D5.5 Research Advancements for the Pilots

HiDALGO2

CENTRE OF EXCELLENCE

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List of Acronyms

Abbreviation / acronym	Description
API	Application Programming Interface
BC	Boundary Condition
BVH	Bounding Volume Hierarchy
CI	Continuous Integration
DB	database
DoE	Design of Experiments
EOP	End of Project
FMU	Functional Mock-up Unit
GUI	Graphical User Interface
HPDA	High-Performance Data Analytics
HPC	High-Performance Computing

Abbreviation / acronym	Description
I/O	Input/Output
KNN	K-Nearest Neighbours
Lod	Level of Detail
LW	Long Wave
MPI	Message Passing Interface
PID	Proportional-Integral-Derivative
POI	Point of Interest
SW	Short wave
UI	User Interface
UQ	Uncertainty Quantification
UX	User Experience
RES	Renewable Energy Sources
HPDA	High Performance Data Analytics
PV	Photovoltaics
AI	Artificial Intelligence
mUQSA	Multiscale Uncertainty Quantification and Sensitivity Analysis
PCE	Polynomial Chaos Expansion
UQ	Uncertainty Quantification
SA	Sensitivity Analysis
EuroHPC-JU	European High Performance Computing Joint Undertaking
FSE	Fire Spread Engine
GPU	Graphics Processing Unit
PGF	porousGasificationFoam
WRF	Weather Research and Forecasting
WUI	Wildland-Urban Interface
CHT	Conjugate Heat Transfer

Executive Summary

HiDALGO2 focuses on the development of high-fidelity simulations to address critical global challenges. This document builds on the foundations of D5.4 [1] by highlighting the research advances achieved within the HiDALGO2 project between M24 and M35 in the five pilot applications: Urban Air Project, Urban Buildings, Renewable Energy Sources, Wildfires and Material Transport in Water. It emphasizes enhancements in solver modelling, accuracy, and versatility, alongside adjustments to the roadmaps based on unforeseen challenges and newly found insights.

For each pilot, specific advancements have been achieved:

- **Urban Air Project (UAP)**: Upgraded solvers, including the integration of RedSim with multi-node, multi-GPU-accelerated configurations, which have significantly improved the simulation of urban airflow and pollutant dispersion. Enhanced pre-processing tools utilizing OpenStreetMap to further support detailed urban environmental modelling. However, to incorporate atmospheric physics features into this pilot and due to a shift in focus, the integration of the digital twin and reduced models using MPI with GPU support and the overall development of the *UAP-FOAM* workflow have been postponed to the next reporting period.

- **Urban Buildings (UB)**: Progress was made in occupancy modelling, weather and geolocation integration, and energy output simulation, enhancing UB's capacity to model energy consumption and indoor environmental conditions. A real-time data validation framework has been implemented, along with a user interface that supports interactive weather and scenario configurations. Planned future additions, such as heating regulation models, aim to further enhance the pilot's simulation of urban building energy and comfort metrics. Challenges in dealing with specific geometric complexities pose a challenge in the generation of watertight meshes.

- **Renewable Energy Sources (RES)**: This pilot is advancing energy prediction models for solar and wind power generation, with progress in coupling models for enhanced accuracy in prediction. The lack of real-world data remains a bottleneck for certain aspects; however, advancements in small and large-scale photovoltaic models provide alternative data sources. Future work includes further refinement of prediction models using uncertainty quantification and visualization improvements.

- **Wildfires (WF)**: The WF pilot has made substantial advancements in simulating wildfire spread in both rural and urban settings, with updated preprocessing for historical wildfire events and coupling of the WRF model to simulate atmospheric interactions. Work is underway on GPU-enabled ensemble simulations, validation of surrogate models, automated vegetation mapping, and VR-ready visualization of fire spread scenarios to inform wildfire risk assessments at varying landscape scales.

- **Material Transport in Water (MTW)**: This new pilot focuses on modelling temperature transport in aquatic environments. Notable achievements include successful fluid-particle coupling and inclusion of temperature transport inside fluid and particles. This model development helps to better understand the fundamental aspects of heat transfer in water and aquatic environments.

This report provides a comprehensive assessment of each pilot’s progress, emphasizing the technical and operational challenges encountered and contributes to WP3 - Exascale Support for Global Challenges and WP4 - Data Exploration and Visualisation. The reported results showcase significant advancements, lay the groundwork for future deliverables, and reinforce HiDALGO2's goal of addressing global challenges through cutting-edge HPC solutions.

1 Introduction

1.1 Purpose of the document

The purpose of this document, Deliverable D5.5, is to report on the progress achieved in the HiDALGO2 project's pilot applications up to month 35 of the project lifetime. It details recent advancements in areas such as solver modelling, simulation accuracy, model versatility, and workflow orchestration. The document emphasizes the continuous efforts made to refine the pilot's performances, contributing to the overarching goal of evolving these applications into effective digital twins.

1.2 Relation to other project work

This deliverable, D5.5, follows on from D5.4 [1]and directly contributes to the work of WP5, which focuses on addressing global challenges through the development of advanced simulation capabilities. The research outcomes and technical developments presented here also relate to and benefit from the efforts of WP3, which focuses on supporting global challenges with exascale computing, and WP4, which handles data exploration and visualization.

1.3 Structure of the document

This document is organized into seven chapters, each addressing a specific aspect of the project's progress and the individual contributions of the five pilot applications.

Executive Summary. Provides an overview of the deliverable's key objectives and highlights the progress achieved across all pilots.

Chapter 1 Introduction. Explains the purpose of the document, its relevance within the broader HiDALGO2 project, and its structure.

Chapters 2 to 6 Focus on the specific research conducted by the UAP, UB, RES, WF and MTW pilots. These chapters present advances made from M24 to M35 in the pilot's model development, solver precision, and versatility.

Each chapter consists of two subsections:

Advances in Model Development

- Summary of key progress in enhancing models and solver accuracy for the pilot.
- Highlights new capabilities and scientific improvements achieved during this phase.

- Focus on advancements in application precision and versatility, showing how these developments impact the quality and reliability of pilot simulations.

Roadmap and Challenges

- Overview of current research challenges and obstacles faced in achieving pilot objectives.
- Description of any adjustments made to the initial roadmap based on findings and emerging needs.
- Key insights gained that inform and shape the future direction and priorities of each pilot's work.

Chapter 7 General Conclusion and Future Outlook. Summarizes the main achievements, challenges, and shifts in the overall roadmap, while providing insights into the next phase of the project with regards to Work Package 5.

2 Urban Air Project

Urban Air Project (UAP) is a high-performance computing framework for simulating airflow in urban environments and, based on the resulting wind fields, evaluating air comfort, air quality, and planning-related KPIs. UAP leverages HPC to handle high-resolution models at city-scale, uses in-house pre-processing tools to generate suitable 3D geometries from open and custom data, i.e. the corresponding 3D meshes. UAP employs dedicated post-processing tools for analysis and visualization. For the air flow computations, UAP applies three optional solvers, which are developed and optimized by the UAP-team according to the EuroHPC compute infrastructure

2.1 Advances in model development

The UAP application consists of pre-processing, computational simulation, and post-processing modules, the latter include visualization and data analytics.

2.1.1 Advances in pre-processing

The main components of the pre-processing module are the 3D geometry modelling and the meshing modules. In the reporting period, one of the main focus points of the UAP development was to significantly improve the UAP geometry modelling properties according to application of UAP for cities. SZE performed an application for the city of Stockholm in collaboration with Stockholm city and the Swedish HPC competence network ENCCS. This application provided with new requirements for the RedSim preprocessing tools mainly due to the use of geographic information system used at the city of Stockholm.

The core of the pre-processing tool advancement are as follows:

- support a new input format, the shapefile format with shp, shx and dbf files that are generated by a geographic information system used by the external users,
- terrain modelling from isolines of the elevations, for an illustration see Figure 1 below,
- integration of the Gmsh mesher, in addition to tetgen and other tools, and extension of the API capabilities such that meshes and other resources can be created with optimized Gmsh through the API, for an illustration see Figure 2 below,
- all pre-processing tools were integrated into the UAP workflow and the HiDALGO2 portal, for an illustration see Figure 3 below.

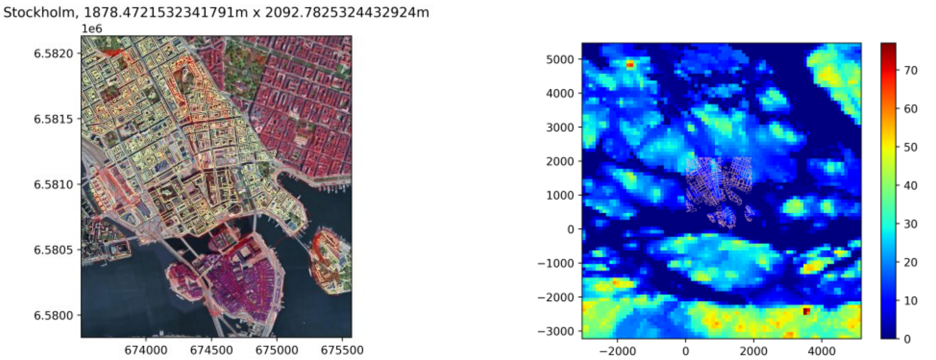

Figure 1. Terrain modelling Input Data from Shape Files provided by the city of Stockholm, overlayed with Google Earth Satellite Data (left) and visualization of elevation map generated from the isolines of the GIS system for terrain modelling (right).

