

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

Xavier Besson¹, Henrik Rusche², Bernhard Peters¹

1: University of Luxembourg



2: Wikki GmbH, Germany



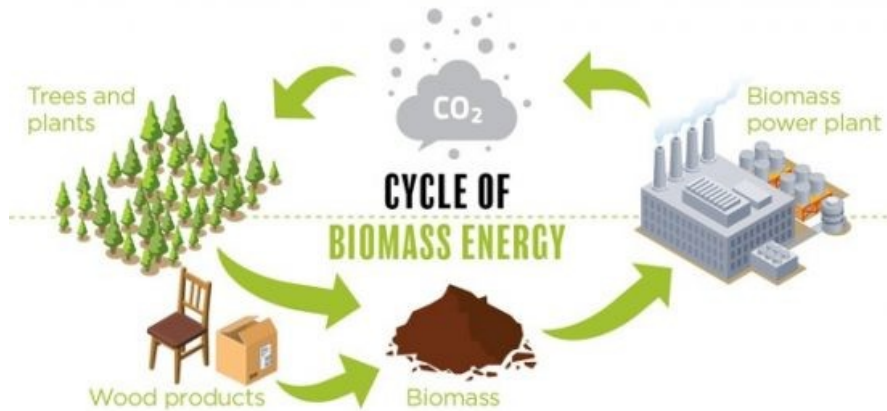
In collaboration with



PEARC'22
Practice and Experience in
Advanced Research Computing
July 10-14, 2022, Boston, MA, USA



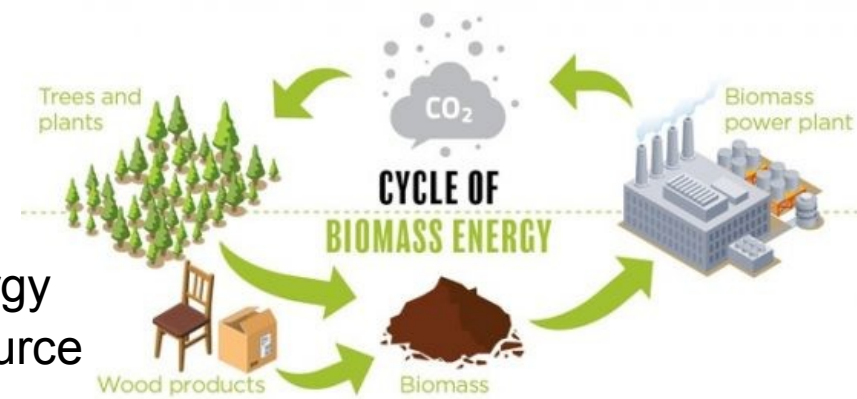
Introduction to Biomass Combustion



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

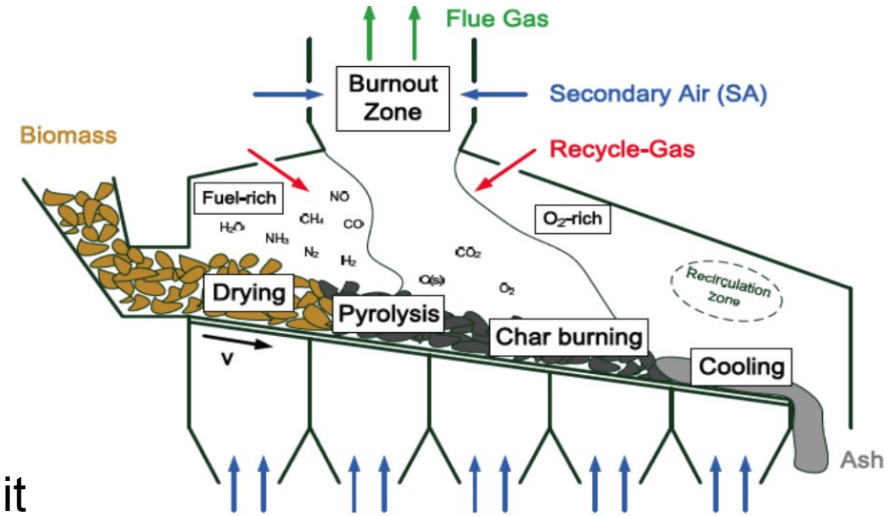
- forward acting grate
- transports the fuel through the furnace

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



[Paces and Kozek, 2011]



Research & Work Objectives

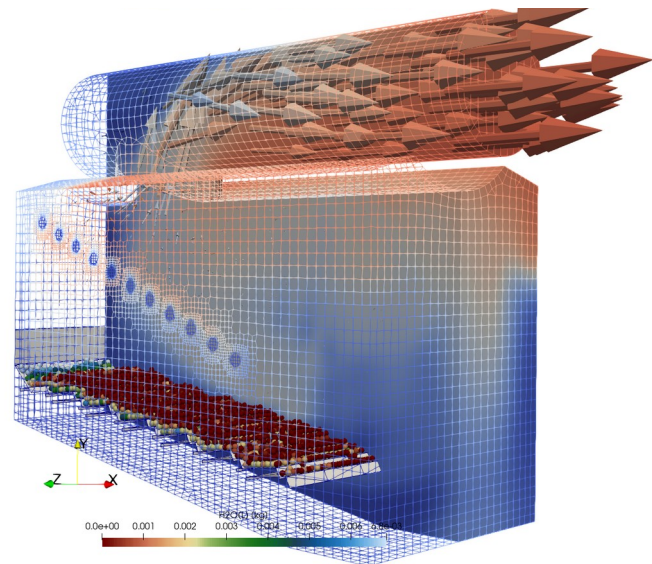
Multi-Physics Simulation of a Biomass Furnace

- Fluid phase with Computational 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)

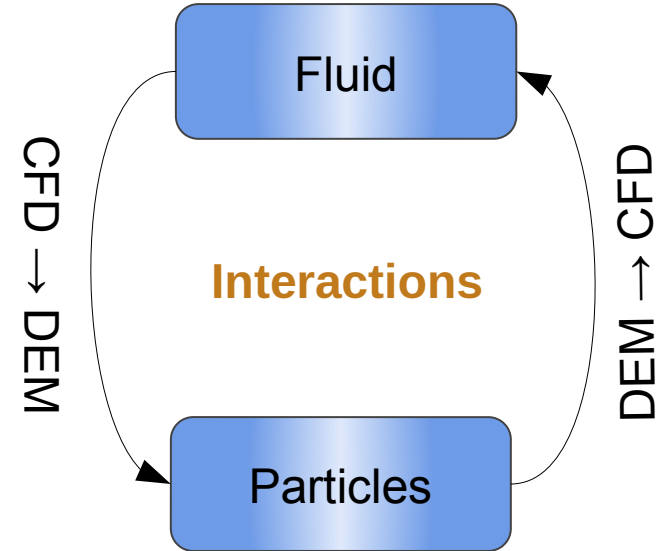
XDEM (Lagrangian) for:

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

OpenFOAM (Eulerian) for:

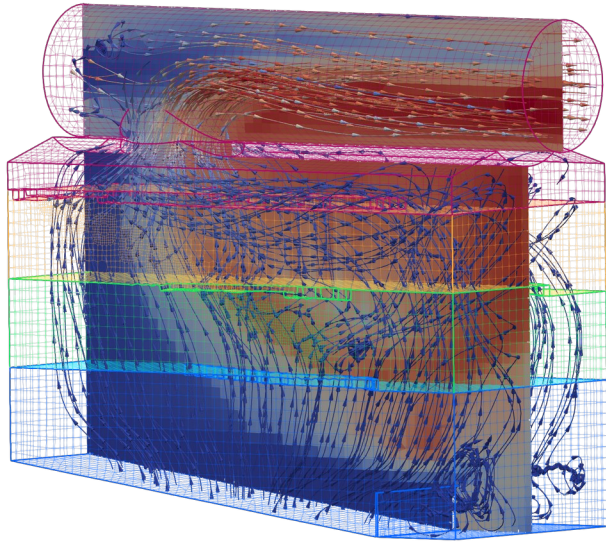
- Flow of gas phase
- Reactions in the gas phase

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

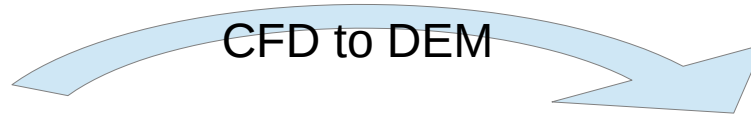


Volume Coupling for Biomass Furnace Simulation

Momentum, Heat and Mass transfer

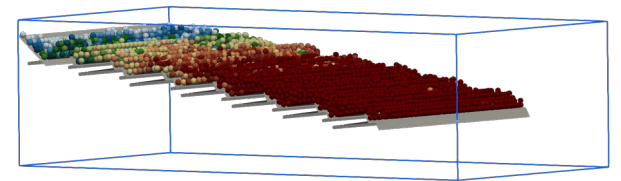


Fluid phase in OpenFOAM

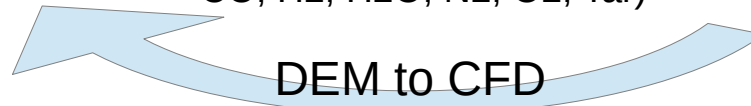


- Fluid *velocity*, density, dynamic viscosity
- *Pressure gradient*
- Temperature
- Thermal conductivity
- Specific heat
- Diffusivity
- Species mass fraction (CH₄, CO₂, CO, H₂, H₂O, N₂, O₂, Tar)

