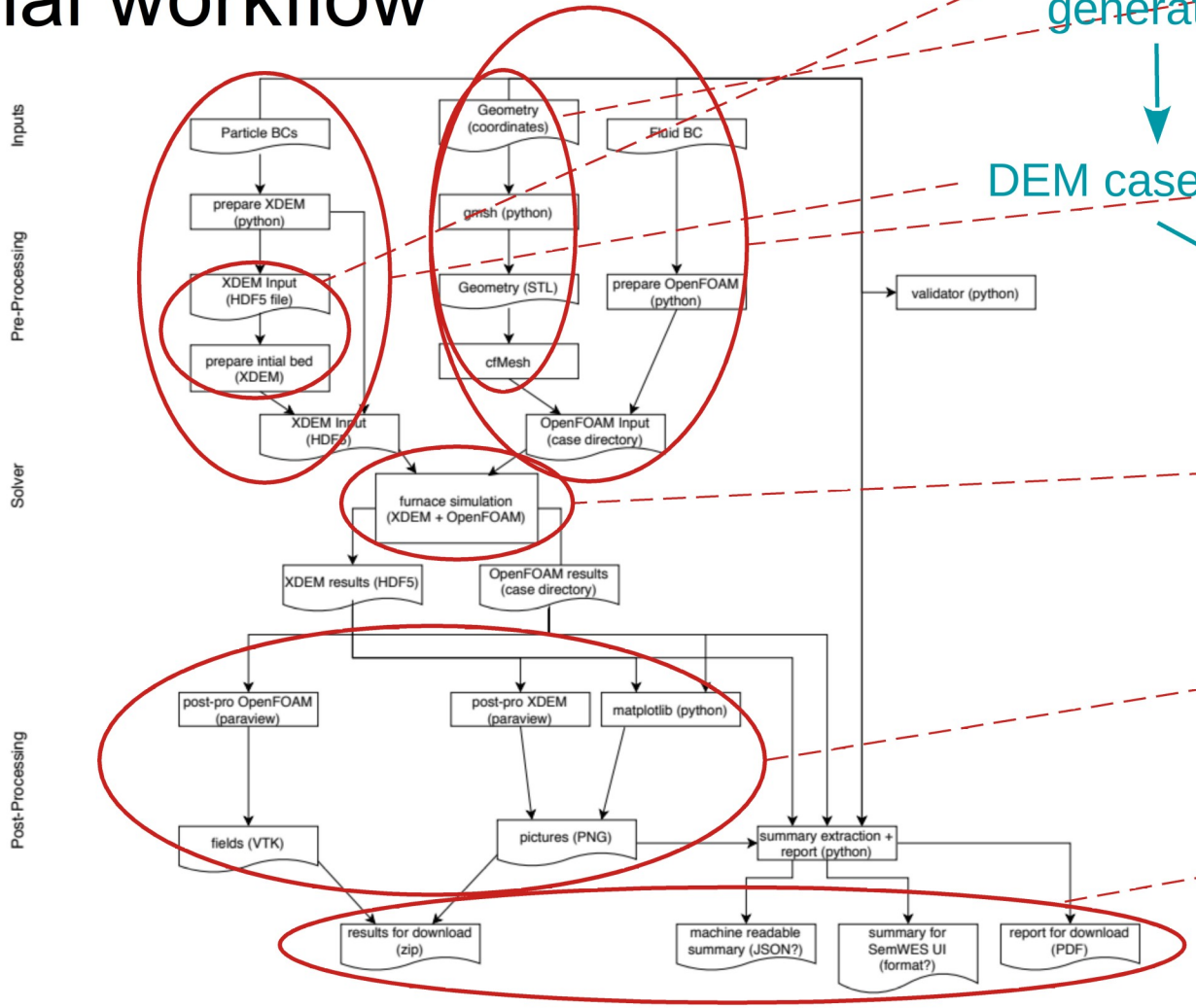
- Designing and implementing a web interface was out of scope