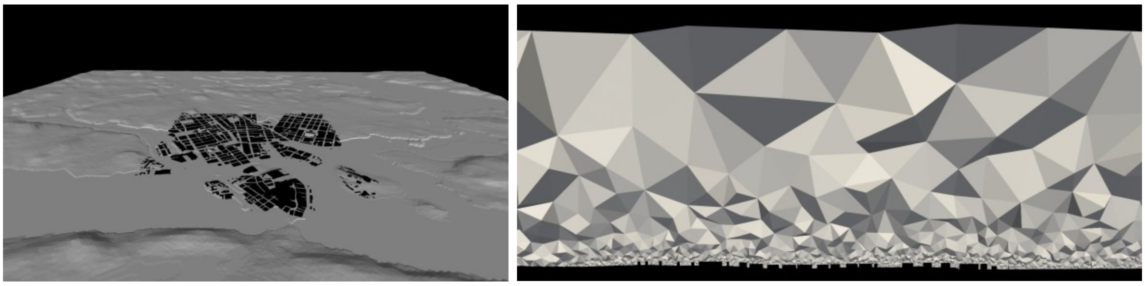

Figure 2. Automated meshing the surface geometry of the ground, with holes for the buildings (left) and a cross-section of the Gmsh-generated 3D volume mesh (right).

2.1.2 Advances in air flow solver development

UAP has three different solvers for the airflow and air quality computation that are *UAP-FOAM*, *RedSim* and *Xyst*. Each solver has advantages and disadvantages over the others, namely:

- *UAP-FOAM* is based on the widespread, flexible *OpenFOAM* code, mainly running on CPUs only,
- *RedSim* is a fully inhouse, compact, native OpenMPI+pthread and OpenMPI+CUDA code running on CPU and NVIDIA GPU clusters efficiently, running on CPU clusters,
- *Xyst* is a proved candidate for exascale and a platform for testing new algorithms.

The advances of these solvers achieved in the reporting period, M24-M35, are reported in the following separate subsections.

2.1.2.1 UAP-FOAM advances

UAP-FOAM solves the incompressible Navier-Stokes equations and scalar transport under atmospheric parameters and settings by using *OpenFOAM*. The application has been updated to *OpenFOAM* com version 2506, including a foam-extend version. Benchmarks with the previous version 2406 and the foam-extend version have been published in cooperation with partners within HiDALGO2 [5]. A new rework done for integration into the MathSO portal, including MathSO CI/CD integration. Further high resolution meshes are created to further investigate model accuracy, including meshes up to 160M cells.

The *UAP-FOAM* development focus was on the support for thermal conduction in order to facilitate the UAP-UBM coupling using Boussinesq approximation, as detailed in D5.7 [6]. Additionally, GPU-based code is being adapted using the OpenFOAM-based *zeptoFOAM* and SPUMA implementations. Preliminary runs using *zeptoFOAM* on NVIDIA architecture are completed, results will be published in D3.3.

2.1.2.2 RedSim advances

In the reporting period the following advances were achieved with RedSim:

- The code has been rewritten to use an OpenMPI + CUDA framework. Thus RedSim runs on arbitrary many CPUs and NVIDIA GPUs.
- RedSIM's parallelization strategy has been reworked from a centralized model (master-slave), to a purely democratic model. The use of MPI I/O provides scalable file exports in Ensight GOLD and VTK, which is crucial for scaling on a large number nodes.
- New mesh partitioning codes integrated, namely Zoltan and ParMETIS. The integration of Scotch is ongoing. Scalability of RedSim was investigated in terms of different mesh partitioning.
- RedSim's Lua-API was reworked from the ground up, in order to maximize its modularity, thus to load multiple meshes, multiple solvers and boundary conditions, store their handles and launch different simulations with different resource combinations.
- Optimization of the code for meshes with tetrahedra only. A separate RedSim code path has been created, which is heavily optimized for simulation on meshes which contain only tetrahedra. This optimized code made possible real-time scenario analysis for relevant problems see Figure 3 below.

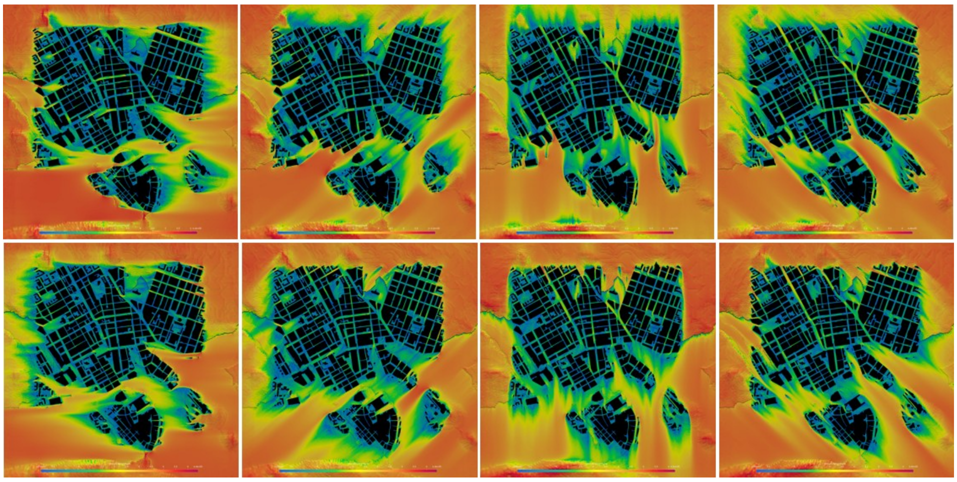

Figure 3. RedSim scenario analysis results done on 2 GPUs for the city of Stockholm. 1 physical hour was simulated on tetrahedral mesh within 1 hour in total.

2.1.2.3 Xyst advances

In the reporting period three new low-speed flow solvers have been added to the Xyst Inciter framework, extending its capability to simulate atmospheric and other incompressible/low-Mach-number conditions. These solvers are part of Xyst's family of Euler and Navier-Stokes solvers designed for complex 3D engineering geometries and efficient execution on massively parallel systems via the Charm++ runtime, which provides asynchronous execution, overdecomposition and automatic load balancing.

The new solvers' numerical correctness has been checked against analytical benchmark problems and further validated using experimental data, with dedicated verification and validation cases.

On the performance side, large-scale tests were carried out on the EuroHPC-JU LUMI supercomputer, where Xyst showed very good strong scaling up to 196,608 CPU cores. Strong scaling was demonstrated for multiple solvers (including LohCG, RieCG and ZalCG, see [8]) without major bottlenecks in computation or I/O.

2.2 Roadmap and challenges

2.2.1 Pre-processing tool

Development and optimization of the pre-processing tool has a ground basis, the existing code. Development of the code to support new features like vegetation by porous zones, increase level of details of buildings (e.g. by adding roof detailed model) are planned.

2.2.2 UAP-FOAM roadmap

Two implementations of the *UAP-FOAM* solver application are still in backlog, having lower priority. First, transitioning to a compressible solver, like *rhoSimpleFoam* and then implementing chemical reactions with *reactingFoam*. While the implementation itself is straight forward, finding the proper numerical schemes and methods require further activities planned which are to be accomplished in the next months. Also, development in this area will need to be finer grained.

Our focus is on further developing the UAP-UB coupling using coupling technologies of preCICE [7]. This tool supports data exchange seamlessly and in a scalable way to facilitate high performance coupled simulation.

On the workflow cleanup, initial steps have been done, including simplification of the code, adjustments to new benchmark methods and adaptation to the GPU implementations. Lessons learned still include high priority on code maintenance and cleanup for more seamless development and integration.

On the roadmap, code cleanup activities are still high priority. Afterwards, porting to GPU will get higher priorities including coupling scenarios and compressible solvers can be properly introduced. If the time still allows, implementation of chemical reactions can be enabled to simulate the nitrogen-oxide-ozone cycle. This reaction, however, needs to be separated from the flow simulation, to be implemented into the incompressible solution, validated and benchmarked against the compressible implementation.

2.2.3 RedSim roadmap

The RedSim algorithm and code are under serious optimization for preparing full machine runs on LUMI, both for CPUs and later on GPUs. This optimization will affect the internal data structure as well, e.g. the handling of ghost cells. SZE started a collaboration with the POP CoE to assess RedSim since M35. The already ongoing POP assessment of RedSim GPU model will require research and modifications on the code. Planned deadlines: M37 (POP-audit), M40 (full machine run on LUMI).

To exploit the full EuroHPC infrastructure by the applications of UAP, especially the AMD GPUs, RedSim will be reimplemented in OpenCL as well. The existing OpenMPI + CUDA path of the code will be continuously maintained. Planned deadline: M44.

