D5.4 Research Advancements for the Pilots

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CENTRE OF EXCELLENCE

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List of Acronyms

Abbreviation / acronym	Description
3D	Three-Dimensional
API	Application Programming Interface

Abbreviation / acronym	Description
BVH	Boundary Volume Hierarchy
CGAL	Computational Geometry Algorithms Library
ChoCG	Continuous Galerkin method of Alexandre Chorin
CO2	Carbon Dioxide
DOF	Degree of Freedom
Dx.y	Deliverable number y belonging to WP x
EC	European Commission
FMU	Functional Mock-up Unit
FSE	Fire Simulation Engine
GIS	Geographic Information System
GPU	Graphics Processing Unit
GUI	Graphical User Interface
HyTeG	Hybrid Tetrahedral Grids
IFC	Industry Foundation Classes
JSON	JavaScript Object Notation
KNN	K-Nearest Neighbours
LaxCG	Continuous Galerkin method of Péter Lax
LES	Large Eddy Simulation
Modelica	Object-Oriented Modelling Language
MPI	Message Passing Interface
MTW	Material Transport in Water
OpenStreetMap	Collaborative Open Geospatial Data Platform
PBL	Planetary Boundary Layer
PDE	Partial Differential Equation
PET	Physiologically Equivalent Temperature
PMV	Predicted Mean Vote
PPD	Predicted Percentage of Dissatisfied
RES	Renewable Energy Sources
SA	Sensitivity Analysis
SLURM	Simple Linux Utility for Resource Management
SME	Small and Medium Enterprise

Abbreviation / acronym	Description
UAP	Urban Air Project
UB	Urban Building
UI	User Interface
UQ	Uncertainty Quantification
VOCs	Volatile Organic Compounds
waLBerla	widely applicable Lattice Boltzmann from Erlangen
WF	Wild Fires
WPx	Work Package x
WUI	Wildland Urban Interface
ZalCG	Continuous Galerkin method of Steven Zalesak

Executive Summary

HiDALGO2 focuses on the development of high-fidelity simulations to address critical global challenges. This document builds on the foundations of D5.3 [1] by highlighting the research advances achieved within the HiDALGO2 project between M11 and M23 across the five pilot applications: **Urban Air Project (UAP), Urban Buildings (UB), Renewable Energy Sources (RES), Wildfires (WF),** and the newly introduced **Material Transport in Water (MTW).** It emphasizes enhancements in solver modelling, accuracy, and versatility, alongside adjustments to the roadmaps based on unforeseen challenges and newly found intel.

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, have significantly improved the simulation of urban airflow and pollutant dispersion. Enhanced pre-processing tools utilizing OpenStreetMap further support detailed urban environmental modelling. However, to incorporate atmospheric physics features into this pilot project 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 pollutant transport in aquatic environments, addressing pollution from microplastics and chemical contaminants. Notable achievements include successful fluid-particle coupling, nearing completion of fluid-scalar coupling, and handling complex boundary conditions across CPU and GPU architectures. While full fluid-particle-scalar integration is ongoing, the MTW pilot is positioned to contribute to sustainable water management through real-world applications in river pollution simulation.

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, including D5.5, 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 D5.4, is to report on the progress achieved in the HiDALGO2 project's pilot applications up to month 23 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 in refining the pilots' performance, contributing to the overarching goal of evolving these applications into effective digital twins.

In addition to providing updates on the four original pilots—Urban Air Project (UAP), Urban Buildings (UB), Renewable Energy Sources (RES), and Wildfires (WF)—this deliverable introduces a new pilot, Material Transport in Water (MTW), which has not been previously covered in D5.3 [1]. The MTW pilot enhances the HiDALGO2 project's scope and strengthens its capacity to tackle global challenges through advanced simulations.

1.2 Relation to other project work

This deliverable, D5.4, follows on from D5.3 [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 the efforts of WP3, which focuses on supporting global challenges with exascale computing, and WP4, which handles data exploration and visualisation.

The introduction of the MTW pilot in D5.4 is a significant development that extends the range of challenges addressed by HiDALGO2. The pilot builds on the methodologies established in D5.3 [1] and introduces new simulation requirements, integrating them with the ongoing work in the other four pilots.

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, the addition of the new MTW pilot, 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 5 Focus on the specific research conducted by the UAP, UB, RES, and WF pilots. These chapters present advances made from M11 to M23 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 6 MTW Pilot. Introduces the MTW pilot, a new addition to HiDALGO2 that was not included in D5.3 [1]. This chapter covers its scientific baseline, research challenges, and progress made up to M23, bringing the MTW pilot in line with the four original pilots before outlining the software developments and strategic roadmap.

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, D5.5.

2 Urban Air Project (UAP)

Urban Air Project (UAP) is an HPC-framework with applications for computing the airflow in cities and based on the computed wind field, the air comfort, air quality, and planning-related KPIs computation. UAP utilizes HPC to deal with high resolution models. It also uses in-house developed pre-processing tools to generate the proper 3D geometry from OpenStreetMap and 3D mesh from the geometry, and post-processing tools for evaluation and visualization.

2.1 Advances in model development

UAP has three different solvers for the airflow and air quality computation, including: UAP-FOAM, RedSim and Xyst. The advances of these solvers achieved in the reporting period, M11-M23, are reported in separate sections.

2.1.1 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 2406, also a foam-extend version is under way. Development has been put forward to MathSO portal and MathSO CI/CD integration. The supporting workflow now introduced portal-supported input download and results upload. A separate workflow for mesh creation is fully separated and integrated. Higher resolution meshes are created to further investigate model accuracy.

2.1.2 RedSim advances

RedSim solves the Euler and Navier-Stokes equations for compressible fluids by using upstream finite volume methods and explicit time-stepping and solves the scalar transport with the implicit Euler time-stepping scheme.

In the reporting period, the MPI and the MPI+GPU-versions of RedSim have been developed and optimized, which support OpenMPI and CUDA libraries. The implementation was also tested on city geometries, including thorough tests for geometry of Győr with up to 512 CPU- and 8 GPU-nodes of the EuroHPC-machine KAROLINA.

According to the findings of the optimizations, several mesh partitioning codes were investigated and added to the code base, namely METIS, ParMETIS, and ZOLTAN. According to our experiments, METIS was not useful for meshes above 10 million cells, ParMETIS above 30 million cells and a partition number above 128. Within all experiments, ZOLTAN 1[1] was the most reliable mesh partitioner.

For the scalar transport, the linear advection-diffusion equation with parameters of the atmosphere have been solved. Both implicit and explicit methods were implemented and used for time stepping.

An essential tool by design, the NVIDIA AMGX solver has been integrated into the RedSim code base. This state-of-the-art linear equation solver tool will be used also for the implicit time-stepping for the airflow computation, of which development is ongoing.

To increase the accuracy of the solvers, which is requested by another industrial applications of RedSim (pipe-flow noise computation) as well, the 2nd-order schemes have been implemented into the parallel code. The algorithm requests linear reconstruction of the physical variables on the cell faces, which requested, in the current solution, a state-interpolation to vertices. This step increased the complexity of the parallelization significantly. Testing the accuracy gain of the 2nd-order scheme over the 1st-order scheme for the urban wind field computation is ongoing.

The preprocessing tool to extract 3D geometry from OpenStreetMap has been further developed to treat issues with the map data.

2.1.3 Xyst advances

Since D5.3 [1] code development in Xyst continued on two different specialized flow solvers: LaxCG and ChoCG, see also [2] for a high-level overview.

LaxCG is a low-Mach-number extension of a hyperbolic solver, whose numerical method, in general, is most effective at moderate to high Mach numbers, computing compressible flows. With the low-Mach-number extension LaxCG becomes effective at computing nearly incompressible (constant-density) flows. Without this extension the simulation of such low-speed flows frequently fails to converge, due to the numerical stiffness as a result of the large ratio of advective and acoustic time scales. After its prototype initial implementation, the LaxCG solver has now been tested, verified, validated, documented, and thus ready for production use.

A new solver was also added to Xyst, named ChoCG. This is a very different solver compared to all existing solvers in Xyst, which are all density-based. ChoCG is a pressure-based solver targeting the time-accurate computation of incompressible (low-speed, exactly constant-density) flows. The algorithm employs a projection scheme to ensure exact divergence-free flow velocities and targets the 2nd-order numerical accuracy in both space and time, as the usual requirement in engineering practice.

[1] ZOLTAN 1 is the original ZOLTAN C-code.

ChoCG solves the incompressible (viscous) Navier-Stokes equations coupled to N transported scalars representing pollutant concentrations. The projection algorithm is believed to be the state-of-the-art (in terms of accuracy and efficiency) for the simulation of time-accurate incompressible flows. In Xyst the projection method is combined with a multi-stage semi-implicit time-discretization and the resulting large linear systems are solved by a preconditioned conjugate gradient algorithm. As all solvers in Xyst, the implementation is an edge-based finite element method for unstructured, tetrahedral meshes. The code is fully asynchronous, parallel, targeting the largest distributed-memory machines. The first prototype implementation of the ChoCG algorithm now works, its verification is currently underway using various test problems, comparing to analytic solutions and to other well-established and published results of the literature. Preliminary tests of strong scalability of this new ChoCG solver implementation shows promising results both at small, $O(10^2)$, as well as larger, $O(10^4)$, number of CPUs, using mesh sizes with $O(10^6)$ and $O(10^8)$ DOFs, respectively, tested on LUMI.