# Internal workflow




Particle bed generation

Mesh generation

DEM case setup

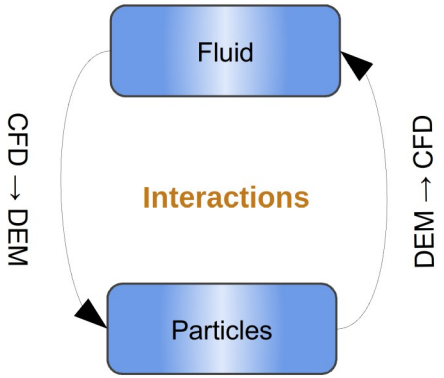
CFD case setup

**HPC Furnace Simulation**

Post-processing

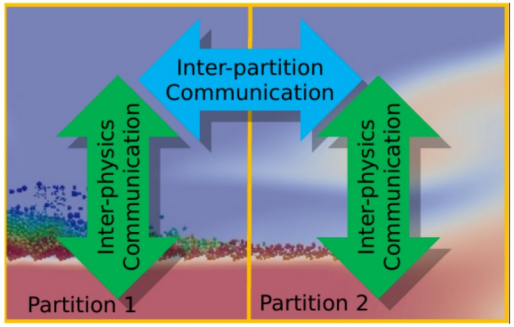
Report

# HPC Biomass Furnace Simulation




## Two-way Direct Coupling

- DEM → CFD and CFD → DEM
- XDEM and OpenFOAM linked into one executable
- All coupling data exchange via shared memory