The advection-diffusion solver to model gaseous pollutant dispersion in a splitting way will be strongly re-implemented both in OpenCL and CUDA, the latter fully optimized for NVIDIA linear algebra solvers. Planned deadline: M38. For modelling particulate material transport coupling with *waLBerla* will be considered and implemented. Planned deadline: M42.

Integration of chemical reactions in the advection-diffusion module will be completed. Also, a non-splitting version of pollutant dispersion will be implemented. Planned deadline: M40.

A prototype of digital twin of the urban air and air pollution will be developed. For the twinning weather sensor data and, optionally, the change of position and release amount of released toxic gases will be live coupled and visualized from the digital twin prototypes. Planned deadlines: M39, M42.

2.2.4 Xyst roadmap

The main task with Xyst is the full integration into the UAP workflow in the portal, testing it under industrially relevant conditions, i.e. application for several cities with a comparison with the RedSim and *UAP-FOAM* solvers.

The overall **expected research results** for the UAP Pilot **are in line** with those described in D5.4.

Table 1. Changes in expected Research Results for UAP Pilot compared to D5.4

Key framework	Status as of M35	Reason for roadmap adjustment	Adjusted / new achievement date
RedSim algorithm	Spatial 1st, 2nd order scheme for Euler and Navier-Stokes equations (MPI+GPU); **Done** advection-diffusion solver for dispersion implemented (MPI+GPU). **Delayed**	Atmospheric physics features (solar radiation) have to be added to the model. Focus shifted to increasing the UAP overall TRL and optimization of the code.	M30->M38
UAP workflow development	Workflow is CI/CD compatible, including file upload/download.	N/A	M30

	Done		
UAP OpenFOAM solver development	Framework updated to v2406, foam-extend framework implementation in progress. **Done**	N/A	M35
UAP digital twin workflow	Prototype for single GPU developed. MPI and MPI+GPU are under development. **In Progress**	Significant improvements achieved. More time is needed for the development of MPI and MPI+GPU than planned.	M36->M37
UAP model order reduction module	Model order - / orthogonal reduction for the airflow simulation implemented in RedSim (single CPU/GPU). MPI-Implementation ongoing. **In Progress**	Implementation done. More time is needed for the optimization of the code.	M36->M38

3 Urban Buildings

The Urban Buildings (UB) pilot has significantly expanded its capability for city-scale building energy and microclimate simulation through the integration of weather-driven Functional Mock-up Units (FMUs), advanced occupancy scenario handling, and a lightweight sun-position FMU that ensures stable performance at scale. To support systematic benchmarking, a sensor time-series database and accompanying API have been deployed, enabling regression-style validation with KNN-based imputation-although full Modelica-to-FMU automation remains an outstanding limitation. Geometry generation has advanced substantially, now supporting watertight multi-storey reconstruction with detailed floor and roof structures, vegetation meshing, and terrain meshing based on constrained Delaunay triangulation. Solar-mask computation has been parallelized using MPI, with a GPU implementation currently underway. The graphical interface has also evolved, introducing weather configuration inputs, vegetation visualization, and a simulation dashboard capable of launching large-scale runs on HPC systems via SLURM. Looking ahead, the roadmap focuses on extending heating-system regulation, integrating WRF-based weather forecasts, and completing the visualization of simulation outputs. Remaining challenges include achieving fully watertight meshes for all geometric edge cases and improving interoperability between LOD1.0 and LOD2.0 model generations. At this stage, shading-mask parallelization, LOD1.0 simulation support, and benchmarking/CI workflows are fully delivered, watertight meshing is approximately 90% complete, and work on result-visualization components is actively progressing.

3.1 Advances in model development

3.1.1 City Geometry Modeling

Significant progress has been achieved in the geometric representation of urban environments to support more accurate and computationally efficient building energy simulations.

The building geometry now contains slabs, separating each storey. This allows visualizing quantities of interest for each thermal zone, instead of aggregating results by building and losing valuable Information.

Additionally, roof geometries are now computed for five different types [2]: flat, gabbled, hipped, conic/pyramidal and skillion. This addition captures architectural diversity and its influence on solar gains and convective exchanges. The inclusion of non-flat roofs presented non-trivial challenges, particularly in the generation of watertight meshes. This required the use of straight skeleton algorithms [3] and related geometric operations to ensure consistent topological relationships among adjoining surfaces.

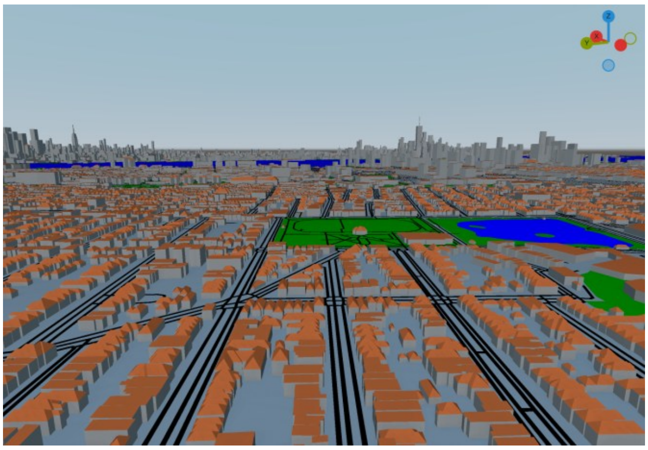

Figure 4. Multiple buildings containing roofs in New York. Visualized using *Ktirio* GUI.

The urban context has been extended to include roads, water bodies, and large paved or green areas such as parks and parking lots. These elements play a key role in defining microclimatic conditions that affect building energy performance. Their integration ensures a more holistic urban energy model that captures both built and unbuilt thermal masses.

Figure 5. Mesh of Strasbourg, containing elevation, green areas, roads, water bodies and buildings. Visualized using *Ktirio* GUI.

Finally, the terrain representation has been substantially optimized. In the previous deliverable, meshing using topography was already supported, although it generated overly refined meshes even in flat areas. This led to excessive computational overhead without added accuracy. The mesh generation process has been optimized from generating around 250,000 vertices per terrain vector tile, to around 500 vertices, reducing mesh complexity by several orders of magnitude while maintaining an acceptable geometric fidelity. This has been done with a contour-based simplification approach. Contour levels are first computed from a 512x512 regular triangular grid, added to a constrained Delaunay triangulation, and simplified using a cost based greedy approach [4] while preserving topological consistency and precision.

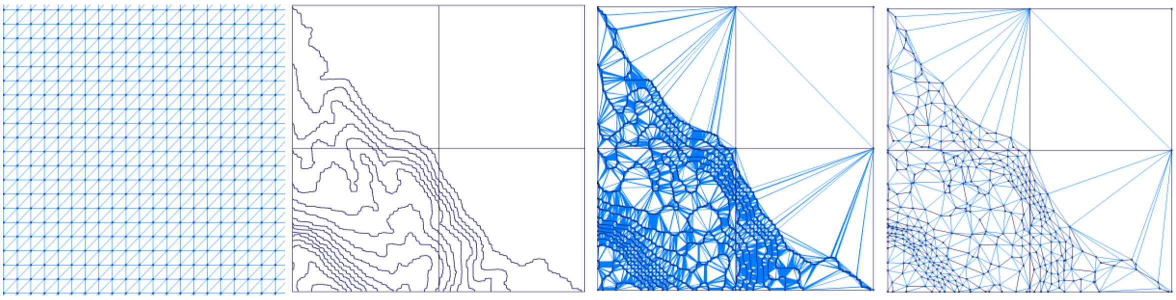

Figure 6. Terrain elevation pipeline: from a structured triangle grid (250k vertices) to a simplified contour level Delaunay triangulation (316 vertices)

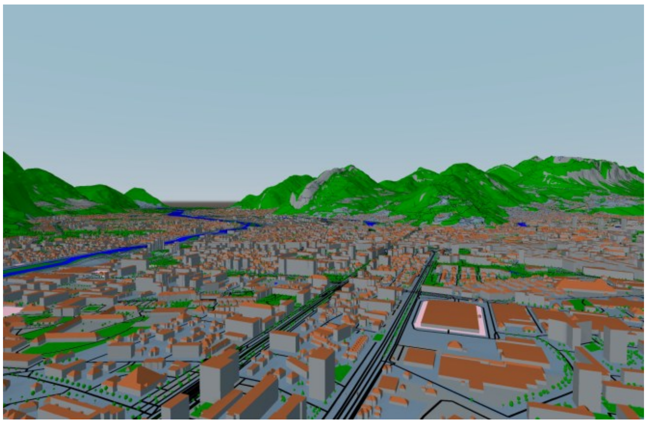

Figure 7. Elevation of mountains in Grenoble, France. Visualized using *Ktirio* GUI.

While these improvements have already been integrated on the Urban Buildings geometry module, work is ongoing to ensure full compatibility and exploitation of these enhancements in the simulation models.

3.1.2 Validation

The validation of the physical models was conducted using the ASHRAE Standard 140-2020 (BESTEST) comparative procedure, focusing on base case: Case 600. This case provides a standardized benchmark for testing the correct implementation of heat transfer, solar radiation, and building energy balance modelling under well-defined boundary conditions.