Since D5.3 [1], a new peer-reviewed journal paper [3] was published by the SZE team, which discusses the algorithm implemented in Xyst as ZalCG and demonstrates saving CPU time by dynamically deactivating partitions of the computational domain combined with automatic load-balancing during parallel simulations of propagating phenomena, such as urban-air pollution scenarios.

2.2 Roadmap and challenges

2.2.1 UAP-FOAM

Currently our work still faces challenges in two implementations of the UAP-FOAM solver application in backlog. 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 which are planned to be accomplished in the next months. Also, development in this area will need to be finer grained.

Second, the current implementation and workflow needs cleanup for a more feasible integration with coupling technologies. Parts of the workflow need to be delegated to other tools, including HPC detection, and environment setup. These updates will facilitate proper ways for coupling mechanisms to be implemented.

For lessons learned, one of the critical tasks of our investigation is to clean up and maintain code properly. This enables us to do code integration and development more seamlessly.

According to the roadmap, code cleanup activities become one of the main tasks planned to be accomplished in the next months. Afterwards, both coupling scenarios and compressible solvers can be properly introduced. Finally, 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.

2.2.2 Xyst

Regarding changes, besides a single new solver in Xyst for constant-density flow, two variants were implemented (see below for more details).

The first lesson learned during the completion and initial usage of LaxCG in Xyst, is that its preconditioning method is problem-dependent due the reference velocity (a model parameter) that the user needs to provide externally. This decreases user-friendliness of this solver since it requires advanced user expertise. Furthermore, we observe, that time-accurate calculations will likely require sub-iterations within every time step. While this is possible, it also likely reduces applicability and utility compared to a projection-type solver, see below.

The implementation of a new ChoCG solver for constant-density flow has been undertaken in next step of our work. Since this is a projection-type pressure-based solver, it does not require sub-cycling for time-accurate flows. One potential challenge with the ChoCG solver will be the requirement to solve the elliptic Poisson equation in each time step, which can be time-consuming and might require advanced preconditioners for fast convergence. Furthermore, this solver can also have scalability problems at large CPU counts, due to the linear solver algorithm and due to the complexity of the preconditioner and its implementation in parallel. Potential remedies for these challenges are to explore different preconditioners, e.g., algebraic multigrid, for the Poisson equation and/or yet a different solver for constant-density flow that altogether eliminates the need to solve a Poisson equation. Ultimately, having multiple types of solvers for the same family of problems should be useful in practice targeting specific application areas.

Table 1 Changes in expected Research Results for UAP Pilot compared to D5.3

Key framework	Status as of M23	Reason for roadmap adjustment	Adjusted / new achievement date
RedSIM algorithm	Spatial 1st, 2nd order scheme for Euler and Navier-Stokes equations; advection-diffusion solver for dispersion implemented (MPI+GPU). **Delayed**	Atmospheric physics features (solar radiation) have to be added to the model.	M18->M30

Key framework	Status as of M23	Reason for roadmap adjustment	Adjusted / new achievement date
UAP workflow development	Workflow is CI/CD compatible, including file upload/download. **Delayed**	Code cleanup is necessary for code release.	M10->M30
UAP OpenFOAM solver development	Framework updated to v2406, foam-extend framework implementation in progress. **Delayed**	Focus shifted on UAP-FOAM workflow development.	M18->M36
UAP digital twin workflow	Prototype for single GPU developed. MPI and MPI+GPU under development. **Delayed**	More time is needed for the development for MPI and MPI+GPU than planned.	M36->M30
UAP model order reduction module	Model order - / orthogonal reduction for the airflow simulation implemented in RedSim (single CPU/GPU). MPI Implementation ongoing. **In progress**	N/A	M36
RedSIM MPI+multi-GPU version	Development and optimization done for 1st and 2nd order spatial discretization. **Done**	N/A	M18->M22
Xyst ZalCG solver	New journal paper published in Computational Physics [3]. **In progress**	N/A	M24 (new)
Xyst LaxCG solver	Prototype implemented. Solver is tested, verified, validated, documented, and ready for production use. **Done**	N/A	M23 (new)
Xyst ChoCG solver	Prototype implementation works, verification ongoing, strong scalability to 65K CPUs on LUMI is promising [2]. **In progress**	N/A	M23 (new)

3 Urban Buildings (UB)

Urban Building pilot focus on improving building energy efficiency and aims to predict energy consumption, thermal comfort and air quality. It operates on both the building and the urban scales. The pilot has advanced in several key areas, including simulation accuracy, geometry modelling, and overall usability. This progress has been facilitated through the integration of various tools such as automatic benchmarking of urban building simulations, data visualization and improved graphical interface.

3.1 Advances in model development

The new GIS2FMU workflow integrates GIS data with FMUs, creating detailed building models by extracting critical information from GIS files and using machine learning to fill gaps. While challenges remain in automating Modelica-to-FMU conversion, the tool sets a strong foundation for realistic urban modelling.

Improvements include enhanced city simulation with weather data integration via the Open Meteo API, versatile FMU models, automatic building generation, and refined energy metrics like Physiological Equivalent Temperature (PET). Geometry modelling has progressed with detailed building reconstructions, vegetation-based shading, and optimized terrain meshing using Delaunay triangulation. Ray tracing for shading masks is being refined with parallel MPI and GPU implementations.

The updated user interface supports data generation, 3D visualization, and simulation management on supercomputers via SLURM pipelines. Future plans for predictive weather modelling and enhanced environmental features will further align the pilot with energy efficiency and sustainability goals.

More details are provided in subsequent sections.

3.1.1 Modelling

Enhancements to the city simulation code include the addition of weather data as an input, selected by users via the Ktirio GUI, utilizing the Open Meteo API. FMU models were made more versatile to handle any weather data and geolocation, enabling accurate sun positioning. A lightweight, building-independent FMU model was introduced to calculate and transmit the sun's position to all models, ensuring uninterrupted execution even if individual building simulations fail. Filters were added to exclude irrelevant buildings with small volumes or areas. Scenarios were developed to assign heating, cooling, and ventilation setpoints by building category, based on schedules, weekdays, or vacation periods. Users can create and allocate custom scenarios or exclude specific building types from simulations.

Building model improvements include an automatic generator for standard models, capable of differentiating between insulated and non-insulated buildings and adjusting floor counts. An ideal heating and cooling flow option was added to maintain set indoor temperatures by counteracting outdoor heat loss or gain, enabling energy consumption and power output calculations. The addition of building-type-specific scenarios, with temperature settings adjusted for occupancy or vacancy, enhances energy consumption modelling and represents a step toward a regulation system.

A new comfort indicator, PET, was implemented alongside PMV and PPD. PET computes the thermal balance of the human body under complex environmental conditions, offering a more versatile and parameter-rich alternative to PMV. Work on a detailed heating system, including pumps, pipes, radiators, and boilers or heat pumps, is ongoing, with a regulation system currently in development.

3.1.2 Reporting

A workflow has been established to facilitate urban-scale analysis, generating reports on weather data, energy consumption, and comfort assessment. Once new features are integrated or simulations for specific geographic locations are executed, the pipeline automatically updates a website [4] featuring a gallery of reference cities, which shown in Figure 1.

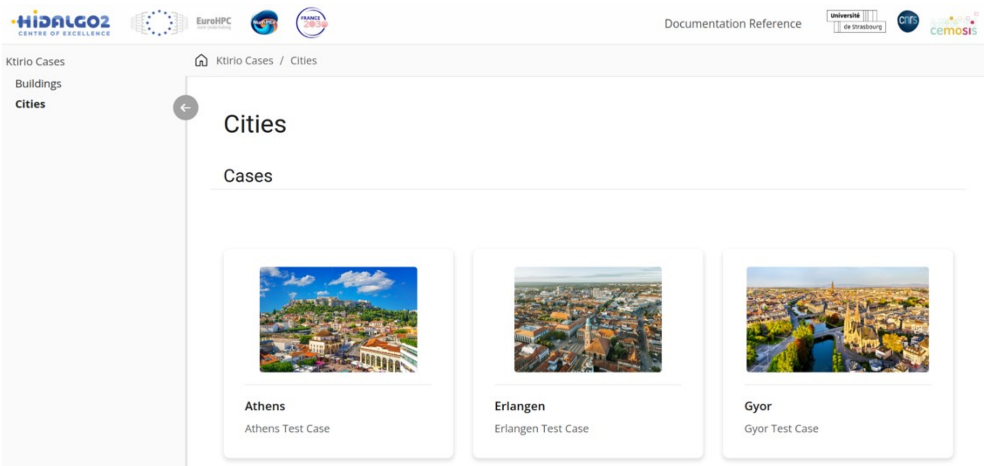

Figure 1 Screenshot of the Ktirio cases website showcasing the city's gallery.

To reduce the need for handling large datasets, key quantities of interest are computed during simulations using a self-developed parallel aggregation tool. These metrics are exported in JSON format at both city and building scales as required.

3.1.3 Validation

Continuous monitoring and validation of application performance are critical. A regularly updated measurement database has been deployed, containing psychrometric data from multiple sensors across various buildings. This time-series database enables automatic comparison and benchmarking of simulation results against actual measurements, ensuring no regressions occur in outputs. The accompanying API facilitates data assimilation.