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



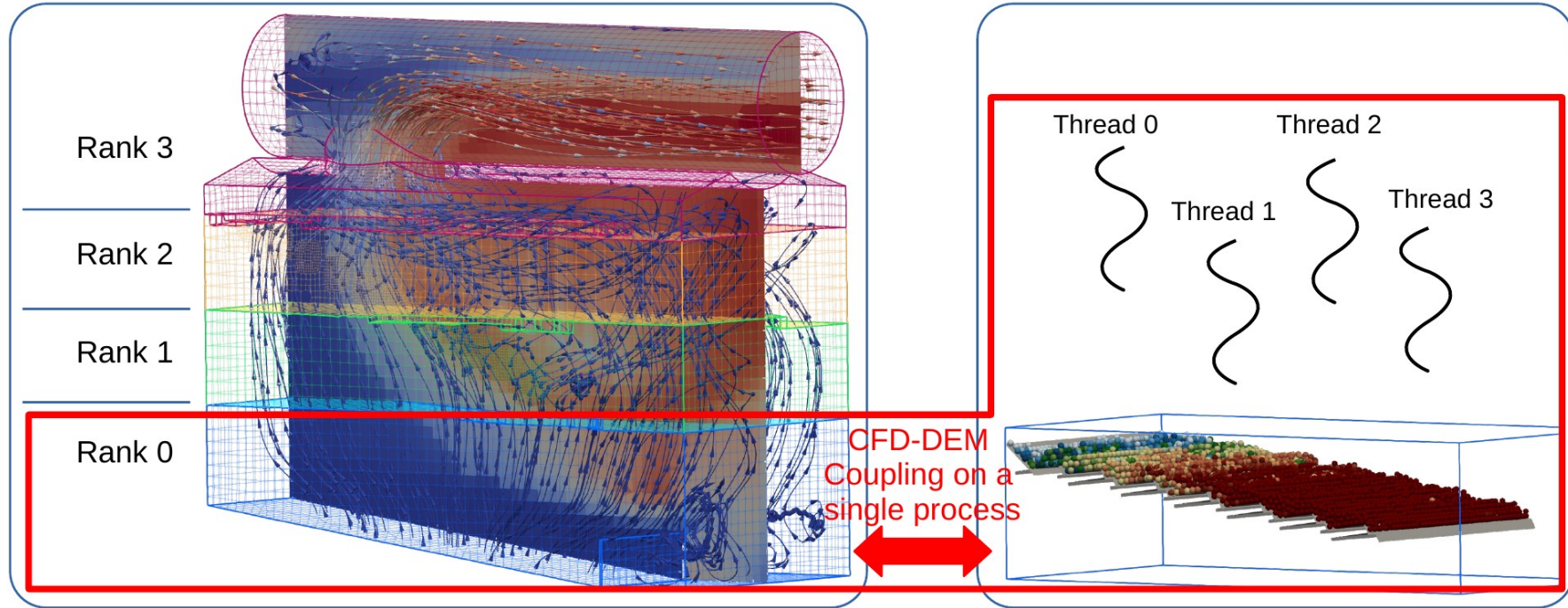
Particles in XDEM



Parallelization approach for Biomass Furnace Simulation

OpenFOAM parallelized with MPI

XDEM parallelized with OpenMP



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

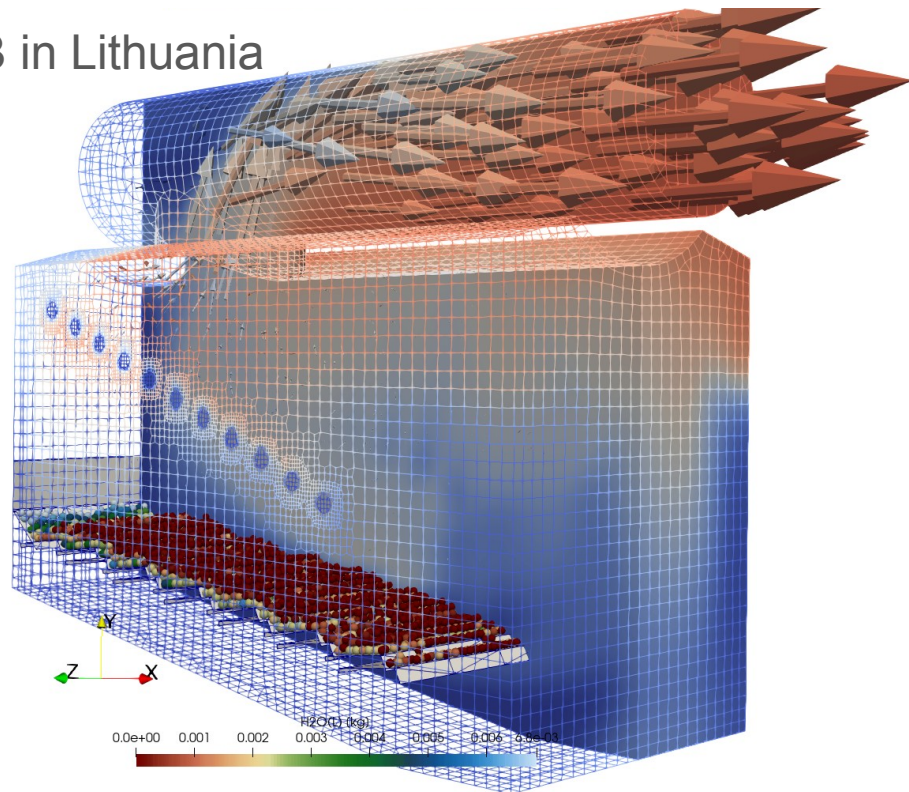
- Dimensions of 2.51m × 1.14m × 2.07m (L × W × H)
- Top exhaust pipe of 0.6m diameter
- 6 primary air inlets from the bottom
- 11 secondary air inlets on each side
- 1 tertiary air inlet on the exhaust pipe

Grates

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

Fuel bed

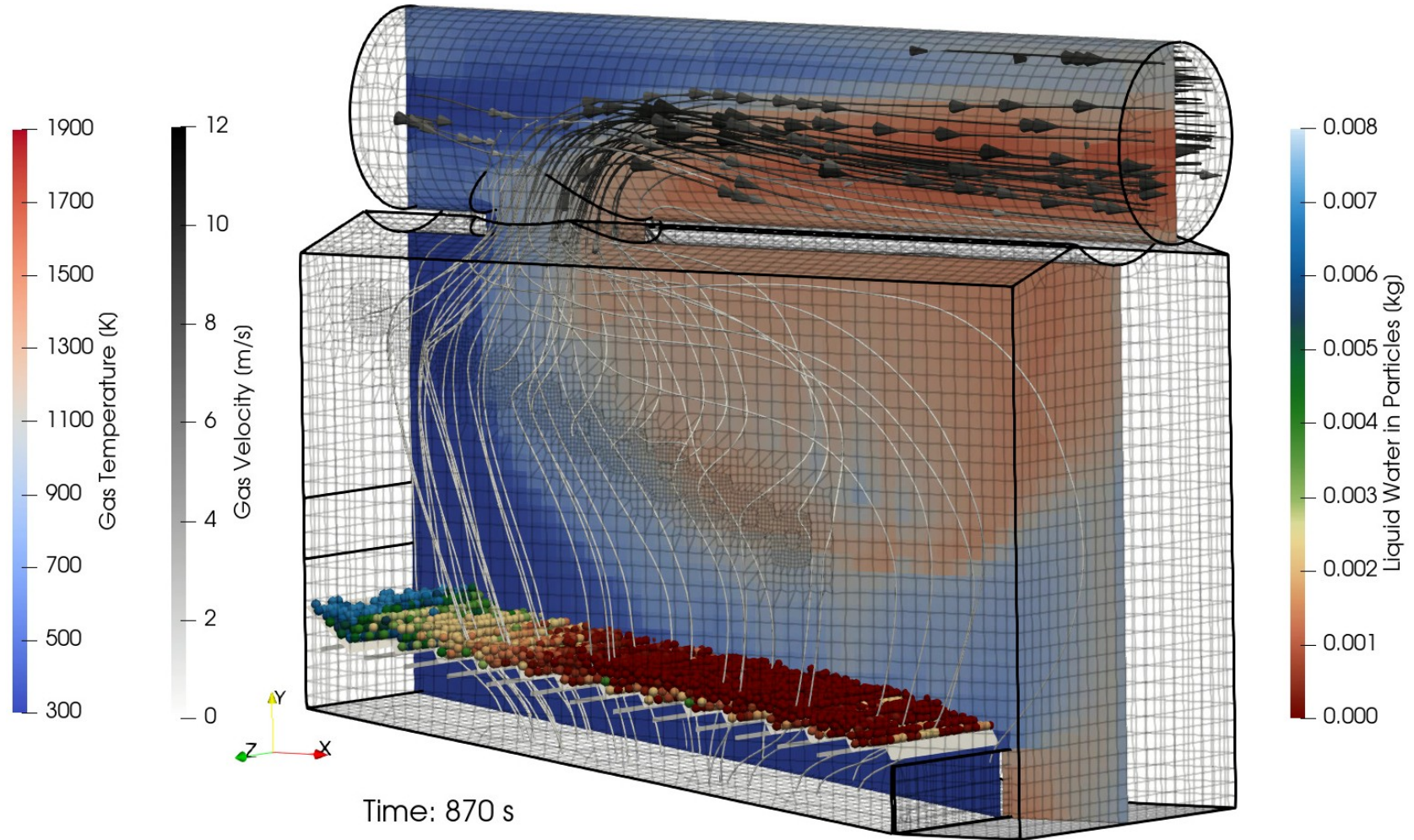
- Initial fuel bed height is 10cm
- Wood particles of 3cm diameter with 40% humidity
- Injected at the top side of the grates at a rate of 439kg/h