Comparative simulations were performed against six state-of-the-art programs (BSIMAC, CSE, DeST, EnergyPlus, ESP-r, and TRNSYS). Across all examined metrics (annual loads, monthly heating and cooling balances, peak hourly demands, and solar radiation indicators) *Ktirio* Urban Building's results are consistent with the documented range of agreement.

The annual heating and cooling loads align closely with the reference values, demonstrating coherent thermal response under both winter and summer conditions. Monthly heating and cooling trends follow the same seasonal evolution as other programs, confirming stable envelope modelling.

Overall, the comparison confirms that the implementation of the main physical models in *Ktirio* conduction, convection, radiation, and solar transmission produces results consistent with those from the established reference programs in ASHRAE 140 Case 600.

Validation will be further extended using additional BESTEST cases and through comparison with real-world measurements. Using data from sensors installed in the IRMA Tower, simulation outputs will be compared against monitored building performance to assess model accuracy under actual operating conditions.

3.1.3 Building Energy Modeling

Significant features and improvements have been made to the physical modelling of buildings. We have made various advances in the accuracy and equations of building models, as well as in their generation and use in city energy simulations.

First, our automatic generator for standard models has been redesigned for greater efficiency and readability. New options have also been added in addition to the choice of number of floors: the number of walls per floor, the presence or absence of windows on the walls, the choice of heating system (ideal, boiler, heat pump), and the number of roof panels. Furthermore, a new workflow has been created to generate FMU datasets modelling buildings. Developers can now create different datasets by selecting various parameters in advance, same as for the standard generator, except that the creator chooses the minimum and maximum values they want for parameters such as the number of floors or walls per floor and provides a list for parameters such as heating systems. This workflow is based on our standard template building model generator and our mo2fmu converter. Once generated, the new datasets are automatically uploaded to our Girder data platform.

Second, we have integrated new heating systems, including a heat pump and a boiler with the associated hydraulic circuit, providing one radiator per floor. The sizing of the boiler, heat pump, and radiators is automatically performed during preprocessing. PID controllers regulate the heat flow through each radiator by modulating a valve according to the setpoint heating temperature.

Third, building on our validation work, we have enhanced the accuracy of the physical models and associated calculations. Diffuse solar radiation is now calculated using an anisotropic sky model instead of the previous isotropic approach. Solar transmission through windows is made dependent on the angle of incidence relative to the glazing. The distribution of solar gains within thermal zones, which was previously only partial, has been corrected. Convective heat transfer now accounts for wall surface roughness. Additionally, window modelling was improved by calculating double panes properties from single pane properties.

Fourth, regarding the numerical simulation part, we are able to run simulations in various configurations:

- with FMU datasets in LoD2.0, thanks in particular to the fact that we can now generate models with a variable number of walls per floor. The user can also switch to LoD3.3 FMUs for a specific building if she provides the corresponding FMU (but it will not necessarily have the right mesh because we provide LoD0 and LoD1 meshes).
- with or without windows on each wall, with a configurable glazed area.
- by selecting the type of heating system to be used.

Capabilities now available to the pilot include:

- Dynamic heating systems & control: boiler/heat-pump variants, PI control, auto-sizing.
- Solar masks & shading with vegetation: BVH-accelerated ray tracing with MPI parallelization.
- Material presets with temperature-dependent properties: for building components.
- Scenario editor: setpoints, ventilation profiles, internal gains, and occupancy.
- End-to-end urban meshing & partitioning: buildings, terrain, roads, water, vegetation; HPC-ready.

Other Development Details:

- Geometric modelling: Harden CGAL pipeline, unify labels/materials DB, and partitioning perf pass for a city-wide robust v2.0 by M36; expand to automated tiling/merge and vegetation/terrain v2.0 by ~M42; freeze toolchain v1.3 with docs/CI by EoP.

- Physical modelling (Geom→Phys): Deliver v1.0 radiative environment (SW direct/diffuse, class reflections; LW two-flux; material presets) injected as boundary conditions by M36; add wind maps, first Evapo-Transpiration parameterization, and coarse runoff/impervious effects by ~M42; provide a calibrated set with district validation by EoP.
- Ensembles & Uncertainty Quantification**:** Provide ensemble v1.0 (batch runs + result collation) and UQ skeleton v1.0 with HPDA integration by M36; add dashboards, scenario management, and surrogate/DoE support ~M42; deliver UQ v2.0 with reproducible benchmarks and public datasets/notebooks by EoP.
- Coupling (WRF & UAP): Achieve WRF→UBM v0.5 and specify/prototype UAP↔UBM façade/roof exchange by M36; reach WRF→UBM v1.0 **(**ops**)** and UAP↔UBM v1.0 (limited area**)** **~**M42; deliver district-scale UAP↔UBM v1.0 with a published coupling API by EoP.

As to the challenges ahead, we can split them into 6 categories:

- Geometry & Meshing: (i) city-scale watertightness with heterogeneous roofs/topologies. (ii) CGAL robustness and partitioning edge cases. (iii) unified labels/materials DB to avoid BC mismatches across tiles.
- Radiative & Microclimate**:** (i) SW/LW calibration with vegetation and deep canyons. (ii) wind/roughness downscaling from WRF with stable temporal interpolation. (iii) view-factor accuracy vs performance.
- Hydro-Thermo Coupling**:** (i) pragmatic Evapo-Transpiration and runoff parameterizations without full hydrology. (ii) wetness-driven optics and energy-balance stability.
- Ensembles & Data Pipelines**:** (i) throughput for multi-city I/O and collation with strict provenance. (ii) HPDA dashboards and reproducible regression at scale.
- UQ & Surrogates**:** (i) cost-aware sampling strategies. (ii) surrogate/DoE coverage of scenario space without bias.
- External Coupling**:** (i) WRF→UBM regridding, latency, horizon-length footprints. (ii) UAP↔UBM flux/energy consistency at façade/roof interfaces with limited-area validation.

3.2 Roadmap and challenges

Based on the core capabilities and validation workflows established in the previous phase, the pilot's focus now shifts toward hardening these pipelines for city-scale deployment and deeper environmental coupling. The roadmap has been slightly adjusted to address specific technical complexities identified during testing, particularly regarding geometric robustness and high-fidelity micro-climate integration.

The following table details the current status of key frameworks and outlines the strategic adjustments made to ensure delivery targets are met.

Table 2. Changes in expected Research Results for UB Pilot compared to D5.4

Key framework	Current status as of M35	Reason for roadmap adjustment	Adjusted / new achievement date
Feel++ - Efficiency/scalability: shading-mask parallelization	Delivered (MPI); GPU implementation remains in progress.	Completed in D5.4; no change.	M18
Ktirio-city - Watertight mesh generation	~90% complete; integrated with non-flat roofs and storey slabs; remaining corner cases.	Added geometric complexity (straight-skeleton roofs) and topological consistency checks extended the effort; D5.4 marked it “delayed/90%”.	M36
Ktirio-city LOD-2.0 mesh generation	On track; LoD2.0 operational with floors and multiple roof types.	Scope expanded beyond D5.4 partial LoD-2.0 to include slabs/roof families.	M36

Key framework	Current status as of M35	Reason for roadmap adjustment	Adjusted / new achievement date
Dymola - LOD-2.0 building-model generation	Completed; extended with FMU-dataset generator (mo2fmu) and automated upload to Girder; integrated heating systems & PID control.	Extension beyond D5.4 baseline (“done”) to support scalable dataset creation and regulation.	M18
Feel++/Dymola/Ktirio-city - LOD-1.0 parallel simulation	Delivered and used for city-scale runs; GUI supports HPC job launch.	No change.	M12
Ktirio-GUI - Result visualization & usability	Partially delivered; weather & vegetation views and HPC launch in place; richer result dashboards ongoing.	Prioritized core modelling/geometry and CI; dashboards/HPDA staged after M35.	M36->M42
Ktirio-city - Benchmarking & CI/CD; physics inputs	Delivered; sensor time-series DB & API underpin continuous regression/validation.	No change.	M18
WRF→UBM (one-way)	v0.2 (partial).	Handling large WRF data volumes and grid-to-building mapping required additional work.	M36->42
UAP↔UBM (two-way coupling)	v0.2 (partial).	Coupling API/specification and validation staged with UAP; limited-area first.	M36->M42->M48

Key framework	Current status as of M35	Reason for roadmap adjustment	Adjusted / new achievement date
Validation - BESTEST + real-data (IRMA sensors)	v1.0 on track; Case 600 agrees with reference tools; ongoing sensor-based regression.	Continuous expansion to more cases and seasons.	M36
Environment geometry (vegetation, terrain, roads, water)	v1.0 delivered (vegetation meshes; simplified topography; roads/water integration); further perf/robustness passes planned.	Consolidation in the geometry toolchain planned with the CGAL pipeline hardening.	M36-> M42
Ensemble framework & UQ	Partial (Ensemble v0.3; UQ v0.1).	Integration and method maturation scheduled after core UB features.	M36

4 Renewable Energy Sources

Sensitivity Analysis revealed that wind direction perturbation is the overwhelmingly dominant factor causing wind speed forecast deviations in leeward urban areas; thus, forecast certainty must focus here. To improve accuracy, HPDA processing computes weighted average forecasts from ensemble simulations, providing a robust input for the AI module. The *RES.energy* AI model, trained on PSNC's PV data, combines historical output with future weather forecasts for reliable solar energy generation prediction. Future accuracy will be further increased by integrating sunlight angle and urban shade mask data from Urban Building (UB) simulations, coupling with which is ongoing.