Measurements are categorized into five fields:

- Psychrometric: temperature, humidity
- Air Quality: CO_2, volatile organic compounds (VOCs)
- Actions: open/close, button press events
- Status: connectivity, signal strength, battery status
- Weather: wind speed, diffuse radiation, air temperature

Currently, the model validation is conducted using summer sensor data, as heating system models are still under development. Summer data, particularly for buildings without air conditioning, provide insights into the building's response to external variations, influenced by geometry, materials, and internal gains (e.g., occupant metabolism and equipment heat output). These comparisons are crucial for validating geometry and material properties in the model. Future work involves collecting heating system power output during the heating season to further refine and validate the models. Figure 2 illustrates the sensor database UI.

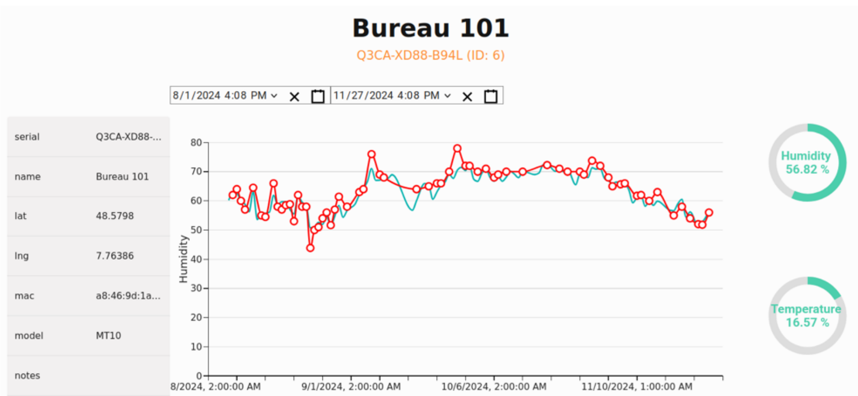

Figure 2 Screenshot of the sensor database UI.

3.1.4 GIS2FMU

Accurate building geometry modelling is essential, including details such as surface materials, thickness, window and door locations, as well as other properties. To achieve this, FMU models are generated from GIS files. The workflow begins with reverse geocoding the buildings in the GIS file, followed by retrieving additional data from various databases to collect information such as materials, window dimensions, positions, and the number of floors. Missing data are imputed using a KNN model, while window and door locations are inferred based on neighbouring buildings.

An IFC file encompassing all buildings in the GIS input is then generated using Ktirio's IFC generator. This IFC file is subsequently converted into a Modelica file, which is further transformed into an FMU model for use in the main application.

However, a technical challenge persists with the software responsible for converting Modelica models into FMU models, preventing full automation of the generation process.

The Figure 3 illustrates some of the capabilities of the tool.

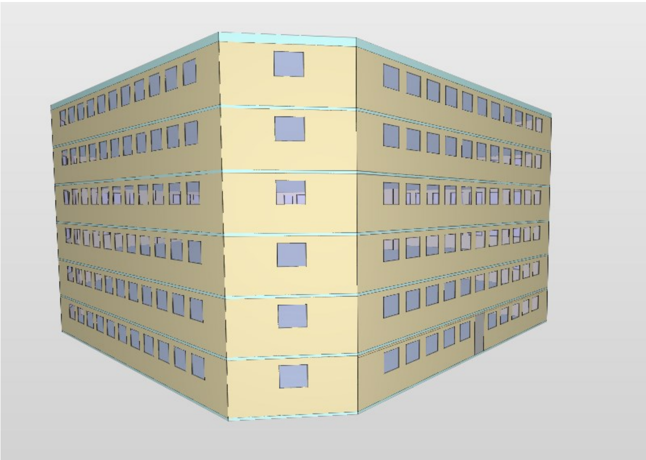

Figure 3 Windows and doors on a generated building IFC, viewed using Solibri.

3.1.5 Geometry modelling

Efforts to enhance the accuracy of urban building models have focused on integrating vegetation components and improving 3D geometry reconstruction. Vegetation is incorporated into the 3D city model, with shading masks generated for buildings based on individual trees sourced from the OpenStreetMap database. Vegetation meshes are included in the overall 3D city representation, ensuring its influence on building simulations is accurately modelled.

Building geometry reconstruction has progressed with methods developed to automatically generate detailed 3D representations, including floors, external walls, and roofs. Terrain meshing using topography is now supported, although the current pipeline generates overly refined meshes, even in flat areas. New strategies, such as isoline computation and constrained Delaunay triangulation (via the CGAL algorithm), are being implemented to address this issue. Work on both vegetation and building geometry improvements remains ongoing, with further refinements planned for the next development phase. Figure 4 illustrates the reconstruction of vegetation in the city of Strasbourg.

Figure 4 Building and Vegetation mesh on Ktirio Gui.

3.1.6 Shading masks evaluation

An advanced algorithm has been developed to compute shading mask coefficients on the 3D city mesh by leveraging solar position data. The method relies on a ray tracing process, implemented using the Boundary Volume Hierarchy (BVH) technique. This approach enhances efficiency and accuracy in modelling shading effects across urban environments.

The algorithm has been parallelized using MPI technology to ensure scalability and faster computation. Additionally, a GPU-based implementation is under development to further accelerate performance and enable larger-scale simulations.

3.1.7 Graphical user interface

Enhancements to the geographic data interface include the addition of a weather UI component, enabling the generation of input data for the Urban Building Pilot. Vegetation geometry visualization is now supported within the 3D scene, providing more comprehensive environmental modelling.

A new simulator UI has been integrated to streamline simulation setup and execution. This interface facilitates task workflows that launch simulations on supercomputers. The pipeline automates input data processing, transfers it to supercomputing resources, and executes the simulation using the SLURM scheduler. Future developments will focus on enabling job monitoring and result retrieval to complete the workflow.

3.2 Roadmap and challenges

3.2.1 Tasks (To-Do)

Heating System Implementation

- Develop and integrate new heating systems, including boiler and heat pump, along with a hydraulic system composed of pump, pipes, expansion vessel, radiator, and valve.
- Implement regulation via closed-loop and/or open-loop systems with PID regulators.
- Timeline: Implementation by Q4 2024, testing and validation by Q1 2025.

Predictive Simulations Using WRF Forecasts

- Integrate Weather Research and Forecasting (WRF) forecasts for predictive simulations.
- Use grid data (e.g., 1 km resolution) to compute indoor indicators, providing specific forecast datasets for each set of buildings within the resolution.
- Timeline: Initial integration by Q1 2025, refinement by Q3 2025.

Building Geometry Improvements

- Enhance city geometry reconstruction by adding support for roofs, windows, and floors.
- Enable coupling of shading masks from LOD1 meshes with simulations using LOD0 buildings.
- Timeline: Development by Q2 2025, full integration by Q4 2025.

Environment Geometry Enhancements

- Support mesh vegetation for new areas such as parks and forests.
- Include terrain geometry like mountains and roads in simulations.
- Timeline: Parks and forests, terrain features by Q1 2025.

Graphical User Interface Enhancements

- Add result visualization features.
- Upgrade UI usability, improving ergonomics and user experience.
- Include points of interest (POI) for selecting specific areas or buildings.
- Timeline: Usability upgrades by Q1 2025, POI integration by Q4 2024.

3.2.2 Challenges

Complexity of Heating System Regulation

- Achieving robust regulation with PID controllers in closed and open loops.
- Integrating detailed hydraulic models without compromising computational efficiency.

Data Requirements for Predictive Simulations

- Handling large-scale WRF forecast data efficiently.
- Ensuring accurate mapping between forecast grids and building sets.

LOD1 and LOD0 Coupling

- Overcoming computational challenges in coupling shading masks from LOD1 meshes with LOD0 simulations.

Vegetation and Terrain Geometry

- Accurately modelling parks, forests, and terrain features while maintaining computational efficiency.

UI Scalability and Usability

- Balancing feature richness with ease of use, especially for novice users.
- Ensuring responsive performance with large datasets.

Table 2 Changes in expected Research Results for UB Pilot compared to D5.3

Key framework	Current status as of M23	Reason for roadmap adjustment	Adjusted / new achievement date
Feel++	Efficiency/scalability. Parallelization of shading mask generation. **Done**	N/A	M18
Ktirio-city	New functionalities. Watertight mesh generation. **Delayed**	90% done. Watertight meshing is still an undergoing development.	M18->M24
Ktirio-city	New functionalities. LOD-1 mesh generation. **In progress**	Partially available.	M12
Dymola	New functionalities. LOD-1 building model generation. **Done**	The models now need to be included in the computational workflow.	M18
Feel++ Dymola Ktirio-city	Efficiency/scalability. LOD-0 parallel simulation. **Done**	N/A	M12

Key framework	Current status as of M23	Reason for roadmap adjustment	Adjusted / new achievement date
Feel++	Data analytics/AI. Leverage of shading mask data for prediction/clustering of buildings. **Done**	The Data has been provided via CKAN and Python code to read the data as well as some notebooks.	M24
Ktirio-Gui	Improve Map view, allow different zones of interest; code refactoring. **Done**	N/A	M21 (new)
Ktirio-Gui	New result visualization features; Improve UI usability. **In progress**	N/A	M30 (new)
Ktirio-city	Improve Benchmarking and CI/CD; improve physics (building types, weather inputs). **Done**	Initial version of website and workflow automated reporting.	M18 (new)
Ktirio-city	Improve geometric modelling; improve physics modelling; improve performance. **In progress**	N/A	M36 (new)

4 Renewable Energy Sources (RES)

In the reported period, model development efforts focused on two key areas: uncertainty quantification (UQ) and sensitivity analysis (SA), and the ability to handle diverse input conditions.