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

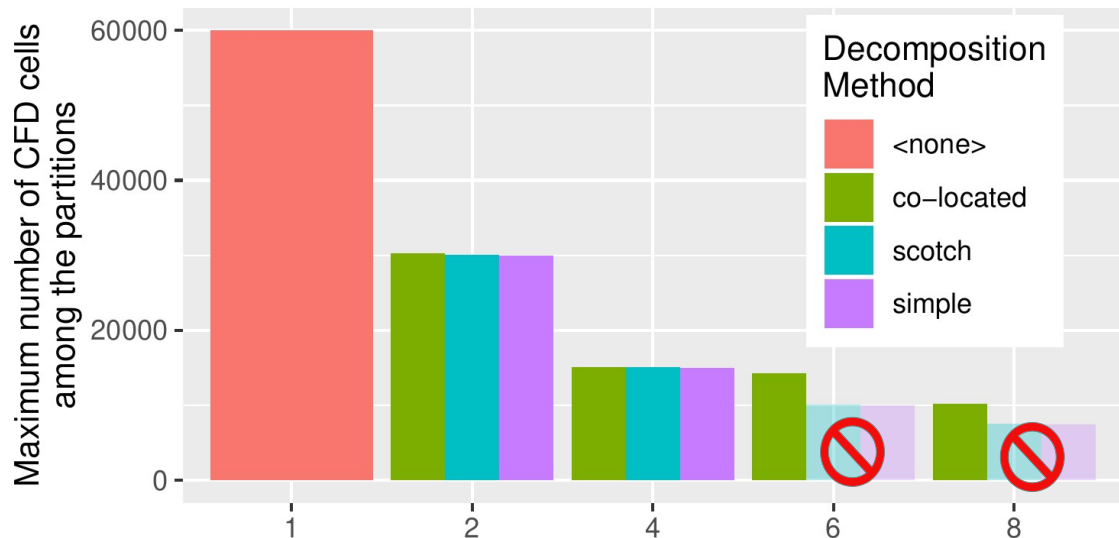
Following performance measurements were carried out on the *Barbora* cluster of the IT4Innovations HPC platform.

Biomass Furnace simulation using XDEM+OpenFOAM



Decomposition and scalability of OpenFOAM

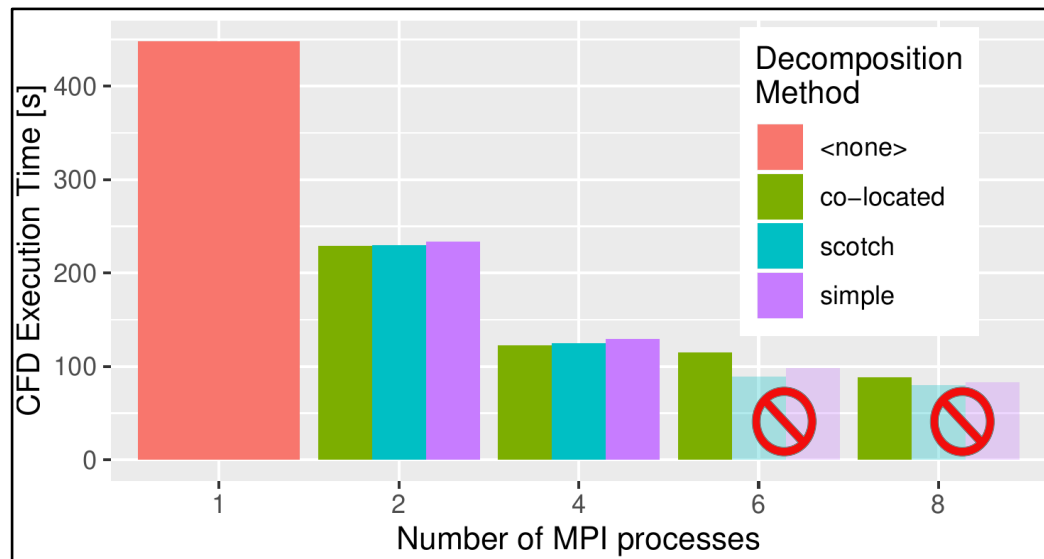
- Execution of the coupled problem, but looking at the **CFD part only**
- Execution time for the first 10s of simulation
- OpenFOAM mesh is relatively small: only 60k cells



Co-located compared to SCOTCH on 8 processes

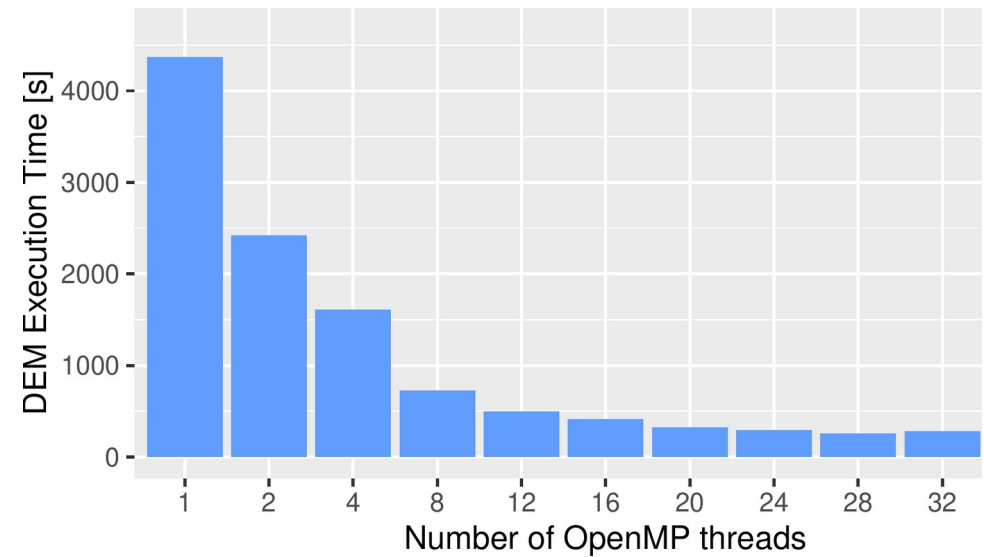
- Load-balancing → +37%
- CFD Execution time → +11% only