4.1 Advances in model development

4.1.1 Uncertainty quantification and sensitivity analysis

The primary objective of this Sensitivity Analysis was to systematically identify the crucial input weather variables that most significantly impact the accuracy of the wind energy generation forecasts produced by the *RES.EULAG* simulation model, which is driven by *RES.WRF* meteorological data. The analysis aimed to increase forecast certainty and focused on the most impactful parameters, ultimately maximizing the credibility of our predictions.

The extensive series of simulations involved perturbing four key weather inputs-horizontal wind speed, wind direction, pressure, and temperature-using the mUQSA toolbox and the computationally efficient Polynomial Chaos Expansion (PCE) method with 256 samples. The analysis, which focused on the resulting deviation in local wind speed, consistently revealed that perturbations in temperature and pressure were negligible, having no meaningful influence on the output, whereas wind direction perturbation was found to be the overwhelmingly dominant factor. Across all analysed scenarios, including variations in mean wind speed and domain size, a perturbation in the forecast wind direction caused the largest absolute contribution to the output wind speed deviation. Crucially, this significant deviation was not uniformly distributed across the domain; it was highly localised within specific, narrow streaks of terrain situated predominantly in the leeward (downwind) areas behind buildings. Windward areas demonstrated a high tolerance to all perturbations. For accurate energy production forecasting in built-up, leeward environments, ensuring the highest possible fidelity and certainty in the input forecast of wind direction is paramount. This variable's influence is so significant that its initial perturbations propagate and sustain considerable effects on the simulation's results, even over time.

4.1.2 Support for ensembles

There is ongoing work on improving the accuracy of RES forecasts by running multiple ensembles. In order to process the results efficiently, HPDA processing is applied. The primary function is to analyse weather parameters (like wind speed, solar irradiance, etc.) across multiple ensemble members-which originate from different model setups and initial data-and across the entire time series. The key task is to compute a weighted average forecast, where each ensemble member's contribution is scaled based on its historical performance and variable-specific accuracy. This approach ensures that the aggregate forecast is more reliable than any single run. This processing is crucial for generating the final, weighted input for the *RES.ENERGY* (AI-based) module and also supports the creation of monthly climatological averages for climate change impact studies. While the current ad-hoc implementation is functional, the work includes plans to port it to a more scalable HPDA software stack to handle future scaling to hundreds of ensembles.

4.1.3 RES.ENERGY first release

The core purpose of the *RES.energy* module is to accurately forecast the electricity output from solar farms based on predicted weather conditions. This involved creating an AI model, which was trained with the data collected over an entire year of real power generation data from PSNC's 1 MWp solar farm, alongside corresponding meteorological forecasts. Through methodical testing of various neural network architectures, we found that the most effective approach was a complex model capable of using both the historical power output and future weather forecasts simultaneously. This design ensures that the system does not only depend on simple correlations-such as solar radiation being the dominant factor-but instead captures the complex interplay of many variables like temperature or visibility, resulting in a reliable and portable forecasting tool that can be quickly adapted for other solar installations.

4.1.4 Increased accuracy of RES.ENERGY

A significant finding in the development of the solar energy prediction module highlights the need to account for a factor beyond standard meteorological variables (such as temperature and solar radiation) that influence photovoltaic (PV) panel efficiency. This critical additional factor is the sunlight angle relative to the PV system and shade mask for urban environment. The current setup defines the UB scenario around the PSNC's established PV installation. The RES and UB simulations are executed in parallel, and upon completion, the combined meteorological and geometric data will be passed to the *RES.ENERGY* module. This integration is expected to yield a more accurate prediction of solar energy generation.

4.2 Roadmap and challenges

- Containerisation for CI/CD, deployment and user usage: The complex RES workflow initially failed to containerise with Apptainer. We adopted **Docker** to manage the two models and Python runner, leveraging its layered structure for easier building. *RES.EULAG* is now provided as a separate layer, and the next step is converting the Docker image to Apptainer/Singularity**.**
- Integration with UB: finalize the integration to feed *RES.ENERGY* with UB data
- Visualisation: integrate SZE solution it within mUQSA portal, where users will be able not only to prepare and run pilot, but also to see the results in graphic form.
- Efficient ensembles processing: to improve accuracy of the RES toolkit, ensemble runs are needed. The first version of HPDA processing tool fails at efficiency when analysing many large files from the ensembles. The second release of this toolkit will address this issue.
- *RES.ENERGY*: the second release is required which will account data from UB model for increased accuracy

Table 3. Changes in expected Research Results for RES Pilot compared to D5.4

Key framework	Current status as of M35	Reason for roadmap adjustment	Adjusted / new achievement date
WRF and EULAG: improved damages prediction	**Done** The damages prediction account for wind direction and excessive speed.	The model takes into account new vertical wind profile to better model the possibility of the damages.	M36 -> M35

Key framework	Current status as of M35	Reason for roadmap adjustment	Adjusted / new achievement date
EULAG, energy module: cloud solution	**In progress** Initial version of Apptainer is ready, though needs to be switched to a docker and test the scalability of the solution.	More work is required to have different models coupled and orchestrated in cloud environment	M36 -> M42
EULAG, energy module; visualisation advancements	**In progress** Proof-of-concept integration with SZE visualization tool;	More work is required to integrate SZE visualization tools inside portal where RES is running	M36 -> M42
EULAG, energy module: uncertainty quantification	**Done** The UQ/SA was applied to assess the sensitivity of the model of perturbations in initial data related to wind fields.	N/A	M36 -> M34
EULAG, energy module: scalability improvements	**In progress**	More work is required improve scalability.	M36 -> M46
Energy module: predictions improved with HPDA/AI methods	**Partially done** The first version of AI-based energy module is ready. The first version of HPDA processing toolkit (for the ensembles) is ready.	Roadmap is adjusted to account second releases for AI based module (using data from coupled models) and for HPDA (improved efficiency)	M36 -> M42

5 WildFires

The Wildfire Pilot has two main objectives: landscape-scale simulation of fire and smoke behaviour on vegetation structures present in the territory, and urbanisationscale simulation of fires affecting populated areas and atmospheric pollutants generated by combustion.

5.1 Advances in model development

5.1.1 Landscape scale

The main objectives at this stage have been accomplished, while still some minor tasks are to be completed in the remaining runtime of the project.

WRF-Sfire has been tested in different areas on most of the EuroHPC-JU machines, demonstrating its suitability for modelling interactions between fire and the atmosphere.

Furthermore, the suitability of the model for simulating smoke dispersion has been verified. Forest fires emit various pollutants that can affect atmospheric chemistry and influence radiative transfer. These include nitrogen oxides (NOx), carbon monoxide (CO), ammonia (NH3), carbon dioxide (CO2), methane (CH4) and particulate matter (PM10 and PM2.5). As a result, air visibility and quality can be affected. Different emission factors have been used for the types of fuels used in the simulations to study the dispersion of pollutants associated with the fire. The emission factors were estimated using the approach based on Fernandes et al., 2022 [9].

Despite the tied coupling between WRF and Sfire that ensures interactions between fire and the atmosphere, such as the release of heat and water vapour that affects air movements, WRF-Sfire does not seem to be suitable for simulating pyroconvective phenomena, so other approaches will be tested during the rest of the project to assess the feasibility of predicting this type of phenomenon.

Ensembles for the operational assessment of uncertainty associated with the atmosphere have been tested and it is planned to include the territory uncertainty too aiming to arrive to 350 members to fully quantify the uncertainty of real fires. So far, tests have been carried out on sets of more than 20,000 cores in Karolina and Discoverer and new tests are planned to scale up to near 90K cores.

A first version of the Fire Spread Engine (FSE) has been ported to GPU and it is now under improvement to include smoke and pollutants dispersion. WRF-FSE coupling will allow simulation of large fires and fire-complexes as the observed over Spain the Summer of 2025. The final objective is to stablish an operational framework for near real time simulation during the 2026 fire-campaign.

5.1.2 Urbanization scale

Since the previous progress report (Deliverable D5.4), we have made substantial progress in using the *OpenFOAM* simulation framework to model the initiation and propagation of wildfires in wildland-urban interface (WUI) areas, where vegetation fuels are represented as reactive porous media. To achieve this, we have followed a stepwise approach of increasing complexity.