4.1 Advances in model development

To address UQ and SA, the mUQSA toolkit (based on QCG), developed under WP2, was integrated into the RES modelling framework. This integration enabled the analysis of the influence of varying weather conditions, particularly wind speed, on the damage to overhead electrical lines in the RES damage scenario. The findings from this analysis were presented at the PPAM 2024 conference [5] and will be published in the conference proceedings. Now the same toolkit is used to study model accuracy by running multiple simulations with perturbed input and model parameters and applying HPDA techniques.

Several enhancements have been made to the model to accommodate diverse input conditions. The mUQSA toolkit, employed for UQ and SA, plays a crucial role in enabling the model to handle various scenarios. In the near future, this capability will be utilized to refine model parametrisation and conduct in-depth accuracy assessments. For further model improvements, the pilot workflow has been separated into distinct phases: pre-processing, mesoscale simulation, local scale simulation, post-processing. Now it will be easier for the user to use different input parameters and data. UQ/SA can be now applied to both or individual models separately.

RES simulations of urban areas necessitate detailed information about buildings, specifically their shape and height. Previously, this data was either sourced from interested parties or manually extracted from geospatial data portals and converted into the 2D shapefile format required by the EULAG model. A significant advancement has been made by enabling the direct integration of OpenStreetMap data into the simulation process. Users can now define a region of interest using WGS-84 coordinates, triggering the automatic retrieval of relevant building information from OpenStreetMap. This data is then seamlessly converted into the appropriate format for EULAG input. There are some advantages of this approach. First of all, accuracy of the model will be improved by using the OpenStreetMap data for the regions where city data was not available or where gather some while ago with lower resolution. Secondly, versatility of the model is also improved by allows pilot users to run the simulation over any region of interest in world, regardless the availability of the building data from local authorities.

In terms of user interface, due to integration with mUQSA toolkit, RES pilot can be used by the users as service. Users can modify input parameters within mUQSA portal and run single simulation or apply UQ and SA for more in-depth analysis. Advancements have been made to visualisation – it is now possible to plot the weather data over GIS data, see Figure 5.

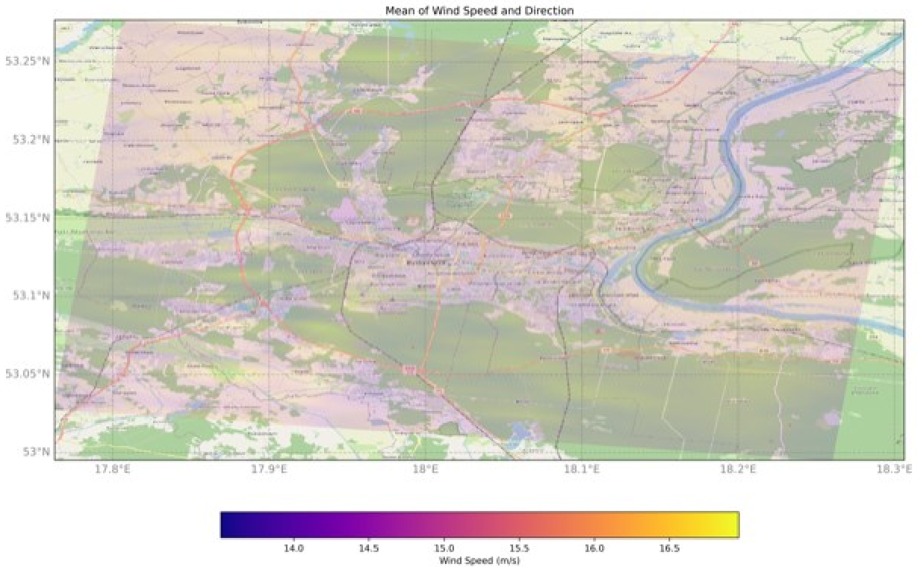

Figure 5 Plotting wind data over GIS data.

4.2 Roadmap and challenges

- <u>Containerisation for CI/CD, deployment and user usage</u> – there is a challenge in making RES pilot available as container to facilitate CI/CD process, deployment on EuroHPC site and for user usage. The workflow contains running two separate models with their own requirements in terms of hardware resources used. Then they are packed and invoked from a runner, Python-based framework, which makes containerisation more difficult. The initial plan to use Apptainer for containerising the RES environment failed. Docker was proposed as a more flexible alternative. Due to its layer-based structure, Git integration for easier building and testing, and compatibility with Apptainer/Singularity, Docker should overcome issues with complex workflow. The Docker container is now built on Ubuntu, installing general libraries, OpenMPI, and Python environment with Conda. The Runner application is installed from a Git repository. The Eulag application, recompiled before each simulation, is added as a separate layer. Future steps include converting the

Docker container to Apptainer/Singularity format and testing it on the cluster for the scalability.

- Integration with UB – there is a new finding in developing energy prediction module for solar panels. Despite weather conditions which affects efficiency of a photovoltaic panel, such as temperature or humidity, there is also another one quite crucial in assessing energy production – sunlight angle against PV system. UB pilot is able to calculate not only the solar mask, but also give information about such angle. The work in integrating this information inside RES pilot is in progress.
- UQ/SA – the next stage in this research involves leveraging UQ and SA to enhance model accuracy, identify critical parameters, and mitigate the impact of uncertainty on the results. Applying surrogate model is also foreseen to speedup computations.
- Visualisation – the next in improving user experience is to provide data visualization results with SZE tool and integrate 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.

There are no changes in the roadmap except for the improved damage predictions, as detailed in Table 3 and Figure 11.

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

Key framework	Current status as of M23	Reason for roadmap adjustment	Adjusted / new achievement date
WRF and EULAG: Coupling models using orchestrator	**Done**, WRF and EULAG are loosely coupled using RES orchestrator (runner component).	N/A	M24->M20
WRF and EULAG: improved damages prediction	The damages prediction account for weather conditions. **Delayed**	In order to account data on materials resistance to different conditions (excessive wind, heat and icing) access to real data from electrical lines owners is needed to propose an improved model.	M18->M36

Key framework	Current status as of M23	Reason for roadmap adjustment	Adjusted / new achievement date
EULAG, energy module: cloud solution	**Work is ongoing** – initial version of Apptainer is ready, though needs to be switched to a docker and test the scalability of the solution.	N/A	M36
EULAG, energy module; visualisation advancements	Proof-of-concept integration with SZE visualization tool; **In progress** Python-based visualization of the damages is ready.	N/A	M36
EULAG, energy module: uncertainty quantification	UQ and SA are used in the damages scenario. Work **in progress** concerns UQ/SA to improve simulations results and apply surrogates.	N/A	M36
EULAG, energy module: scalability improvements	**In progress**	N/A	M36
Energy module: predictions improved with HPDA/AI methods	**In progress**	N/A	M36

5 Wildfires (WF)

The wildfire pilot focuses on modelling the initiation and spread of a flame front, as well as the emission and dispersion of smoke, over vegetation structures (forest fuels) in the territory. Special attention has been given to wildfires affecting populated areas (wildland-urban interface or WUI) to assess potential impacts due to heat emission and the presence of atmospheric pollutants. In line with recent wildfire events, simulating these phenomena requires calculating the fire-atmosphere interaction and how it modifies and conditions the spread and behaviour of the flame front and the smoke plume.

5.1 Advances in model development

For the Wildfires (WF) pilot, two scales have been defined to tackle the problem: landscape scale and urbanization scale.

5.1.1 Landscape scale

Considering landscape-scale HPC simulations, the WRF-SFIRE software has been installed and tested. The objective at this scale is to study the initiation and spread of fire fronts and smoke plumes of wildfires that extend over large areas, as well as to model fire-atmosphere interaction and its effect on wildfire behaviour.

A workflow has been proposed, comprising several stages:

- Acquisition of initial static data, such as the digital terrain model and vegetation cover.
- Collection of data for atmospheric characterization, like ERA5 reanalysis.
- Conversion of static and meteorological data to WRF format.
- Simulation design and parametrization: calculation domain, resolution, and MPI processing strategy.
- Execution of the preprocessing phase.
- Fire-atmosphere modelling in real conditions.
- Export and interpretation of results.

One of the biggest challenges in these simulations has been obtaining atmospheric grids with resolutions greater than 1 km (e.g., 200 m) and corresponding fire simulation grids with resolutions finer than 100 m (e.g., 20 m).

Several model physics parametrizations have been tested to conduct an initial analysis of wildfire behaviour and atmospheric interactions, focusing on wind field disturbance. Both Planetary Boundary Layer (PBL) parametrization and the alternative use of the LES vortex model have been evaluated.

Smoke emission and dispersion have also been simulated using passive tracers, demonstrating both the utility and necessity of parallel computing and integrating results into advanced visualization experiences in virtual reality. The chemical and physicochemical interaction model in smoke plumes (CHEM) was deemed unnecessary for the pilot's initial objectives.

Reframe software has been integrated into a suite of tests to evaluate scalability in HPC environments. The first results were published in deliverable D3.1 [6], showing progress according to plan.

In the WF pilot for landscape scale, work has begun to integrate MeteoGrid's Fire Spread Engine (FSE) with the mesoscale WRF model as an alternative to SFIRE, and its execution in HPC environments using OpenMP, MPI, or hybrid solutions. This new solution will be named WRF-FSE.

MeteoGrid has also begun adapting FSE for execution in GPU ensembles. This serves a dual purpose: to train neural networks that capture the model's simulation capabilities for operational use and to perform HPDA risk analysis over large areas and UQ processes associated with all simulation stages (FSE as a surrogate for WRF-SFIRE).