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



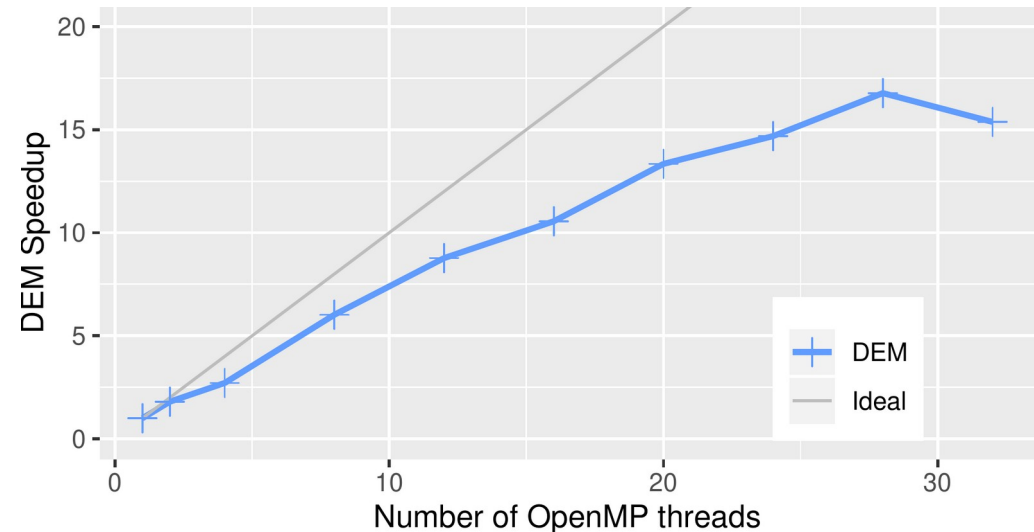
Scalability of XDEM

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



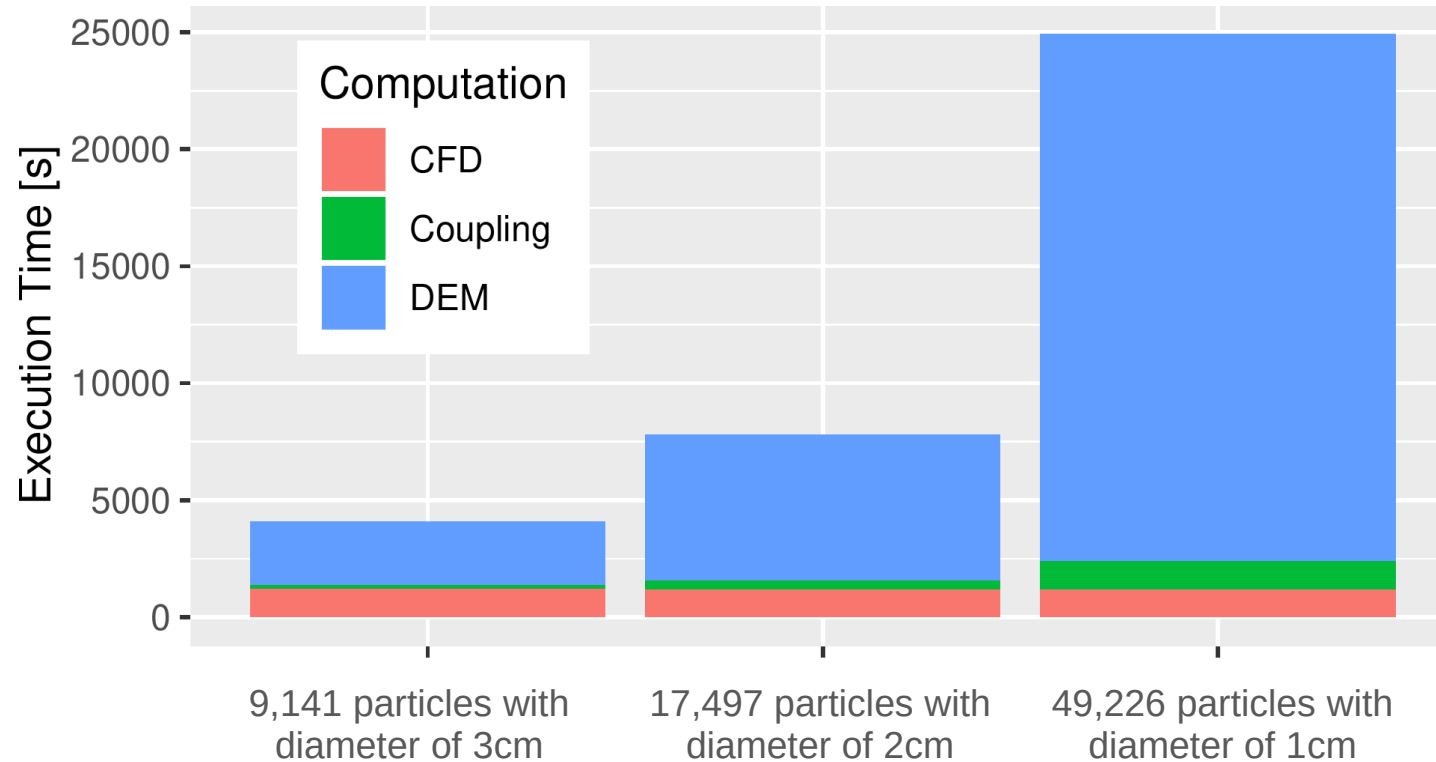
XDEM speedup of 16.8 with 28 threads

- 60% efficiency for 9k particles



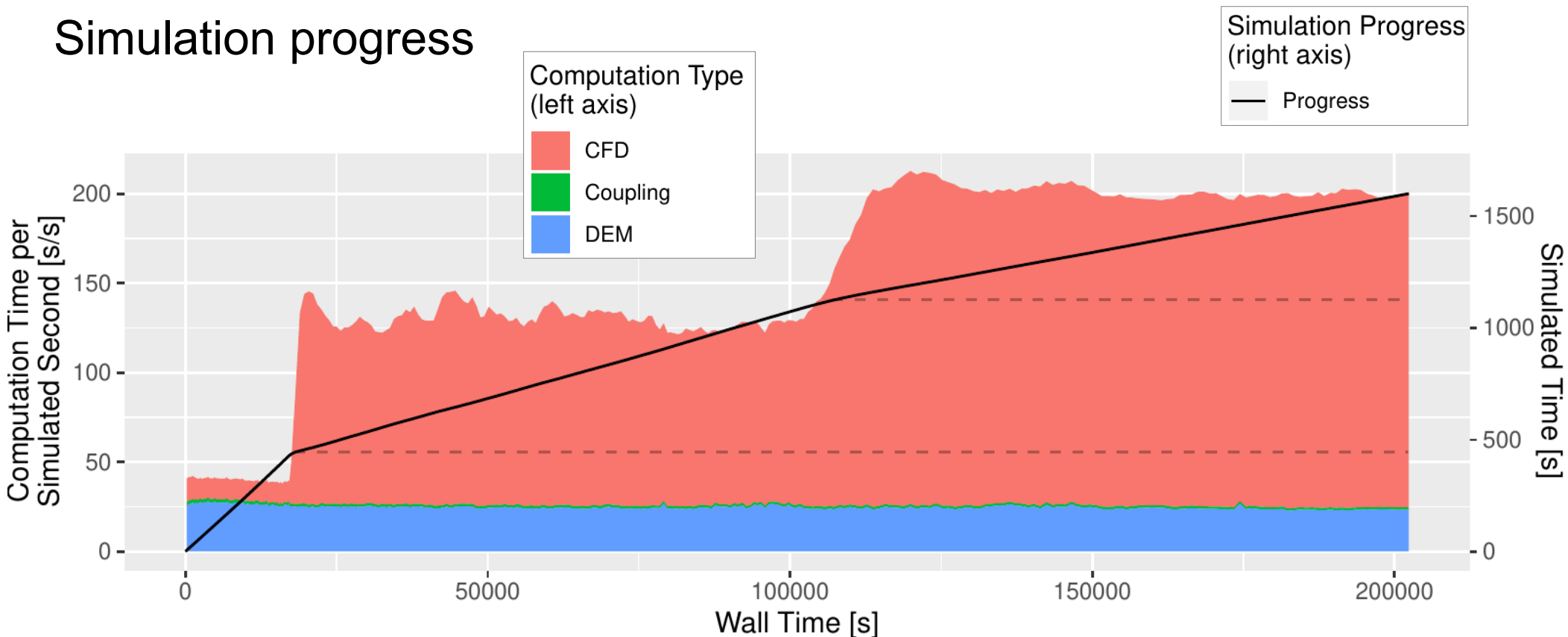
Influence of the number of particles

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



⇒ Workload between CFD and DEM changes with the furnace setup

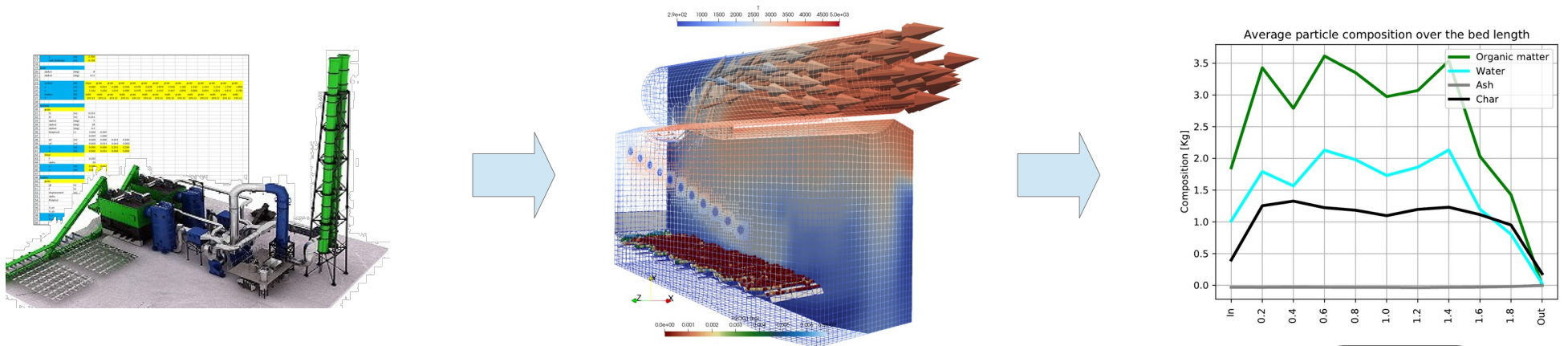
Simulation progress



- 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



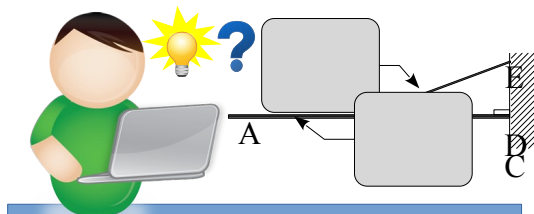
<https://www.cloudifacturing.eu>



- **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



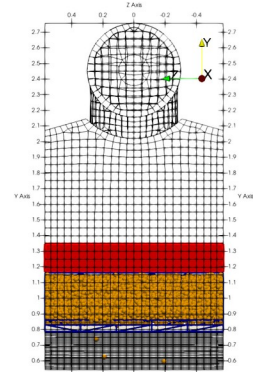
Visualize the results

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

Spreadsheet Input File

Automatic generation of the CFD+DEM case

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



A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1	Unit																
2	Variable																
3	x1	[m]		2.500													
4	x2	[m]		0.070													
5	y1	[m]		2.222													
6	y2	[m]		0.570													
7	Fuel pipe																
8	r	[m]		1.257													
9	z	[m]		0.000													
10	connecting_pipe																
11	x	[m]		0.557													
12	y	[m]		0.000													
13	secondary_air_pipe																
14	x	[m]		2.455													
15	y	[m]		0.000													
16	L	[m]		2.700													
17	inlet_diameter	[m]		0.330													
18																	
19																	
20	alpha1	[deg]															
21	alpha2	[deg]															
22																	
23	inlet																
24	x	[m]		0.000	0.054	0.286	0.346	0.578	0.638	0.870	0.930	1.162	1.222	1.454	1.514	1.746	1.806
25	y	[m]		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
26	z	[m]		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
27	inlet																
28	alpha1	[deg]															
29	alpha2	[deg]															
30	beta	[deg]															
31	l1	[m]		0.014													
32	l2	[m]		0.241													
33	alpha1	[deg]		7													
34	alpha2	[deg]		28													
35	alpha3	[deg]															
36	beta(alpha)	[°]		1.000	0.000												
37	beta	[°]		0.000	1.000												
38	alpha	[°]		0.000	0.000	0.241	0.264										
39	beta	[°]		0.000	0.014	0.044	0.000										
40	gamma	[°]		0.000	0.000	0.241	0.264										
41	delta	[°]		0.000	0.014	0.044	0.002										
42	theta	[°]															
43	phi	[°]		0.205													