5.1.2.1 Simulation of wind advection effects on turbulent flame diffusion around buildings.

We first implemented a simplified scenario consisting of a detailed 3D model of a building and a block of vegetation (green hedge) located directly in front of its main façade. The vegetation was replaced by a methane (CH_4) burner with equivalent thermal properties. The methane flow rate (0.6 kg/s) was calibrated to produce a 3-meter flame length, corresponding to a linear fire intensity of 4,220 kW/m, representative of this type of vegetation burning in a wildfire.

For this purpose, the *fireFoam* solver was used and carefully parametrized to simulate, as accurately as possible, the generation and turbulent diffusion of flames, taking into account that methane (CH_4) combustion is stoichiometric and does not produce any secondary by-products such as smoke or soot. This simplification is acknowledged, since in wildfires, soot plays a major role in heat transfer processes and significantly influences the turbulent diffusion of heat, mass, and momentum.

The purpose of these simulations is to analyse how combustion dynamics and flame distribution interact with the building structure, identifying zones where flame impingement occurs-particularly on thermally thin components that could contribute to structural involvement.

Special care has been taken to ensure numerical stability and consistent results. The base mesh resolution was set to 10 cm, and the time step was automatically adjusted to maintain a Courant number below 0.9. This aspect is especially critical in turbulent flame diffusion, where local accelerations caused by vorticity play a key role.

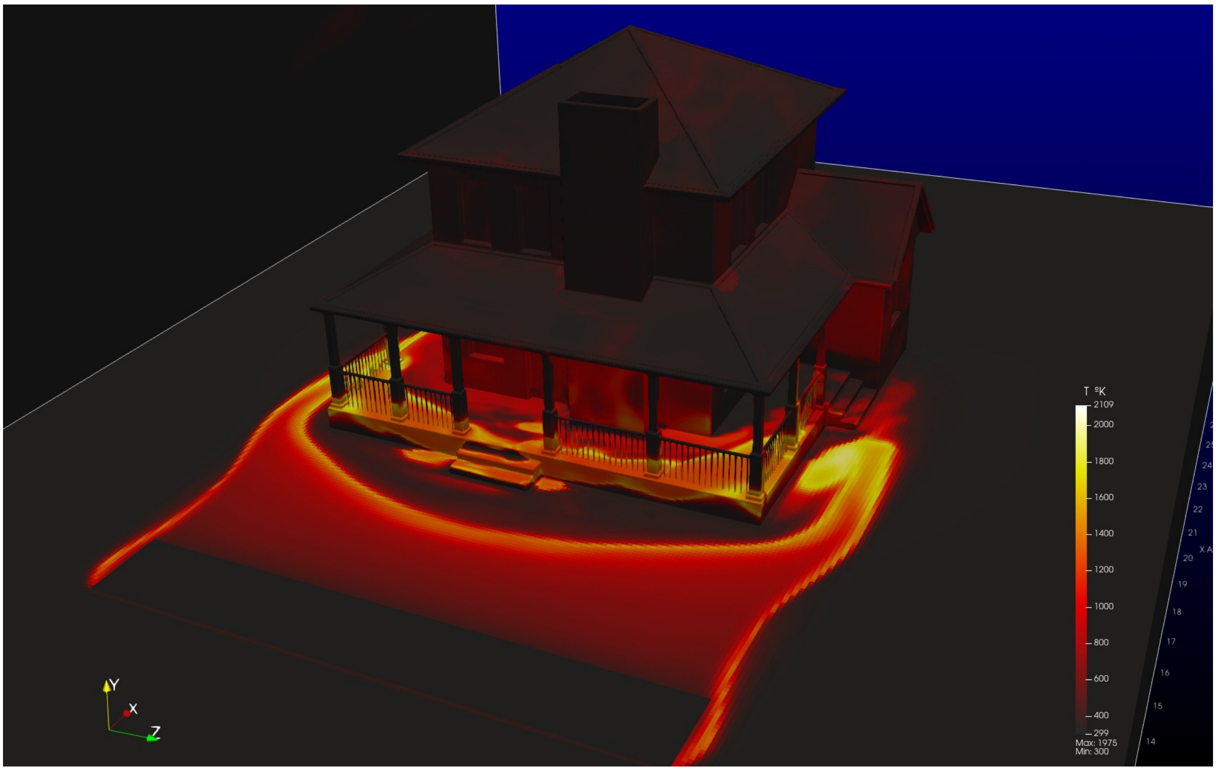

Figure 8. Result of the temperature distribution (K) caused by flame impingement on the surfaces of a structure.

5.1.2.2 Simulation of combustion in reactive porous media.

Forest fuels can be described as porous media composed of a solid phase-interpreted as uniform particles-and a gaseous phase forming the surrounding matrix. Porous media exhibit distinctive characteristics in gas flow behaviour, and in the case of wildland fuel combustion, several coupled processes must be considered: drying, pyrolysis, and oxidation, along with heat transfer through conduction, convection, and radiation within and between the solid and gaseous phases. Additionally, by-products such as charcoal and tar gas are generated, both of which participate in the overall combustion and flame generation processes.

For this purpose, we employed the *porousGasificationFoam* (PGF) solver (Zuk et al, 2022), which couples all these phenomena, making it particularly well-suited for simulating reactive porous beds such as forest fuels. During this reporting period, progress has been made in problem definition, parametrization, and reaction and kinetics specification, as well as in progressive simulations, starting from inert pyrolysis processes and advancing toward coupled combustion and turbulent flame diffusion.

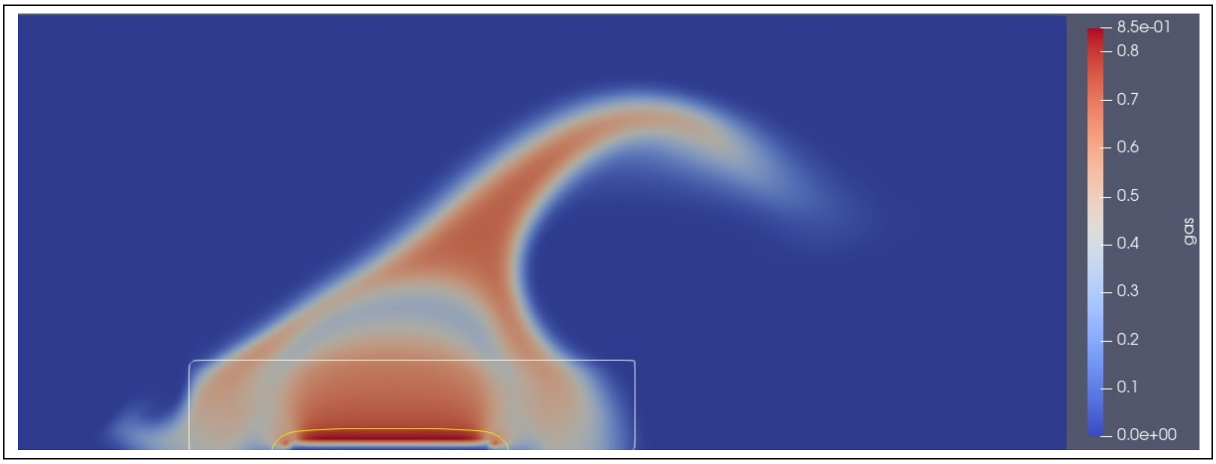

Figure 9. Emission of pyrolysis gases caused by the heating of a reactive porous material block (green hedge) under the effect of a heat-emitting surface.

A detailed selection of the base cell resolution and time step has been carried out to ensure numerical stability, both with respect to the Courant number and the requirements of the chemical kinetics. The latter forces very small-time steps when using high-resolution cells, as required for fuel bed-scale analysis. At coarser resolutions-for example, when analysing fires at the community or urban-scale-average values are used, which partially mitigates this effect.

These simulations have been developed using a multi-scale approach of increasing complexity: the fuel bed scale, the building environment scale, and the urban settlement scale. For this class of simulations, it is essential to describe the spatial distribution of biomass participating in combustion and the corresponding porosity, both expressed as three-dimensional matrices.

To achieve this, we have developed a novel workflow that derives vegetation structure descriptions from detailed 3D geometric models reflecting individual plant architecture. Through fractal sampling of their components, we generate point clouds with associated biomass values, enabling the volumetric estimation of biomass and porosity fields.

As such, *OpenFOAM/PGF* simulations are closely integrated with this biomass and porosity 3D mapping workflow, which is particularly valuable for testing fuel mitigation strategies, silvicultural treatments, and evaluating their impact on wildfire propagation within the WUI. Furthermore, these simulations allow us to calculate smoke emission and dispersion resulting from local combustion processes around buildings.