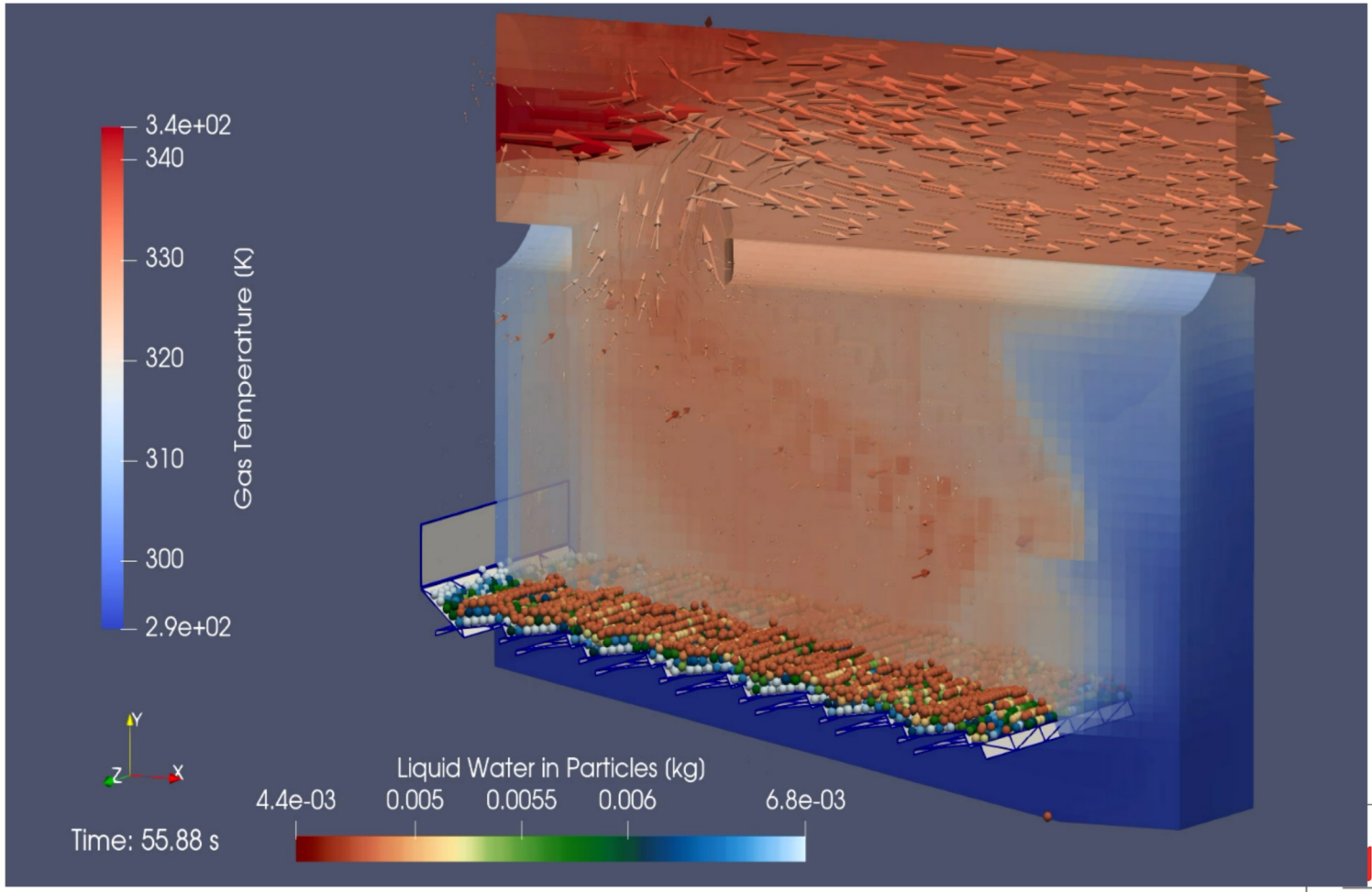

## Hybrid Parallelization Scheme

- OpenFOAM running in parallel using **MPI**
- XDEM parallelized using **OpenMP**

## HPC Execution

- Portable execution using Singularity
- HPC Job submission using SemWES
- Execution on IT4Innovations HPC platform

# Biomass Furnace simulation using XDEM+OpenFOAM



# Summary and Future Work

## Multi-Physics Biomass Furnace Simulation

- Cloud-based interface and submission portal
- HPC execution back-end

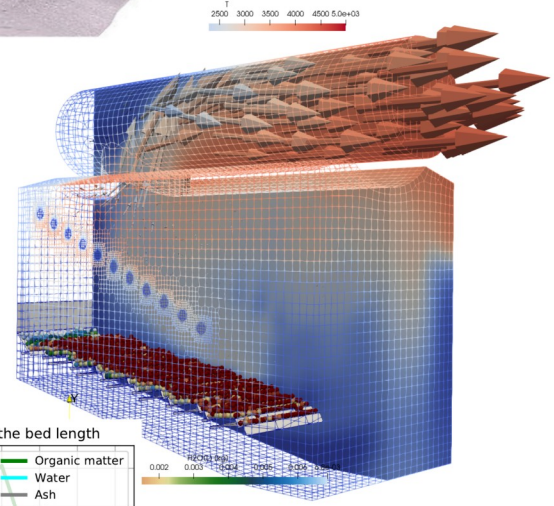
→ **Application as a Service (AaaS)**

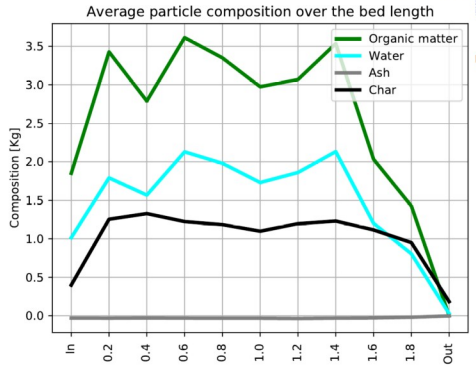
## Simplified Workflow for end user

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

## Part of the CloudiFacturing project

- Experiment 15 BioOpt
- To be integrated in the Digital Marketplace
- Target audience: SMEs





# Thank you for your attention!

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

Contact: xavier.besseron@uni.lu

More details about the CloudiFacturing BioOpt Experiment:
http://luxdem.uni.lu/projects/2020-CloudiFacturing_BioOpt/

# Acknowledgement

The project CloudiFacturing receives funding from the European Union's Horizon2020 research and innovation programme (Grant No. 768892).