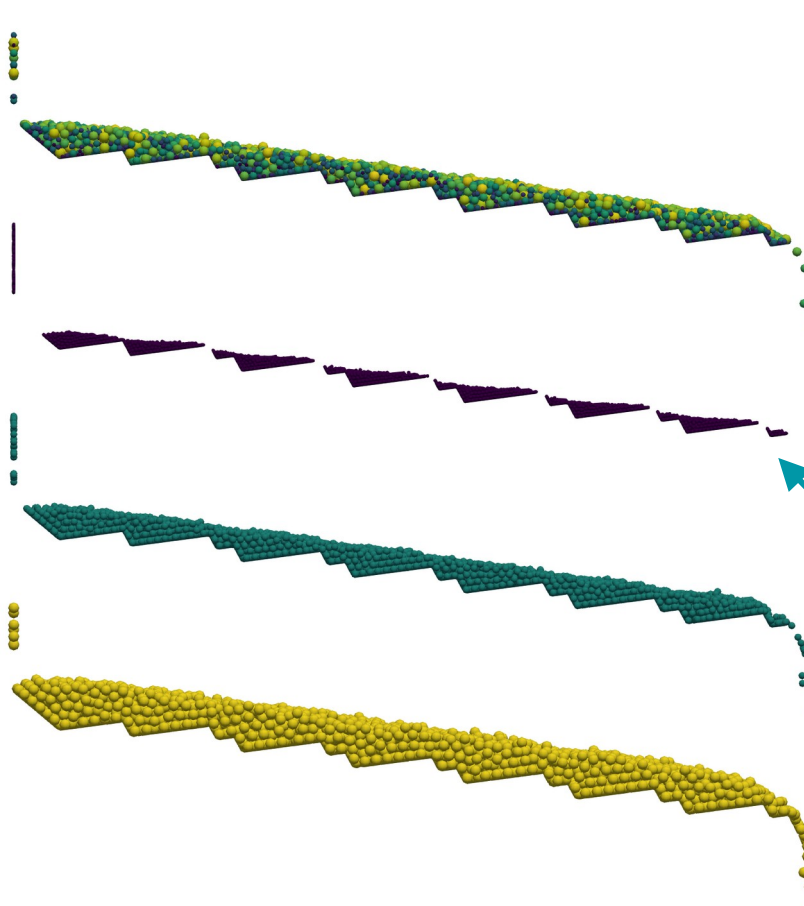
Furnace and grates geometry

A	B	C	D	E	F
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_H	[kg/kg]	0.000		
15	Y_N	[kg/kg]	0.004		
16	Y_S	[kg/kg]	0.000		
17	Y_Cl	[kg/kg]	0.000		
18	Y_Ash	[kg/kg]	0.010		
19	Y_H2O	[kg/kg]	0.400		
20			1.000		
21					
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		BeechWoodLignin(S)		
28					

Fuel composition

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	name	x	y	z	u	v	w	boundary	condition					
2		[m]	[m]	[m]	[m]	[m]	[m]	[m]	[m]	[m]	[m]	[m]	[m]	[m]
3	sec_ar1	0.247	1.904	-0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
4	sec_ar2	0.284	1.863	-0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
5	sec_ar3	0.543	1.782	-0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
6	sec_ar4	0.690	1.721	-0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
7	sec_ar5	0.838	1.659	-0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
8	sec_ar6	0.986	1.598	-0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
9	sec_ar7	1.134	1.537	-0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
10	sec_ar8	1.281	1.476	-0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
11	sec_ar9	1.429	1.415	-0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
12	sec_ar10	1.577	1.353	-0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
13	sec_ar11	1.725	1.292	-0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
14	sec_ar12	0.247	1.904	0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
15	sec_ar13	0.284	1.863	0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
16	sec_ar14	0.543	1.782	0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
17	sec_ar15	0.690	1.721	0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
18	sec_ar16	0.838	1.659	0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
19	sec_ar17	0.986	1.598	0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
20	sec_ar18	1.134	1.537	0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
21	sec_ar19	1.281	1.476	0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
22	sec_ar20	1.429	1.415	0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
23	sec_ar21	1.577	1.353	0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
24	sec_ar22	1.725	1.292	0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
25	sec_ar23	0.247	1.904	-0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
26	sec_ar24	0.284	1.863	-0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
27	sec_ar25	0.543	1.782	-0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
28	sec_ar26	0.690	1.721	-0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
29	sec_ar27	0.838	1.659	-0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
30	sec_ar28	0.986	1.598	-0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
31	sec_ar29	1.134	1.537	-0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
32	sec_ar30	1.281	1.476	-0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
33	sec_ar31	1.429	1.415	-0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
34	sec_ar32	1.577	1.353	-0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
35	sec_ar33	1.725	1.292	-0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
36	sec_ar34	0.247	1.904	0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
37	sec_ar35	0.284	1.863	0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
38	sec_ar36	0.543	1.782	0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
39	sec_ar37	0.690	1.721	0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
40	sec_ar38	0.838	1.659	0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
41	sec_ar39	0.986	1.598	0.570	0.000	0.000	1.000	0.061	0.017652	343.15	0.0000	0.0000	0.0000	0.2314
42	sec_ar40	1.134	1.537	0.570	0.000	0.000	1.000	0						