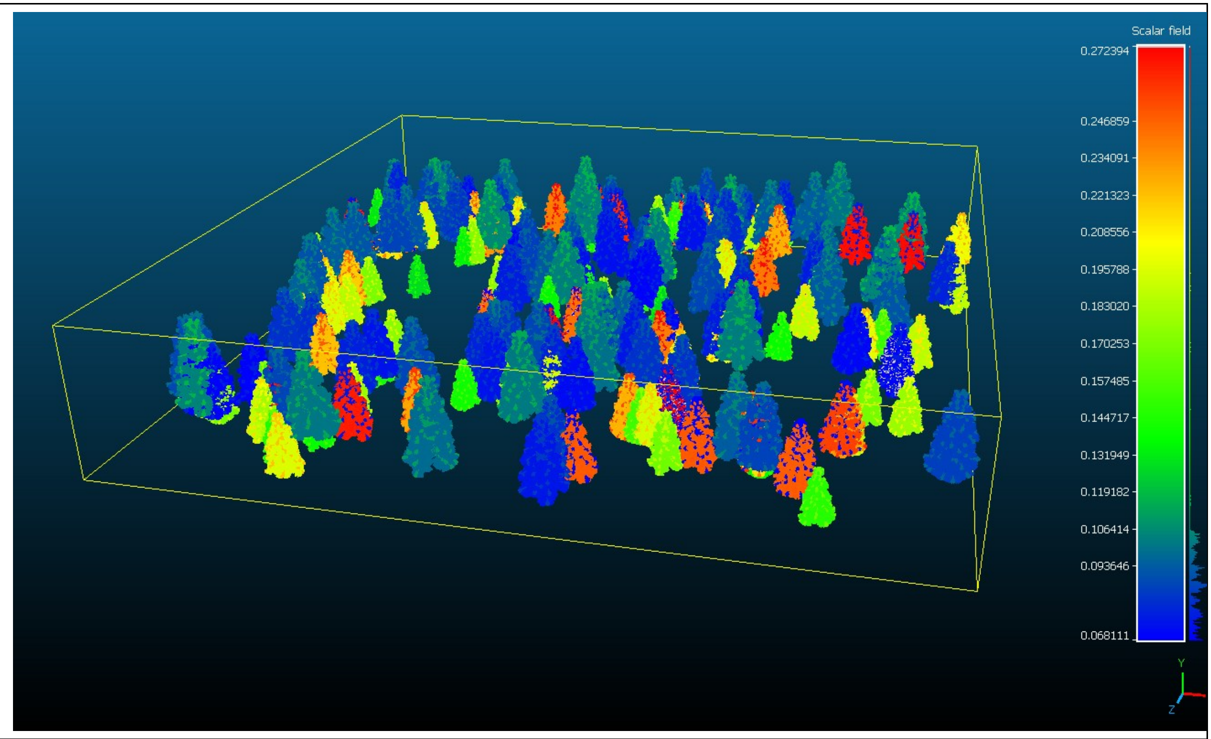

Figure 10. Example of biomass distribution obtained by sampling the detailed 3D models of each plant within a vegetation structure. The result is a point cloud that is later aggregated into voxels representing the combined distribution of biomass and porosity.

5.2 Roadmap and challenges

The roadmap for the identified research challenges are grouped in three chapters:

1. WRF/SFIRE and FSE applications (landscape):
   - Efficient ensembles solution for WRF-Sfire uncertainty quantification solution.
   - WRF-FSE coupling and improvement, including CI/CD containerisation
   - Deployment of the coupled WRF-FSE version during the 2026 firefighting campaign to validate its operational behaviour.
2. *OpenFOAM/PGF* (urbanization):
   - Handling of great meshing schemes to allow the urbanization environment domain
   - Simulation of smoke production and dispersion
   - Considering live and dead fuels in PGF solver
3. Unreal Engine vegetation description and visualization:
   - Improvement of demonstrators for use in preparedness and training activities.

- 3D-Immersive video for MetaQuest 3

Table 4. Changes in expected Research Results for WF Pilot compared to D5.4

Key framework	Current status as of M35	Reason for roadmap adjustment	Adjusted / new achievement date
WRF-SFIRE UQ-QCG	Final release	No change. Progressing as planned	M42
OpenFOAM / PGF	2025: Fuel bed, single house simulation domain. Scalability integration. GPU porting analysis	Progressing as planned. GPU porting analysis is still ongoing.	M36
OpenFOAM / PGF	2026: Urbanization environment domain	Progressing as planned.	M42
Unreal Engine	WRF-SFIRE VR Demonstrator	Finalized in month 34. New versions adapted to the new case studies are currently being developed.	M34->M42
Unreal Engine	*OpenFOAM/PGF* VR Demonstrator	Progressing as planned.	M42
Unreal Engine	3D-Immersive video for MetaQuest 3	Progressing as planned.	M42

6 Material Transport in Water

In the earlier deliverable D5.4, the Material Transport in Water (MTW) pilot was introduced, marking the first deliverable in which MTW contributed to the research advancements within the pilot activities. During this phase, fluid-scalar coupling mechanisms were developed, including both one-way and two-way coupling approaches. Additionally, initial strategies and conceptual frameworks for extending the model toward fluid-scalar-particle coupling were discussed, setting the foundation for the subsequent developments presented in the current deliverable.

6.1 Advances in model development

Significant advancements have been achieved in the pilot model development since the previous deliverable (D5.4). In D5.4, the capability of *waLBerla* to simulate fluid-scalar coupling was presented in detail, while the fluid-scalar-particle coupling was identified as a key future objective. Since then, the model has evolved substantially to incorporate and validate this coupling mechanism.

During M28, the first milestone was achieved by integrating particles with constant and uniform temperatures into the coupling framework. This marked the first successful realization of fluid-scalar-particle coupling within the *waLBerla* environment. The implementation was rigorously validated to ensure numerical accuracy and physical consistency.

In the subsequent period, between M29 and M30, the model was further extended to enable conjugate heat transfer (CHT) with identical thermophysical properties for both fluid and particles. This represented a major development milestone, as it introduced the ability to resolve temperature fields within particles, allowing for heat conduction within the particles.

From M31 to M35, the model capabilities were significantly enhanced to account for different thermophysical properties between particles and the surrounding fluid. This improvement reflects a more realistic physical representation of particle-laden thermal flows, where such property variations naturally occur. The extended model has been thoroughly validated using both single-particle and multi-particle test cases involving transient motion within the simulation domain.

All CHT kernels have been implemented using lbmpy and are fully code-generated, ensuring optimized performance and compatibility across both CPU and GPU architectures. This modular and portable design supports scalability and efficient deployment for large-scale simulations.

With the current status of the model, it is planned to submit a paper demonstrating the robustness of the current CHT model in hand.

6.2 Roadmap and Challenges

The forthcoming development steps appear highly promising, though certain challenges are anticipated. The current model demonstrates strong accuracy for low-Prandtl-number cases. However, high-Prandtl-number scenarios have yet to be fully explored. It is expected that, within specific parameter constraints, the model will remain stable and accurate for Prandtl numbers up to 7, corresponding to water.

A major challenge moving forward will be the application of the model to realistic, high-fidelity parameter ranges that reflect real-world physical conditions. In such cases, the numerical stability and robustness of the model remain uncertain. Consequently, extensive testing and validation under realistic operating conditions will be essential to ensure the reliability and predictive capability of the developed framework.

Apart from this due to the establishment of model to its current state, we were able to come up with strategies to approach the tasks of ensembles and uncertainty quantification. This work would begin partially until the end of M36 and strictly taken forward from M37 onwards.

Table 5. Changes in expected Research Results for MTW Pilot compared to D5.4

Key framework	Current status as of M35	Reason for roadmap adjustment	Adjusted / new achievement date
waLBerla: Validations	Done	N/A	N/A
lbmpy-implementation of SRT/TRT collision operators	Done	N/A	N/A
waLBerla, lbmpy - code porting towards GPU	Almost in the finishing stages, would be complete by end of January or start feb	Time consumed to get the pipeline running on CPU and synchronize it with GPUs	M38->M39

Key framework	Current status as of M35	Reason for roadmap adjustment	Adjusted / new achievement date
waLBerla - runs for the ensembles and uncertainty quantification scenarios	Codes porting is done; simulation runs planned beginning end of January	Time taken to strategise the key scenario for a relevant study for uncertainty quantification and ensemble scenarios	M42

7 Conclusions

In general, from M24 to M35 significant progress has been achieved across all five pilots, accompanied by some notable challenges:

I. Urban Air Pollution (UAP):

The UAP pilot achieved significant progress in urban airflow and air-quality modelling during this period. The workflow was successfully applied to real-city scenarios, most notably Stockholm, enabled by major improvements in geometry processing, terrain handling, and meshing. All three solvers-*UAP-FOAM*, *RedSim*, and *Xyst*-advanced in performance, scalability, and GPU readiness. RedSim's new MPI+CUDA framework and Xyst's strong scaling on LUMI notably strengthened UAP's exascale potential. Some planned activities, such as surrogate modelling and extended atmospheric physics, have been postponed focussing on real-application deployment. Overall, UAP is now well positioned for upcoming coupling tasks and for progressing toward a digital-twin-ready urban air-quality platforms.

II. Urban Buildings (UB):

The UB pilot recorded major advancements in both modelling fidelity and workflow robustness. Significant improvements in geometry generation-including watertight multi-storey buildings, complex roof typologies, terrain simplification, and environmental features-substantially increase the realism of urban simulations. Parallel ray-traced shading expanded FMU libraries, new heating system models, and improved radiative and convective formulations strengthen the physical accuracy of building energy predictions. Validation against ASHRAE BESTEST confirms correct implementation of core thermal processes. Remaining challenges lie in generalising the geometry pipeline across diverse urban topologies and extending microclimate coupling with atmospheric and air-quality models. Overall, the UB pilot is on a strong trajectory toward scalable, city-wide digital building simulations.