Over 10,000 simulations have been performed and analysed by ICCS, specifically in outlining a strategy for identifying simulation shapes and comparing them with real-world fire perimeters using AI inference engines. These procedures and collaborations with ICCS are expected to continue with the GPU version of FSE-Ensembles.

A strategy for quantification and validation of uncertainty (VUQ) has been designed and tests are scheduled for the upcoming months with the help of HLRS.

5.1.2 Urbanization scale

The detailed simulation of fire spread in wildland-urban interface (WUI) areas, where buildings and vegetation coexist, is conducted with specific numerical models such as FDS (Fire Dynamics Simulator) or OpenFOAM/fireFOAM. These simulations require a detailed description of geometric elements (such as houses) and non-geometric or porous elements (such as vegetation).

Progress has been made in simulating vegetation generation and evolution (Procedural Vegetation Spawner) in Unreal Engine to facilitate realistic WUI environments.

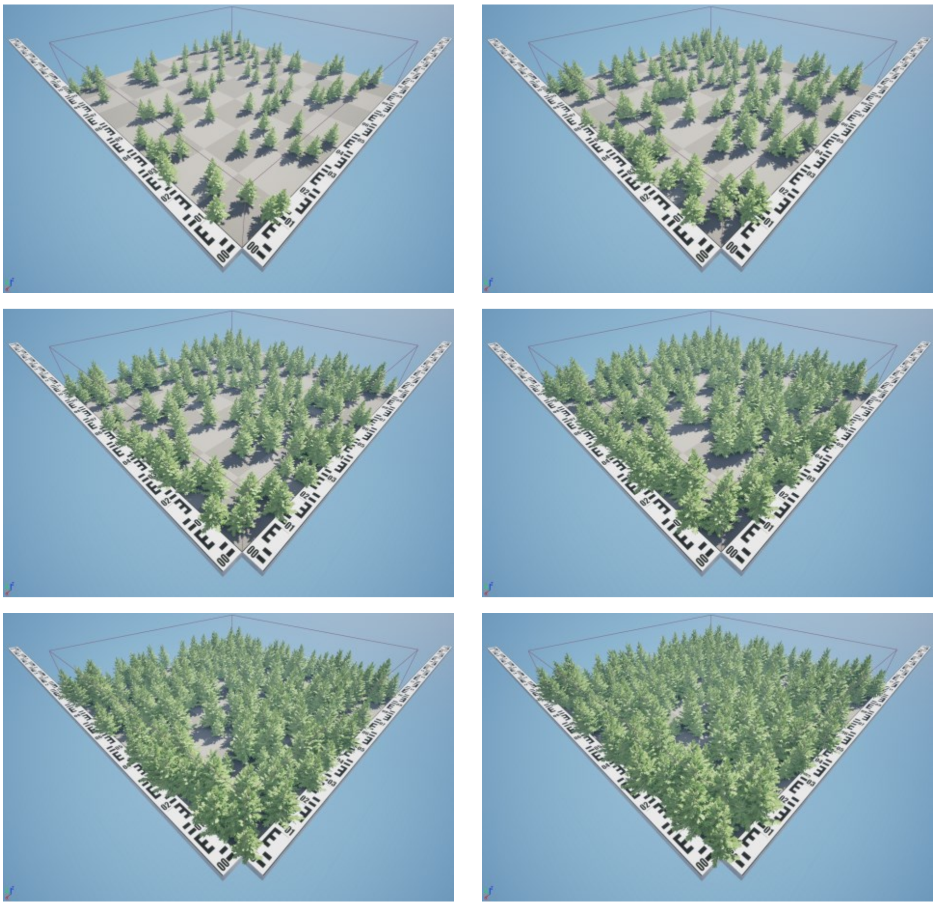

Figure 6 Example of creating a complex vegetation structure and its evolution over time using a Procedural Vegetation Spawner.

Figure 6 shows an initial tree density of 100 individuals per hectare. Basic rules for seed dispersal, growth, and competition for space and light have been defined. Using them with a Procedural Vegetation Spawner, realistic results are achieved as can be seen in the succession of images shown in the same figure. A specific method has also been developed, including software for sampling the resulting geometry (especially vegetation) and creating point clouds that store biomass distribution information for combustion. This Python-based software is designed for parallel processing, dividing the scene into blocks and assigning tasks to multiple processors. The biomass point cloud will be used as input for combustion and fire propagation models (OpenFOAM/fireFOAM or FDS) in the next phase. These point clouds are currently being generated for both real and idealized WUI scenarios.

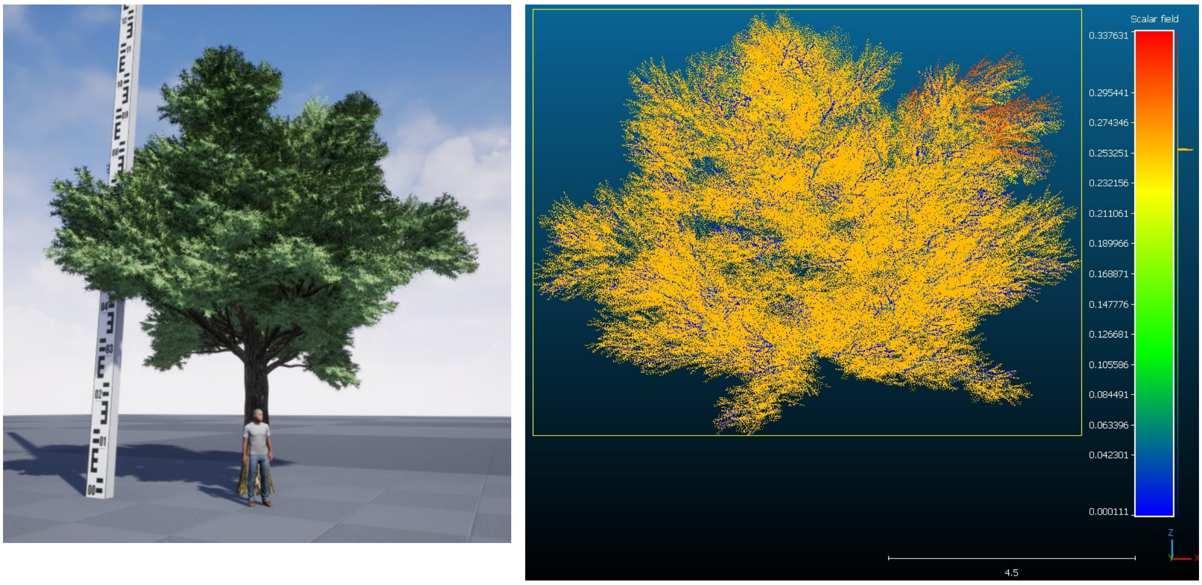

Figure 7 Example of biomass distribution estimation in a detailed 3D model of *Tilia heterophylla.*

Figure 7 shows an example of this technique to obtain an estimate of the biomass distribution for a 3D model of Tilia heterophylla. This method involves generating a point cloud fractal to sample components relevant to wildfires, specifically leaves and small branches. The estimated total biomass is 113.45 kg, the bulk volume is 821.9 m^3, and the calculated bulk density is 0.13 kg/m^3, closely matching real-world data.

OpenFOAM/fireFOAM has been installed and initial tests on HPC systems have commenced. HLRS assistance will be required in certain aspects. To this end, specific technical meetings will be held to discuss issues related to the combustion of porous elements in fireFOAM, such as porous element modelling and interpreting combustible materials as particles (similar to FDS's particle combustion model).

5.1.3 Visualization

In terms of visual simulation, integration of results from WRF-SFIRE calculations has advanced, particularly regarding volumetric smoke emission and propagation using VDB format. This includes the optical effect of light on smoke plumes and integration with 3D CESIUM geometry through Google Tile Service in Unreal Engine.

As previously mentioned, workflows for developing WUI environments with complex vegetation structures (various layers, species, ages, etc.) and coupling them with numerical models via burnable biomass distribution have been established in Unreal Engine.

Progress has also been made in developing demonstrators illustrating WRF-SFIRE numerical simulations, notably those of the 2019 Cadalso-Almorox wildfire, with model outputs generated every minute. A snapshot of this simulation is shown in Figure 8. One demonstrator will be available for the upcoming review meeting.

Figure 8 Integration in Unreal Engine of fire-atmosphere interaction simulation and smoke dispersion for the 2019 Amorox-Cadalso fire.

The technique for creating hybrid 360° immersive videos in virtual reality has progressed to integrate complex wildfire scenarios and simulations, especially at the detailed urbanization level.

All these methods and techniques are designed for use in the development of demonstrators, which will encapsulate the data and results of simulations performed on HPC facilities, as explained later.