Spreadsheet settings and many more



	A	B	C	D	E	F	G	H	I
1	Position			Normal (inwards)				Boundary Condition	
2	zone	x	y	z	n_x	n_y	n_z	max_flux	temp
3	[m]	[m]	[m]	[m]	[m]	[m]	[m]	[kg/s]	[K]
4	rec_ar1	0.047	1.804	-0.570	0.000	0.000	1.000	0.061	0.017652
5	rec_ar2	0.394	1.843	-0.570	0.000	0.000	1.000	0.061	0.017652
6	rec_ar3	0.543	1.782	-0.570	0.000	0.000	1.000	0.061	0.017652
7	rec_ar4	0.690	1.721	-0.570	0.000	0.000	1.000	0.061	0.017652
8	rec_ar5	0.838	1.659	-0.570	0.000	0.000	1.000	0.061	0.017652
9	rec_ar6	0.986	1.598	-0.570	0.000	0.000	1.000	0.061	0.017652
10	rec_ar7	1.134	1.537	-0.570	0.000	0.000	1.000	0.061	0.017652
11	rec_ar8	1.282	1.476	-0.570	0.000	0.000	1.000	0.061	0.017652
12	rec_ar9	1.430	1.415	-0.570	0.000	0.000	1.000	0.061	0.017652
13	rec_ar10	1.577	1.353	-0.570	0.000	0.000	1.000	0.061	0.017652
14	rec_ar11	1.725	1.292	-0.570	0.000	0.000	1.000	0.061	0.017652
15	rec_ar12	1.873	1.231	-0.570	0.000	0.000	1.000	0.061	0.017652
16	rec_ar13	2.021	1.170	-0.570	0.000	0.000	1.000	0.061	0.017652
17	rec_ar14	2.169	1.109	-0.570	0.000	0.000	1.000	0.061	0.017652
18	rec_ar15	2.317	1.048	-0.570	0.000	0.000	1.000	0.061	0.017652
19	rec_ar16	2.465	0.987	-0.570	0.000	0.000	1.000	0.061	0.017652
20	rec_ar17	2.613	0.926	-0.570	0.000	0.000	1.000	0.061	0.017652
21	rec_ar18	2.761	0.865	-0.570	0.000	0.000	1.000	0.061	0.017652
22	rec_ar19	2.909	0.804	-0.570	0.000	0.000	1.000	0.061	0.017652
23	rec_ar20	3.057	0.743	-0.570	0.000	0.000	1.000	0.061	0.017652
24	rec_ar21	3.205	0.682	-0.570	0.000	0.000	1.000	0.061	0.017652
25	rec_ar22	3.353	0.621	-0.570	0.000	0.000	1.000	0.061	0.017652
26	rec_ar23	3.501	0.560	-0.570	0.000	0.000	1.000	0.061	0.017652
27	rec_ar24	3.649	0.499	-0.570	0.000	0.000	1.000	0.061	0.017652
28	rec_ar25	3.797	0.438	-0.570	0.000	0.000	1.000	0.061	0.017652
29	rec_ar26	3.945	0.377	-0.570	0.000	0.000	1.000	0.061	0.017652
30	rec_ar27	4.093	0.316	-0.570	0.000	0.000	1.000	0.061	0.017652
31	rec_ar28	4.241	0.255	-0.570	0.000	0.000	1.000	0.061	0.017652
32	rec_ar29	4.389	0.194	-0.570	0.000	0.000	1.000	0.061	0.017652
33	rec_ar30	4.537	0.133	-0.570	0.000	0.000	1.000	0.061	0.017652
34	rec_ar31	4.685	0.072	-0.570	0.000	0.000	1.000	0.061	0.017652
35	rec_ar32	4.833	0.011	-0.570	0.000	0.000	1.000	0.061	0.017652
36	rec_ar33	4.981	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
37	rec_ar34	5.129	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
38	rec_ar35	5.277	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
39	rec_ar36	5.425	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
40	rec_ar37	5.573	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
41	rec_ar38	5.721	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
42	rec_ar39	5.869	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
43	rec_ar40	6.017	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
44	rec_ar41	6.165	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
45	rec_ar42	6.313	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
46	rec_ar43	6.461	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
47	rec_ar44	6.609	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
48	rec_ar45	6.757	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
49	rec_ar46	6.905	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
50	rec_ar47	7.053	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
51	rec_ar48	7.201	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
52	rec_ar49	7.349	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
53	rec_ar50	7.497	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
54	rec_ar51	7.645	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
55	rec_ar52	7.793	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
56	rec_ar53	7.941	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
57	rec_ar54	8.089	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
58	rec_ar55	8.237	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
59	rec_ar56	8.385	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
60	rec_ar57	8.533	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
61	rec_ar58	8.681	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
62	rec_ar59	8.829	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
63	rec_ar60	8.977	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
64	rec_ar61	9.125	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
65	rec_ar62	9.273	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
66	rec_ar63	9.421	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
67	rec_ar64	9.569	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
68	rec_ar65	9.717	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
69	rec_ar66	9.865	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
70	rec_ar67	10.013	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
71	rec_ar68	10.161	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
72	rec_ar69	10.309	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
73	rec_ar70	10.457	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
74	rec_ar71	10.605	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
75	rec_ar72	10.753	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
76	rec_ar73	10.901	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
77	rec_ar74	11.049	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
78	rec_ar75	11.197	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
79	rec_ar76	11.345	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
80	rec_ar77	11.493	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
81	rec_ar78	11.641	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
82	rec_ar79	11.789	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
83	rec_ar80	11.937	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
84	rec_ar81	12.085	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
85	rec_ar82	12.233	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
86	rec_ar83	12.381	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
87	rec_ar84	12.529	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
88	rec_ar85	12.677	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
89	rec_ar86	12.825	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
90	rec_ar87	12.973	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
91	rec_ar88	13.121	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
92	rec_ar89	13.269	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
93	rec_ar90	13.417	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
94	rec_ar91	13.565	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
95	rec_ar92	13.713	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
96	rec_ar93	13.861	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
97	rec_ar94	14.009	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
98	rec_ar95	14.157	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
99	rec_ar96	14.305	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
100	rec_ar97	14.453	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
101	rec_ar98	14.601	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
102	rec_ar99	14.749	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
103	rec_ar100	14.897	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
104	rec_ar101	15.045	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
105	rec_ar102	15.193	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
106	rec_ar103	15.341	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
107	rec_ar104	15.489	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
108	rec_ar105	15.637	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
109	rec_ar106	15.785	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
110	rec_ar107	15.933	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
111	rec_ar108	16.081	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
112	rec_ar109	16.229	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
113	rec_ar110	16.377	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
114	rec_ar111	16.525	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
115	rec_ar112	16.673	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
116	rec_ar113	16.821	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
117	rec_ar114	16.969	0.000	-0.570	0.000	0.000	1.000	0.061	0.017652
118	rec_ar115	17.117	0.						