III. Renewable Energy Sources (RES):

The RES pilot achieved substantial progress in sensitivity analysis, ensemble-based forecasting, and AI-supported renewable energy prediction. The identification of wind-direction uncertainty as the most influential driver of wind-energy forecast variability is a key scientific outcome that guides the refinement of model coupling strategies. The first release of the RES.ENERGY neural-network model, trained on real PV-farm data, demonstrates the feasibility of integrating HPC weather forecasts with AI-based renewable prediction. Ongoing work on containerisation, scalable ensemble processing, and UB-RES coupling will further enhance operational readiness. These results establish robust groundwork for high-certainty, data-driven renewable energy forecasting workflows.

IV. Wildfires (WF):

The WF pilot made major strides in both landscape-scale and urban-scale fire modelling. WRF-SFIRE simulations successfully ran on multiple EuroHPC systems with demonstrated scalability, supporting high-resolution studies of fire-atmosphere interaction. The GPU-accelerated Fire Spread Engine and ongoing coupling with atmospheric and smoke-transport models provide a promising path toward near-real-time operational capability. At the WUI scale, the integration of *OpenFOAM* and *porousGasificationFoam* models enabled detailed simulation of pyrolysis, flame spread, and smoke generation in complex-built environments. Additionally, new workflows for vegetation structure reconstruction and VR-ready visualisation broaden the utility of wildfire simulations for both analysis and emergency-management scenarios. The WF pilot is now well-positioned to deliver multi-scale fire-behavior predictions with strong scientific and societal relevance.

V. Material Transport in Water (MTW):

The MTW pilot has progressed rapidly from early fluid-scalar coupling to a fully validated framework for conjugate heat transfer in fluid-particle systems. The newly developed models support temperature evolution within particles, heterogeneous thermophysical properties, and GPU-accelerated execution-all essential for realistic simulations of thermal transport in aquatic environments. Validation against single particle and multi-particle scenarios demonstrates numerical stability and physical correctness. The upcoming challenges relate to extending the model to high-Prandtl-number regimes, performing large-scale ensemble simulations, and integrating uncertainty quantification workflows. Overall, the MTW pilot has transformed into a robust simulation tool capable of addressing complex water-borne transport phenomena.

Next Steps

I. Urban Air Project

Future work for the UAP pilot will focus on finalizing the integration of atmospheric physics, advancing digital-twin prototyping, and consolidating GPU-enabled workflows. In parallel, efforts will be directed toward strengthening multi-solver coupling with the Urban Buildings (UB) pilot and the WRF framework. Building on these developments, RedSim and Xyst will be further advanced toward exascale readiness, alongside the completion of preprocessing extensions for vegetation representation and high-detail urban geometry.

II. Urban Buildings

Future efforts will prioritize the completion of watertight geometry v2.0, the extension of micro-climate coupling (WRF ↔ UBM and UAP ↔ UBM), and the hardening of radiative and micro-climate models for robust city-scale simulations. This will be followed by the delivery of visualization dashboards, ensemble and uncertainty-quantification tools, and district-scale coupled simulations to support operational digital-twin deployment.

III. Renewable Energy Sources

Future work will focus on finalizing the UB-RES coupling and upgrading the RES.ENERGY module to incorporate geometric shading and refined ensemble-based HPDA workflows. These efforts will be followed by improvements in containerization, scalability, visualization integration, and forecast accuracy through the deployment of second-generation AI and HPDA modules.

IV. Wildfires

Future activities will advance WRF-SFIRE and FSE-WRF coupling toward near-real-time operational readiness, including the development of GPU-accelerated fire-spread and smoke-dispersion models. In parallel, PGF/OpenFOAM simulations for wildland-urban interface (WUI) scenarios will be extended, vegetation-biomass workflows will be unified, and VR demonstrators will be delivered for both landscape- and urban-scale fire scenarios.

V. Material Transport in Water

Future work will extend the model toward high-Prandtl-number regimes, refine robustness under realistic physical conditions, and initiate ensemble and uncertainty-quantification studies on upgraded GPU pipelines. In addition, the new conjugate heat transfer (CHT) model will be applied to complex water-environment scenarios, and large-scale demonstrations will be prepared to support forthcoming publications.

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Appendix

The following 5 figures show the main research activities within the five pilots, as well as the milestones in each of them. Milestones in blue refer to deliveries of partial functionality, deliveries that will make it possible to evaluate the progress of the activity and check the progress in functionality. Milestones in red refer to deliveries of the research lines that are explained in respective chapter of the pilot.

UAP roadmap figure

Table 6. Main research activities in the UAP Pilot and the main milestones in each of them

Roadmap figure	Before M24	M25-M27	M28-M30	M31-M33	M34-M36	M37-M39	M40-M42	M43-M45	M46-M48
Optimisation of preprocessing tools									♦
UAP UQ					♦				
UAP coupling frameworks; WRF, UB,Wildfires									♦
UAP airflow and air quality (*simpleFOAM/pipmpleFOAM/reactingFOAM*)									
Thermal simulations with UAP *reactingFOAM*									
RedSIM in the UAP framework				♦					
RedSIM digital twin prototype for the city of Györ						♦			

Further Physics in RedSIM								◆ (red)	
RedSIM AI version							◆ (red)		
Xyst solver development									
UAP digital twin							◆ (red)		

UB roadmap figure

Table 7. Main research activities in the UB Pilot and the main milestones in each of them

Roadmap figure	Before M24	M25-M27	M28-M30	M31-M33	M34-M36	M37-M39	M40-M42	M43-M45	M46-M48
Improve benchmark dataset									◆ (red)
Improve geometric modelling					◆ (blue)			◆ (red)	
Improve CI/CD/CB									
Improve heat transfer modelling					◆ (red)				
Improve graphical user interface					◆ (blue)			◆ (red)	
Support HPDA and ML									◆ (red)
Coupling UB and UAP					◆ (blue)			◆ (red)	
Coupling UB and MTG					◆ (blue)			◆ (red)	

RES roadmap figure

Table 8. Main research activities in the RES Pilot and the main milestones in each of them

Roadmap figure	Before M24	M25-M27	M28-M30	M31-M33	M34-M36	M37-M39	M40-M42	M43-M45	M46-M48
RES + UQ/QCG					◆				◆
RES Coupling models - coupling using orchestrator static					◆			◆	
RES HPDA/AI - module for energy prediction					◆		◆		◆
RES AI performance analysis and optimization									◆
RES visualization							◆		◆
Definition and development of new RES functionalities	◆				◆				◆

WildFires roadmap figure

Table 9. Main research activities in the WF Pilot and the main milestones in each of them

Roadmap figure	Before M24	M25-M27	M28-M30	M31-M33	M34-M36	M37-M39	M40-M42	M43-M45	M46-M48
Coupling WRF with Sfire modules on HPC			◆ (red)						
Coupling *OpenFOAM*/*fireFoam* for wildland urban interface	◆ (blue)				◆ (red)				
WRF-Sfire HPDA/AI for fire prediction spread	◆ (blue)				◆ (blue)			◆ (red)	
WRF-Sfire high resolution parameterization improvement	◆ (blue)				◆ (red)				
WRF-Sfire + UQ/QCG	◆ (blue)						◆ (red)		
Sfire performance improvement				◆ (red)					
Visualization of vector fields and particle tracers in Unreal Engine		◆ (red)							
Wildfires-UAP coupling					◆ (blue)		◆ (red)		
GPU FSE model (data calculation for HPDA/AI/UQ)					◆ (blue)		◆ (red)		
OpenFOAM/*PGF* Single house domain			◆ (blue)		◆ (red)				
OpenFOAM/PGF Urbanization domain						◆ (blue)	◆ (red)		
WRF-Sfire demonstrator				◆ (blue)			◆ (red)		
OpenFOAM-fireFoam demonstrator					◆ (blue)			◆ (red)	

MTW roadmap figure

Table 10. Main research activities in the MTW Pilot and the main milestones in each of them

Roadmap figure	Before M24	M25-M27	M28-M30	M31-M33	M34-M36	M37-M39	M40-M42	M43-M45	M46-M48
one-way fluid-scalar coupling validation	◆ (red)								
two-way fluid-scalar coupling validation	◆ (red)								
fluid-particle-scalar coupling validation /showcase				◆ (blue)				◆ (blue)	◆ (red)
Surrogate model fluid-scalar coupling									
Benchmark and scaling runs for fluid-scalar								◆ (red)	
Benchmarking and scaling runs for fluid-scalar-particle					◆ (blue)	◆ (blue)	◆ (blue)	◆ (blue)	◆ (red)
Further physical validations and evaluation of a complex setup						◆ (blue)	◆ (blue)	◆ (blue)	◆ (red)
Visualization of simulations						◆ (blue)	◆ (blue)	◆ (blue)	◆ (red)

Legend:

◆ (red): full release

◆ (blue): partial release