5.2 Roadmap and challenges

The development of the wildfire pilot is progressing as planned, and the following challenges have been identified for future reporting periods:

5.2.1 Landscape scale

- Simulation of historical wildfire events with fire-atmosphere interaction that have had significant social, economic, and environmental impacts:
  - Llutxent Fire 2018 (Spain)
  - Varnavas Fire 2024 (Greece)
  - Pedrógão Grande Fire 2017 (Portugal)

- Coupling the FSE fire simulation engine with the WRF model to create the coupled WRF-FSE solution. This includes simulating the spread through the tree canopy and its relationship with surface fire spread. Fire-atmosphere interaction will be coupled through the generated heat flux and moisture injected into the atmosphere.
- Enhancing parallel computing performance and scalability of WRF-FSE. Optimizing the design of the number of domains and their division into tiles. Improving preprocessing times and I/O operations.
- Incorporating physicochemical processes in the calculation of smoke generation and dispersion: WRF-CHEM coupling.
- Incorporating the LES vorticity model for more detailed simulations of smaller regions and comparing it with PBL parametrizations.
- Simulating actual cases with WRF-*real*, configuring boundary conditions using actual atmospheric data, and implementing data assimilation procedures.
- Adapting FSE to GPU/CUDA and using it in ensemble simulations over large territories.
- Uncertainty analysis and quantification, HPDA methods for sensitivity analysis of the territory to wildfire spread, and development and application of AI engines for the operational use of simulations.

5.2.2 Urbanization scale

- Generation of procedural vegetation structures in wildland-urban interface (WUI) scenarios, including buildings and simulating different strategies for forest fuel mitigation (firebreaks, fuel load reduction, vegetation moisture control, etc.).
- Automatic generation of three-dimensional biomass distribution maps (point clouds) and their equivalent in 3D voxel grids.
- Testing combustion calculations in FDS using the volumetric biomass description from the previous step.
- Adaptation of the FDS particle combustion method to OpenFOAM/fireFOAM.
- Meshing methods and domain partitioning for parallel computation.
- <u>Implementation Phase 1</u>: simulation of a single house and its surrounding vegetation:
  - Scenario description. Structure geometry. Interpreting vegetation as particles.
  - Meshing and domain partitioning for parallel computation.
  - Calculation of airflow through vegetation and around the house. Effects of porous materials (vegetation) under different assumptions.
  - Calculation of fire initiation and spread in the vegetation surrounding a house. Estimation of heat fluxes impacting the structure. Effects of preventive treatments, such as forest fuel mitigation.

- Calculation of smoke production and dispersion due to local vegetation combustion.
- Implementation Phase 2: simulation of a housing development and its surrounding vegetation:
  - Scenario description. Location of houses, roads, streets, and other infrastructure. Description of vegetation structure using Procedural Vegetation Spawner.
  - Interpreting vegetation as particles, biomass distribution, and generation of input files for physical simulation.
  - Meshing and subdivision of the domain for parallel computation.
  - Calculation of airflow through the housing development and the effect of porous materials (vegetation) under different configurations (e.g., different preventive treatments such as firebreaks).
  - Calculation of fire initiation and spread within the development. Effects of vegetation discontinuities and preventive treatments (fuel load mitigation). Estimation of heat fluxes on structures.
  - Calculation of smoke production and dispersion due to local combustions.

5.2.3 Visualization

- Development of a hybrid method for immersive 360º videos with virtual reality scenarios.
- Integration of smoke and flames produced in OpenFOAM/fireFOAM into Unreal Engine using VDB files. Creation of bridge software that interprets OpenFOAM/fireFOAM results as VDB files.
- Creation of demonstrators. Demonstrators are interactive-immersive applications that enable intuitive data exploration and visualization of HPC simulation results. They are developed around case studies where specific scenarios are presented for user decision-making.
  - Demonstrator 1. Simulation of the Almorox-Cadalso fire. Landscape-scale visualization of fire evolution and smoke propagation over the 3D model of the territory.
  - Demonstrator 2. Simulation of fire initiation and spread around a house. Effect of preventive measures and impact on the house.
  - Demonstrator 3. Simulation of fire initiation and spread within a housing development, under varying weather conditions (wind) and fire origin points. Effect of preventive actions and impact on buildings and infrastructure.

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

Key framework	Current status as of M23	Reason for roadmap adjustment	Adjusted / new achievement date
WRF-SFIRE	First WRF-SFIRE Reframe. Tests carried out **as planned**.	N/A	M11
WRF-SFIRE Reframe	First evaluation tests. Carried out **as planned**.	N/A	M15
WRF-SFIRE Reframe	Data Analytics/AI/WRF-Sfire HPDA/AI first release. Validation still **in progress**.	WRF-Sfire HPDA/AI first release in validation phase.	M12->M26
WRF-SFIRE UQ-QCG	VVQ strategy defined, first tests are planned for Dec 24. First Release **delayed.**	To establish a better strategy for UQ implementation.	M18->M28
WRF-SFIRE UQ-QCG	First ensembles **in progress.**	Subrogated model in development.	M24->M26
WRF-SFIRE UQ-QCG	Final release **Planned**	N/A	M48
SFIRE	**In progress**	A hackathon to analyse improvements is planned in M24.	M36
Open-FOAM / fireFOAM	2025: Single house simulation domain. Scalability integration. GPU porting analysis. **Planned**	N/A	M36 (new)
Open-FOAM / fireFOAM	2026: Housing environment domain. **Planned**	N/A	M44 (new)
Unreal Engine	WRF-SFIRE: VR Demonstrator. 3D-Immersive video for MetaQuest 3. **Planned**	N/A	M36 (new)
Unreal Engine	OpenFOAM: VR Demonstrator. 3D-Immersive video for MetaQuest 3. **Planned**	N/A	M44 (new)

6 Material Transport in Water (MTW)

This chapter introduces the MTW pilot, covering the information missing in D5.3 [1], including scientific baseline, research challenges, and progress made up to M23. This pilot is being developed by the partners at Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU). The pilot has been part of HiDALGO2 since M18, and therefore, a detailed scientific baseline and use case definition of the MTW pilot, which was previously not included in deliverable D5.3, are outlined.

6.1 Scientific baseline and use case definition

Simulation of transport processes in water are critical in the context of the current environmental challenges faced across the globe. To provide a broader insight into some commonly faced issues, examples are detailed below.

- **Environmental protection:** Understanding how pollutants (like chemicals, nutrients, or microplastics) disperse and move in water bodies is crucial for predicting the impact of industrial discharge, agricultural runoff, or oil spills. The advection-diffusion equation models how these pollutants are carried by the flow velocity (advection) and spread due to molecular motion (diffusion).
- **Regulatory Compliance:** Many countries have regulations governing water quality. Simulations help authorities to predict the spread of contaminants and guide interventions to minimize environmental impact.
- **Aquatic Ecosystem Health:** Temperature and salinity gradients in oceans drive water movement and influence biological processes in aquatic environments. Understanding the transport of temperature and dissolved substances like oxygen or nutrients allows researchers to model how ecosystems respond to environmental changes, including warming waters due to climate change.
- **Pollutant Dispersion in Drinking Water:** Contaminants in water supplies pose significant health risks. Simulating the movement of pollutants helps in the design of filtration and remediation systems and assists in emergency responses to accidental spills or contamination events. This is a matter of high priority for public health eternally and for generations to come.

The above scenarios are just a few examples and there are many more applications showing the necessity of simulating transport processes in water. In the HiDALGO2 project, the partners from FAU strive to develop efficient simulation software for the simulation of scalar transport processes in water. Simulating transport processes involves the numerical modelling of fluid, particles and the quantity that is being transported such as saline concentration, pollution or temperature. It also involves the coupling of these different physical phenomena hence making this a complex multiphysics simulation that requires highly efficient codes and HPC architectures to perform advanced numerical simulations. A description of utilized simulation frameworks and their specific couplings is given in D5.6 [7].

6.2 Discussion of Requirements

For the successful implementation and verification of the MTW-pilot, the following requirements have been identified:

- Access to EuroHPC clusters to run the benchmarks and scaling runs.
- Create a database for local code development and FAIR storage.
- Use experimental data for comparison of simulation results for improving the model reliability.
- A suitable real-world application scenario to showcase the efficiency and scalability of the software tools at hand.

6.3 General Status of MTW-pilot as of M23

The work on this pilot started in M18 and the following has been achieved until M23:

- Identification of required software and tools for the pilot development.
- Adoption of the existing numerical methods for the various physical effects present in this pilot.
- Access to several EuroHPC machines such as Leonardo, LUMI, Vega.
- Identification of possible collaborators for various work package tasks.
- Continuous development of the pilot's models as described in subsection 6.4.

This information is given to bring the MTW-pilot in line with the four original pilots. An updated version from D5.3's [1] visualization of the five pilots' progress is given in the appendix Figure 13.

6.4 Advances in model development

The development of the pilot started in M18, and significant progress has been made since. The highly scalable waLBerla open-source simulation framework [8], based on the lattice Boltzmann method (LBM), is used to describe the dynamics of fluids. The framework flexible and modular software design makes it easy for portability of codes without loss in performance. To describe the sediment transport in riverbeds, the MTW pilot accounts for interacting solid particles along the fluid flow. These particle interactions are modelled using discrete element method (DEM). As both media effect one another, a two-way coupling of fluid and particles has already been established. The coupling has been realized using the partially saturated cells method and has been tested and validated both on CPU and GPU. The particle dynamics is solved using a module of waLBerla called mesapd that is coupled with waLBerla to account for the fluid-particle coupling.

In addition to sediment transport involving only fluid and particles, the current pilot includes an additional scalar field, such as saline concentration, pollutants, or temperature, which is transported along with the fluid and particles. This scalar transport coupled to the fluid-particle coupling is what constitutes the main ideology of the MTW.

The main goal of this pilot is to establish an efficient and performance-portable fluid-particle-scalar coupling. This is achieved in two phases: the first phase focuses on establishing the coupling between the fluid and scalar, while the second phase incorporates the coupling between the scalar and particles. The coupling between fluid and particles has already been established in the waLBerla framework using the PSM method that works on both CPUs and GPUs as stated above.