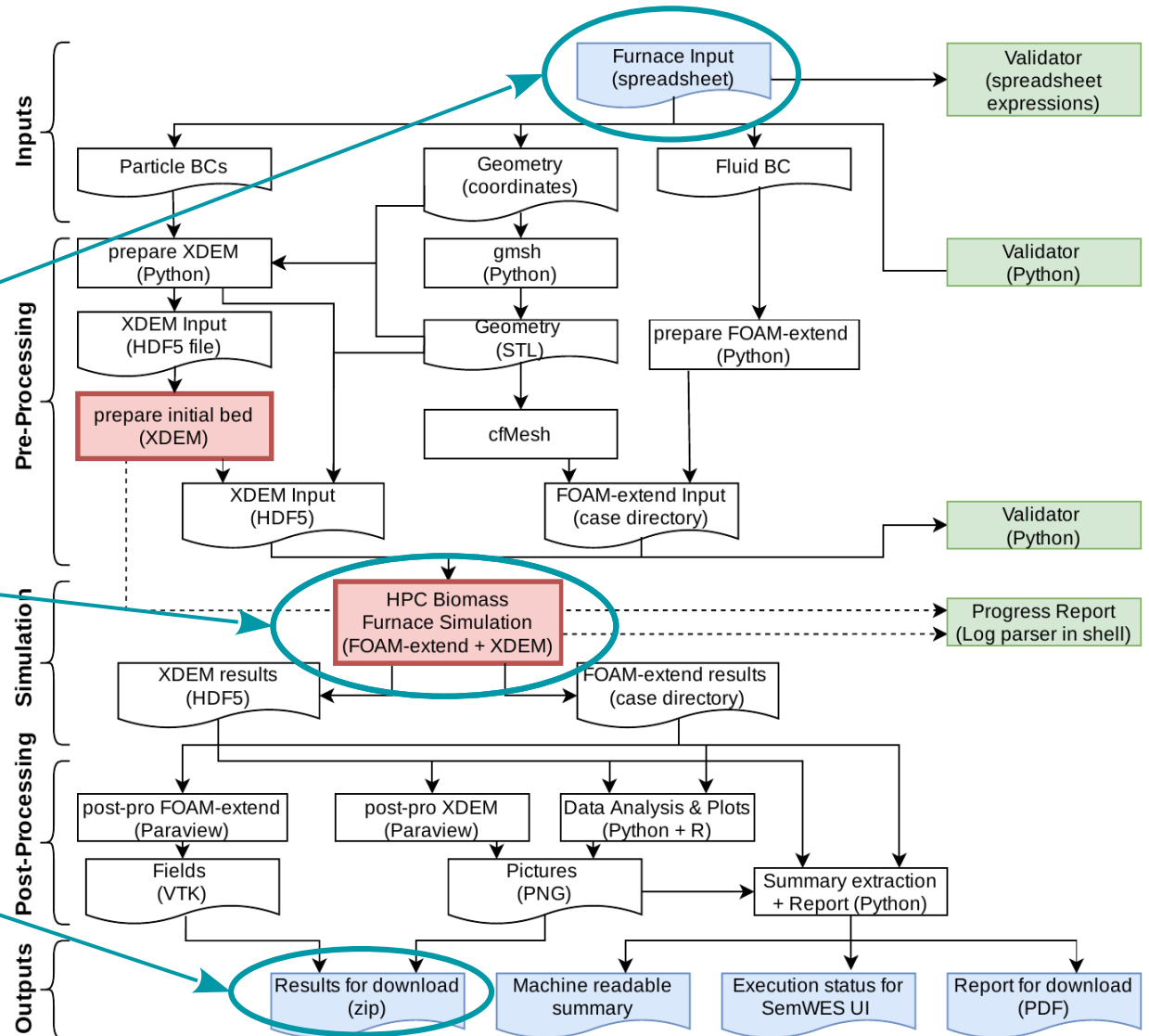
Internal workflow

executed in the Singularity container

User Input

Parallel Biomass Furnace Simulation

Simulation Output



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

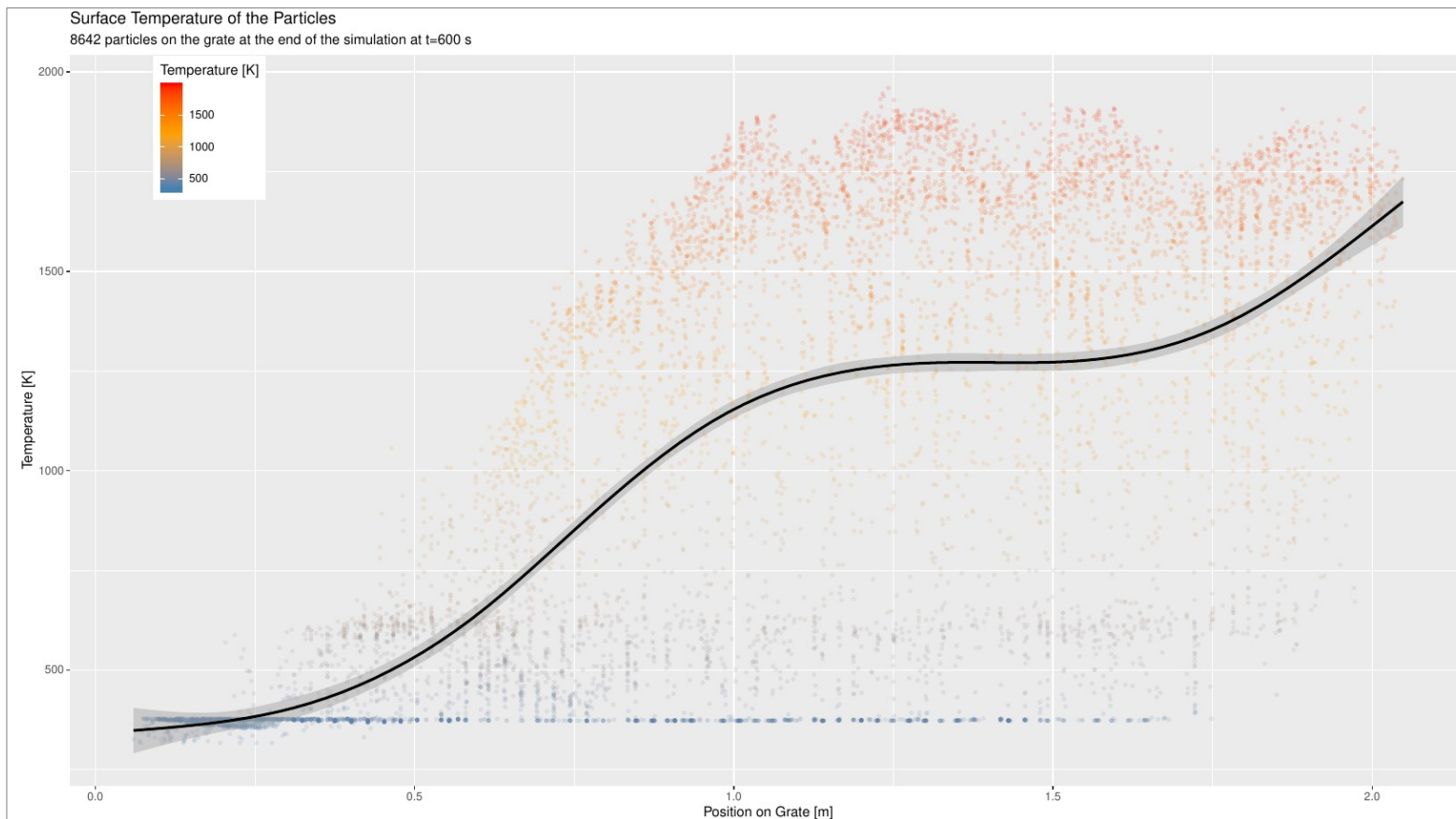
Extracts of the Simulation Reports

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
```

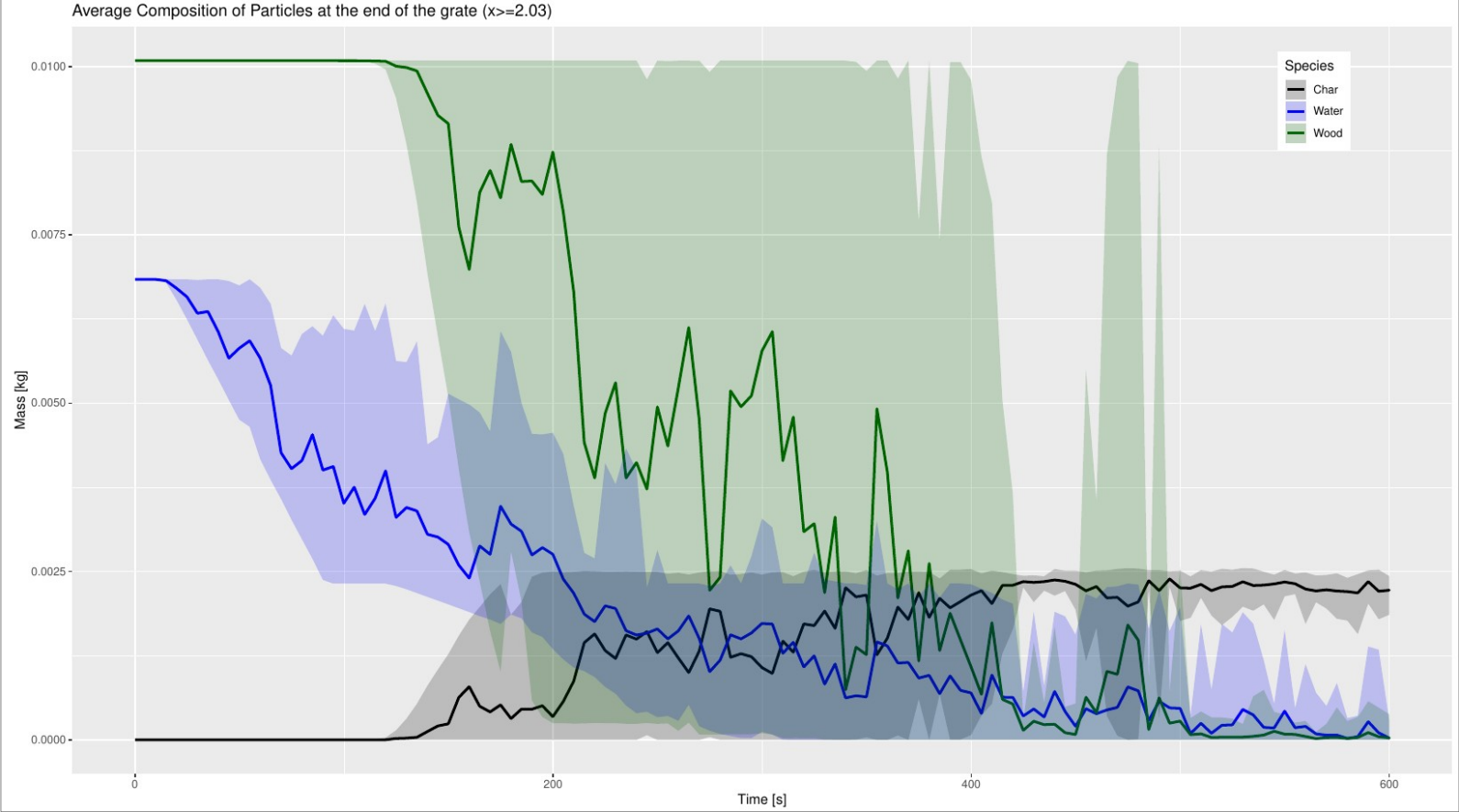
Average properties at exit of the exhaust pipe

Extracts of the Simulation Reports



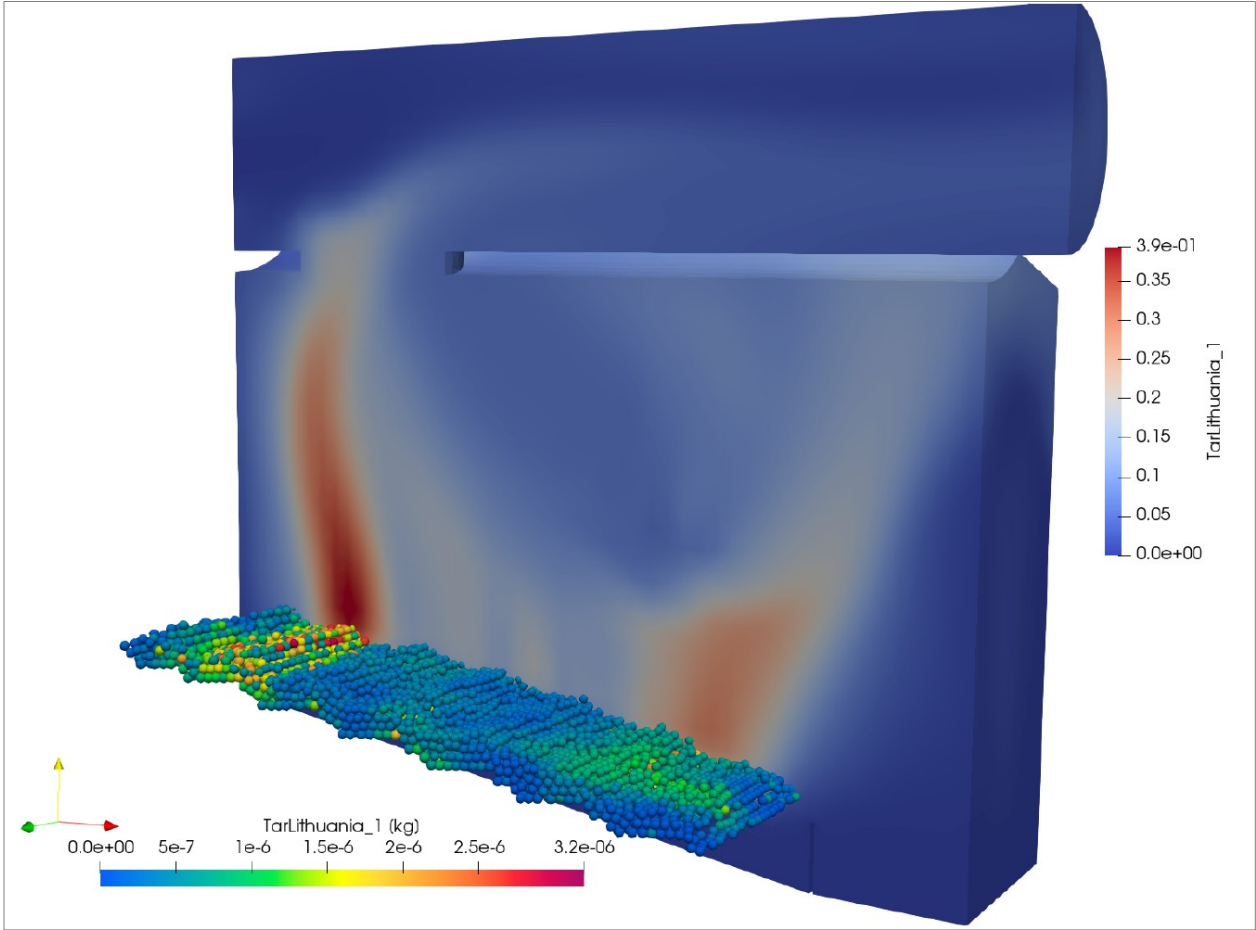
Surface temperature of the particles along the grate

Extracts of the Simulation Reports

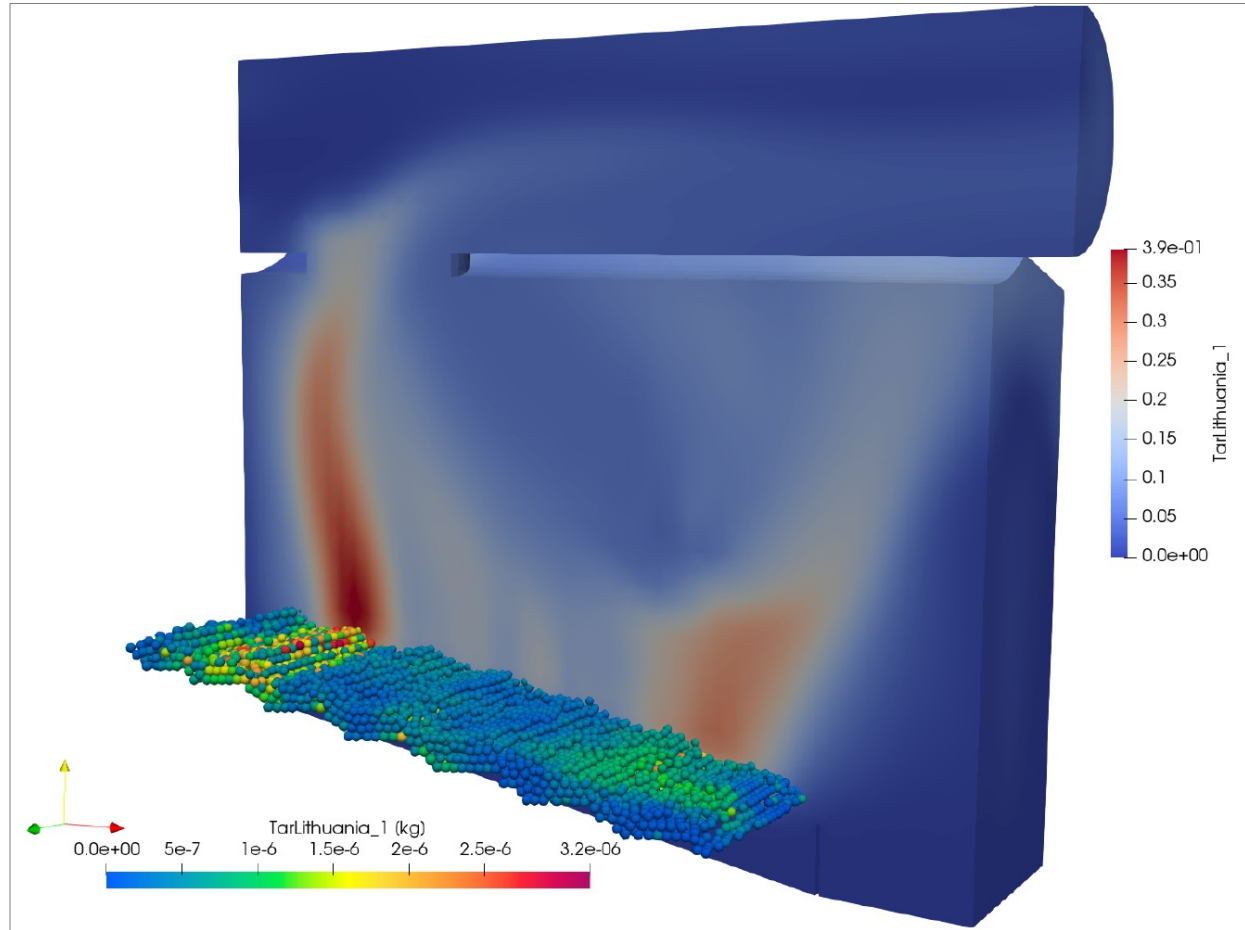


Evolution of particle composition at the exit of the grate

Extracts of the Simulation Reports