Multiple complex scenarios were simulated and tested to analyse fluid-particle coupling. Additionally, this coupling has been extended to include electrostatic effects from charged particles. This is called the fluid-particle-charge coupling. For this charged coupling, several validations and verifications have also been done. This established charge coupling gives a strong foundation for establishing the fluid-particle-scalar coupling by using several combined software tools, and physics-based schemes.

As of M23, a one-way coupling between the fluid and scalar has been established, supported by thorough verifications and validations. The lattice Boltzmann method is used for solving both fluid dynamics and scalar transport. LBM for fluids leads to the Navier-Stokes equations which govern the fluid motion. In a similar way, LBM for the scalar leads to the advection-diffusion equation which governs the scalar transport. The scalar can be anything here, for example, temperature, saline concentration, pollution, etc. The velocity of the fluid as well as the gradient in the scalar magnitudes from one point to another is what drives the transport of the scalar. The approach of using LBM for solving the scalar is explicit in time.

At FAU, lbmpy is developed as a Python-based package designed to generate fast and efficient C implementations of lattice Boltzmann codes. Hence, lbmpy is used for generating the kernels for both the fluid and scalar lattice Boltzmann codes. Initially, a working showcase has been developed and tests were performed to verify and validate the fluid-scalar coupling against some classical benchmarks in literature resulting in promising agreement.

Initially, a one-way coupling was planned, where the scalar transport is influenced by the fluid but not the other way around. However, in nature there are several flows in which both scalar and fluid influence each other such as Rayleigh Bernhard convection. Thus, it is important to have a two-way coupling in place, as it broadens the scope for simulating more complex scenarios. Currently, efforts are focused on establishing a two-way coupling. The two-way coupling will be completed in the coming months.

6.5 Challenges and Roadmap

The forthcoming steps appear promising yet may present certain challenges. As mentioned a validated and tested working version of the two-way coupling between the scalar and fluid dynamics is anticipated to be available within a few months capable of running on both CPU and GPU architectures.

The next challenge is then the formulation of the coupling among the three quantities; fluid, particles, and scalar. Each of the individual physics models for particles, fluid, and concentration is functioning adequately. The fluid-particle coupling is well established, and the fluid-concentration coupling is nearing completion. Nevertheless, the fluid-particle-scalar coupling requires careful consideration due to potential complexities related to boundary conditions and load balancing. An improved showcase for the MTW pilot is expected to be presented within the coming months. The idea would be to have the river-bed or a sediment transport application in which there is a scalar such as temperature. The river-bed and sediment transport have fluid-particle coupling and further fine tuning this application towards incorporating the scalar effects would be the task for the future.

Another challenge is the planned utilization of the HyTeG [9] finite element simulation framework. The initial objective of coupling HyTeG with waLBerla was to solve the advection-diffusion equation implicitly using HyTeG and integrate this solution with waLBerla. However, two significant issues have emerged:

- HyTeG is currently not supporting GPU architectures; it is designed for CPU usage only. As high-performance computing (HPC) increasingly shifts towards leveraging GPUs, and the fact that the HiDALGO2 project is focusing on the use of the EuroHPC's extensive GPU resources, relying solely on CPU technology is not feasible.
- The grid structures employed by HyTeG and waLBerla differ significantly. Consequently, coupling these frameworks can be unfavourable on GPUs as it necessitates interpolation between the data structures, leading to increased computational overhead and potential inaccuracies. Furthermore, a strong coupling approach aimed at minimizing data input/output may not be feasible without extensive and intrusive adjustments to both framework's cores to integrate necessary communication and orchestration subroutines.
- To support GPUs we will either have to adapt the HyTeG framework or use code generation technology to provide an alternative solver for the scalar problem.

Solutions are currently being explored to enhance the implicit PDE solver and tackle the identified challenges.

Table 5 Expected Research Results for MTW Pilot

Key framework	Research Goal	Current status as of M23	Foreseen date of achievement
waLBerla	One-way coupling fluid-scalar.	**Completed** on CPU and GPU.	completed
waLBerla	Two-way coupling fluid-scalar.	Working on showcase and physical validations. **In progress**	M25
mesapd	Particle integration with fluid-scalar.	**Not yet started**	M30
lbmpy	Development of portable kernels for the pilot.	Constantly **in progress**, working for CPU and GPU.	M48
waLBerla	Fluid-scalar coupling showcase.	**Not yet started**	M27
waLBerla + mesapd	Versatile MTW riverbed showcase on GPU and CPU.	**In progress**	M33
HyTeG	Coupling fluid-scalar with implicit PDE solver.	**In progress**	M40
waLBerla + mesapd, HyTeG	GPU portability.	Constantly **in progress**.	M48

7 Conclusions

This deliverable, D5.4, reports the substantial step forward in HiDALGO2's mission to develop high-fidelity simulations addressing critical global environmental challenges. Documenting the ongoing achievements and research findings of the five pilot applications, including (i) Urban Air Project (UAP), (ii) Urban Buildings (UB), (ii) Renewable Energy Sources (RES), (iv) Wildfires (WF), and (v) the newly introduced (from M11 to M23) Material Transport in Water (MTW). It provides insights into model development, accuracy, versatility, and the adjustments of the currently 44 research milestones that build the strategic roadmaps for each pilot.

The MTW pilot expands HiDALGO2's scope by addressing material transport challenges in water systems, showcasing the consortium's adaptability to evolving global needs. To catch up with the foundational progress documented for the other four pilots in D5.3 [1], the newly added pilot outlines its scientific baseline and use case definition in chapter 6.1, its requirements in chapter 6.2, and the general status of this pilot as of M23 in chapter 6.3.

In general, from M11 to M23 significant progress has been achieved across all five pilots, accompanied by some notable challenges:

i. **Urban Air Project:** Significant advancements have been made in airflow and pollutant dispersion simulations, with the RedSim solver now equipped with NVIDIA AMGX for enhanced linear equation solving and improved computational efficiency. Other notable achievements include upgrades to OpenFOAM, enabling more accurate and detailed wind field predictions, essential for urban air quality assessment and planning.

ii. **Urban Buildings (UB):** Progress in the UB pilot focuses on improved simulation models for energy efficiency, air quality, and indoor comfort. Key developments include custom integration of weather data, occupancy scenarios, and energy parameters, as well as enhanced thermal comfort indicators. These advances, supported by ongoing efforts in building geometry reconstruction and sensor data validation, bolster UB's potential for informed urban planning applications.

iii. **Renewable Energy Sources** (RES)**:** The RES pilot has made strides in its predictive models for solar and wind energy output. Through the development of independent photovoltaic systems, RES is refining its ability to forecast energy production, even amidst data limitations. Efforts to further couple WRF and EULAG models, along with a focus on uncertainty quantification, aim to optimize predictions and broaden application scenarios.

iv. **Wildfires (WF):** The WRF-SFIRE application for wildfire simulation in landscapes has been installed and tested on various EuroHPC machines. Potential issues and performance are analysed. Real-world wildfire simulations have been conducted. Improving scalability is necessary, so future solutions and developments will be explored, such as the use of the new FSE fire propagator. With FSE, a solution for HPDA and AI by simulating ensembles of wind scenarios and fire origins is designed. The integration of WRF-SFIRE results, particularly volumetric smoke, into immersive VR experiences developed in Unreal Engine has been achieved for training, awareness, and planning purposes.

v. **Material Transport in Water (MTW):** Focusing on pollutant transport within aquatic systems, the MTW pilot has successfully integrated fluid-particle coupling for pollutant tracking and advanced scalar transport modelling, supporting both CPU and GPU architectures. These advances position MTW to provide essential insights into water quality and pollution management, addressing the complex challenges of river and aquatic ecosystem preservation.

Since the last reporting period, 18 new research goals have been identified increasing HiDALGO2's the total number of research milestones from 26 to 44. In this time, the five scientific pilots have collectively achieved 13 of those milestones, including early completion of two, eight remaining on schedule, and nine research goals have seen timeline adjustments to address technical complexities, data dependencies, and resource needs. For example, the integration of atmospheric physics into UAP workflows shifted from M18 to M30, while enhancing damages prediction for RES required external data, extending this milestone from M18 to M36. This signifies the substantial advancement toward the overarching goals of HiDALGO2. To ease the overview of HiDALGO2's progress of the main research activities within each pilot and the main milestones for each of them, a visual representation is provided in Figure 9, Figure 10Figure 11Figure 12, and Figure 13 (see appendix).

In D5.3 [1], four working groups were identified: **WRF**, **Coupling Urban Simulations**, **Coupling Forest Fires and Air Pollution**, and **Visualization**. The last group is focused on Task 4.4, which involves Visualization Techniques; current progress for this task can be found in D4.6 [10]. The other working groups address synergies between the pilots and are actively being explored as part of Task 5.6, *Synergy and Coupled Simulations*. Preliminary outcomes from these efforts are documented in D5.1 [11].

Next Steps:

- **UAP**: Continue enhancing solver capacity and MPI integration to support city-scale simulations on GPU clusters.
- **UB**: Extend model features by incorporating heating systems and further automating data validation processes.
- **RES**: Advance prediction models, focusing on uncertainty quantification and visualizations for improved usability.
- **WF**: Refine coupling of fire simulation engines and atmospheric models while developing VR demonstration tools.
- **MTW**: Integrate scalar-fluid coupling into MTW to fully address aquatic pollution dynamics and GPU compatibility.

Deliverable D5.5 will continue monitoring these efforts, providing an updated analysis of progress and outcomes for the final phase of HiDALGO2. The update of pilot-specific and targeted next steps not only influence the tasks outlined in WP5 but guide each pilot's contributions to HiDALGO2's broader objectives. This includes efforts in **Scalability, Optimization, and Co-Design (Task 3.2)**, **Ensemble Scenarios (Task 3.3)**, **Innovative HPC Technologies (Task 3.4)**, **High-Performance Data Analytics (Task 4.2)**, **Artificial Intelligence for Global Challenges (Task 4.3)**, **Visualization Techniques (Task 4.4)**, and **Uncertainty Quantification (Task 4.6)**. These interconnected efforts are set to drive HiDALGO2 towards scientifically robust solutions for tackling global challenges.

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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.

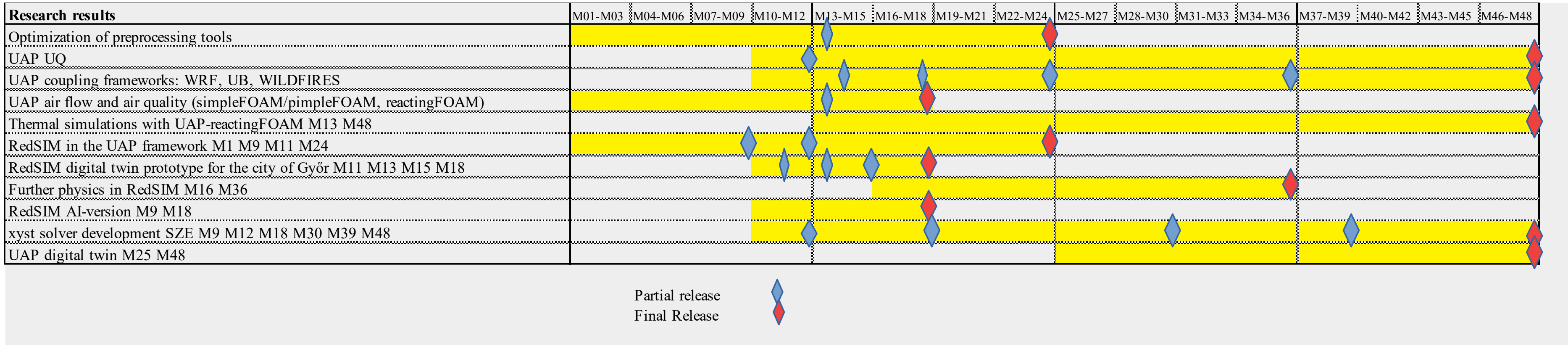

Figure 9 Main research activities in the UAP Pilot and the main milestones in each of them.

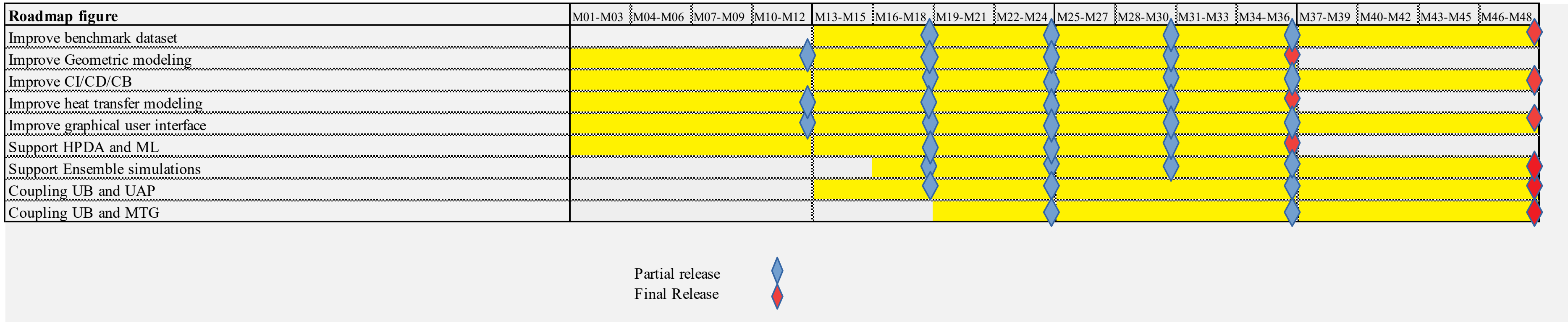

Figure 10 Main research activities in the UB Pilot and the main milestones in each of them.

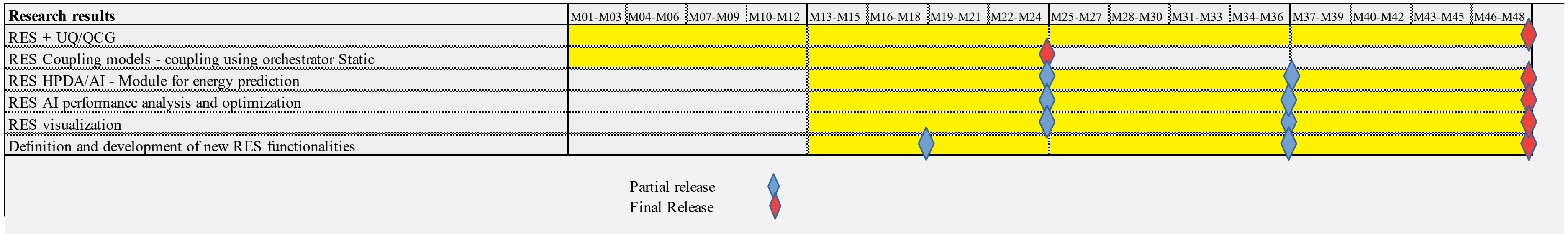

Figure 11 Main research activities in the RES Pilot and the main milestones in each of them.

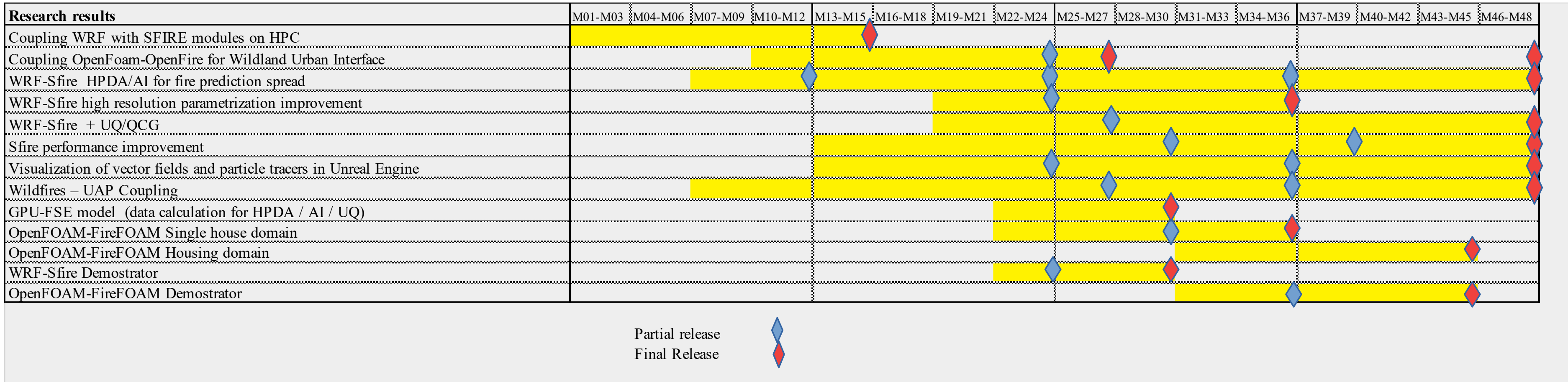

Figure 12 Main research activities in the WF Pilot and the main milestones in each of them.

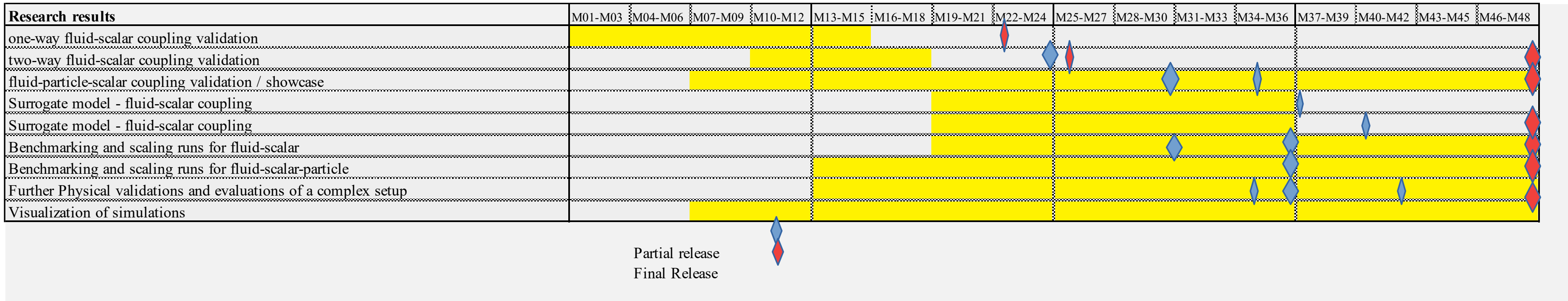

Figure 13 Main research activities in the MTW Pilot and the main milestones in each of them.