Tar content of the particles and in the gas



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



IT4Innovations
national supercomputing
center

Multi-Physics Biomass Furnace Simulation

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

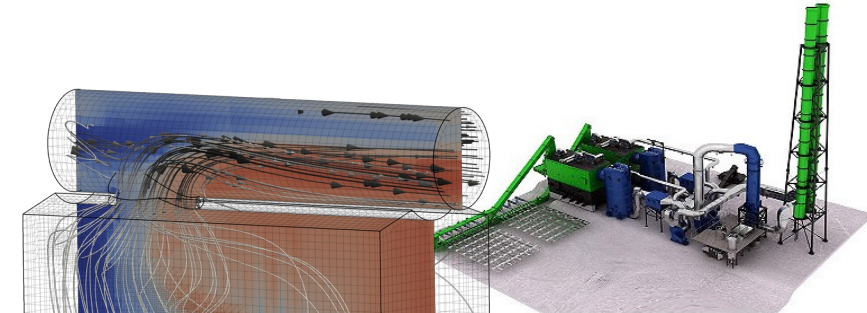
Cloud-based interface and submission portal

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

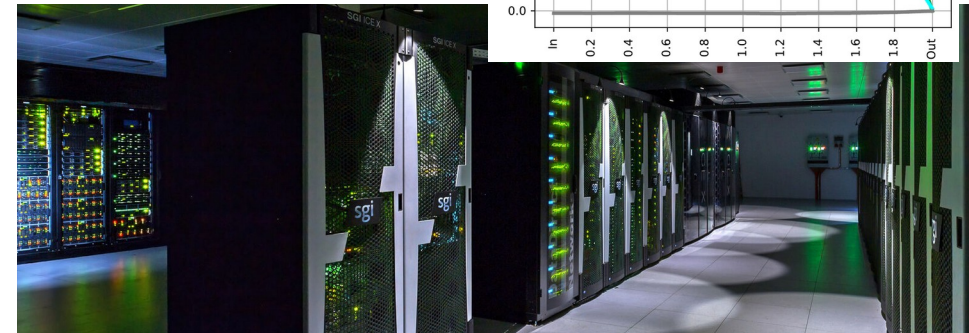
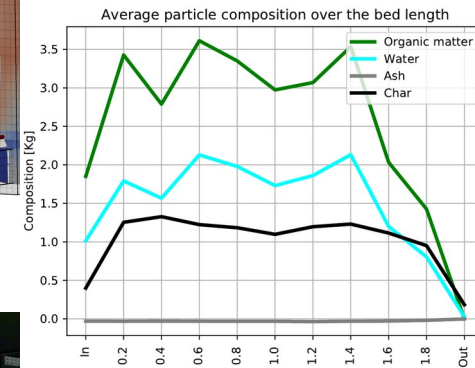
Simplified Workflow for end user

- 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)**



Time: 1200 s



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, and 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

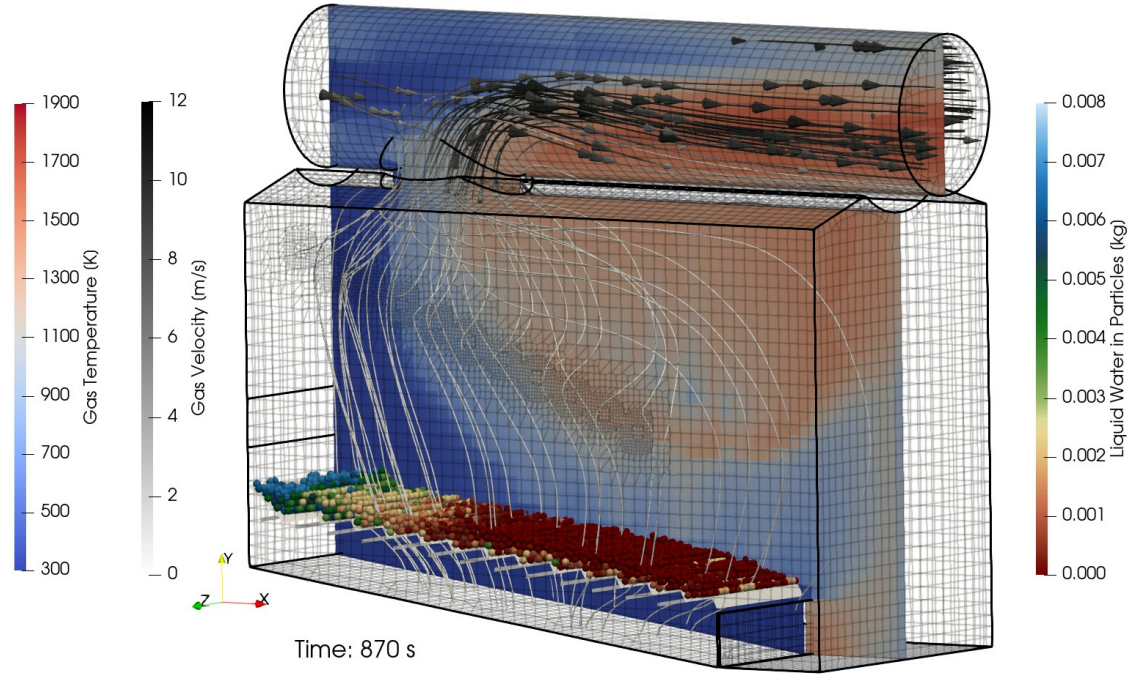
Next Steps

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

