

# **D5.7 Implementation Report on Pilot Applications**



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Lead Participant	MTG	Lead Author	Luis Torres
Contributors	MTG, PSNC, SZE, FAU, UNISTRA	Reviewers	Jesús Gorroñogoitia (ATOS)
			Vasiliki Kostoula (ICCS)

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# **Document Information**

List of Contributors	
Name	Partner
Luis Torres	MTG
David Caballero	MTG
Leydi Laura Salazar	MTG
Jaime Ribalaygua	MTG
Michał Kulczewski	PSNC
Wojciech Szeliga	PSNC
Krzysztof Kotecki	PSNC
Filip Depta	PSNC
Christophe Prud'homme	UNISTRA
Vincent Chabannes	UNISTRA
Philippe Pincon	UNISTRA
Gwenollé Chappron	UNISTRA
Ravi Kiran Ayyala	FAU
Harald Koestler	FAU
Zoltán Horváth	SZE
József Bakosi	SZE
Mátyás Constans	SZE
László Környei	SZE

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Document name:	D5.7 Implementation Report on Pilot Applications					Page:	3 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



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Luis Torres	MTG	03/06/2025			
Quality Manager	Rahil Doshi (FAU)	06/06/2025			
Project Coordinator	Marcin Lawenda (PSNC)	06/06/2025			

Document name:	D5.7 Implementation Report on Pilot Applications					Page:	4 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



# **Table of Contents**

Docum	ent Information	3
Table of	of Contents	5
List of	Tables	7
List of	Figures	7
List of A	Acronyms	7
Execut	ive Summary	10
1 Intr	oduction	11
1.1	Purpose of the document	11
1.2	Relation to other project work	11
1.3	Structure of the document	11
2 Urb	oan Air Project implementation status	13
2.1	Current status on software development and implementation	13
2.2	Challenges faced and future plans	15
3 Urb	oan Building Model implementation status	16
3.1	Current status on software development and implementation	16
3.2	Challenges faced and future plans	21
4 Re	newable Energy Sources implementation status	23
4.1	Current status on software development and implementation	23
4.2	Challenges faced and future plans	25
5 Wil	dfires implementation status	26
5.1	Current status on software development and implementation	26
5.2	Challenges faced and future plans	32
6 Ma	terial Transport in Water implementation status	35
6.1	Current status on software development and implementation	35
6.2	Challenges faced and future plans	36
7 Pilo	ot couplings implementation status	37
7.1	Current status on UAP-UBM coupling	37
7.2	Current status on UBM-RES coupling	39
7.3	Current status on UAP-WF coupling	40

Document name:	D5.7 Implementation Report on Pilot Applications					Page:	5 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



7.4	Current status on UBM-WRF coupling	40
7.5	Current status on RES-WRF coupling	43
7.6	Current status on MTW-WF coupling	43
8 Co	onclusions	44
Refere	ences	45

Document name:	D5.7 Implementation Report on Pilot Applications					Page:	6 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



# List of Tables

Tahla 1	Comparative overview of	counling approaches	22
		coupling approaches	 . 22

# List of Figures

Figure 1. Workflow of the Ktirio Urban Building from inputs (left) to outputs (right), orchestration (middle top), data management (top) and the actual application (middle).	17
Figure 2. Screenshots of the report for the city of Luxembourg on cases.ktirio.fr	19
Figure 3. Visualisation of Ktirio Urban Building simulation of Paris and suburbs. The colour shows th	
useful energy.	20
Figure 4. Visualisation of the domain used in the first case of the wildland-urban scenario.	28
Figure 5. Results of the simulation of flame advection around a house in different time steps (in	
seconds) in the first case of WUI scenario using fireFoam solver. Visible flame temperature threshol	d
is 723 °K	30
Figure 6. Top left: detailed architectural model of a single-family house. Top right: surface	
temperatures of the building in °K at timestep 8 s. Bottom left: visible flame surrounding the house	
(723 °K). Bottom right: visible flame boundary colored by velocity magnitude. Note the acceleration	
within the vortices	31
Figure 7. An example of a 3D distribution of biomass around houses	34
Figure 8. Figure demonstrating the temperature distribution in domain with fluid, particles and	
temperature effects	36
Figure 9. First one way coupling between UAP and UBM. Top panels represent the initial data from	
Ktirio Urban Buildin, bottom left panel displays the mesh and bottom right the temperatures in the air	r
and at the walls of the buildings	38
Figure 10. Strasbourg greater area overlaid by temperature field computed by WRF	42

# List of Acronyms

Abbreviation / acronym	Description
AI	Artificial Intelligence
AoS	Array of Structures
CD	Continuous Deployment
CFD	Computational Fluid Dynamics
CI	Continuous Integration

Document name:	D5.7 lr	nplementation Repo	Page:	7 of 48			
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



CPU	Central Process Unit
DMP	Data Management Platform
Dx.y	Deliverable number y belonging to WP x
EC	European Commission
ECMWF	European Centre for Medium-Range Weather Forecasts
EESSI	Electronic Exchange of Social Security Information
FAU	Friedrich-Alexander University
FSE	Fire spread engine
GIS	Geographical Information System
GPU	Graphics Processing Unit
GUI	Graphical User Interface
HPDA SA	High-Performance Data Analytics Sensitivity Analysis
HPC	High-Performance Computing
ICCS	Institute of Communication and Computer Systems
I/O	Input / Output
JSON	JavaScript Object Notation
LBM	Lattice Boltzmann Method
Lidar	Light Detection and Ranging
MPI	Message Passing Interface
MTG	MeteoGrid
MTW	Material Transport in Water
NOAA	National Oceanic and Atmospheric Administration
OSM	OpenStreetMap
PI	Proportional-Integral control
PSM	Partially Saturated Cells Method
PSNC	Poznan Supercomputing and Networking Center
PV	Photovoltaic
RES	Renewable Energy Sources
SIMD	Single instruction, multiple data
SoA	Structure of Arrays
SZE	Széchenyi István University
UAP	Urban Air Project

Document name:	D5.7 Implementation Report on Pilot Applications						8 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



UB	Urban Buildings
UBM	Urban Building Modelling
UCM	Urban canopy model
UNISTRA	University of Strasbourg
UQ	Uncertainty Quantification
WF	Wildfires
WP	Work Package
WRF	Weather Research & Forecasting Model
WUI	Wildland-Urban Interface

Document name:	D5.7 Implementation Report on Pilot Applications						9 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



## **Executive Summary**

This deliverable is part of a series of reports documenting the results and progress of the HiDALGO2's pilot applications in our efforts to address global challenges by leveraging high-performance computing (HPC). D5.7, which covers up to month 29, is an update of the information presented in D5.6 [33] and aims to provide an overview of the advances implemented since month 18 in the use cases and in the couplings between them. Additionally, it outlines the technical advancements and developments expected to be achieved until the end of the project.

In addition to updating the overall progress in the development of these pilots, this deliverable allows to contrast the compliance of the research and development activities against the strategic roadmap contained in D5.6 [33]. It includes the functional improvements achieved in each pilot as well as the steps in the improvement of the possible couplings between them, although a detailed description of the proposed solutions for the couplings between the different pilots is not addressed, as this is already described in D5.1 [34] and will be detailed at the end of the project in D5.2.

This delivery shows the results obtained during this last year in the different pilots of the project and the state of implementation of the proposed solutions in each one of them. All the pilots have advanced towards the fulfilment of the pursued objectives, prioritizing functional or scalability aspects according to the maturity status of the models used in each one of them. The status of the couplings between the models used in the different pilots that have started to be developed or those still in the planning phase is also shown.

It also shows the challenges encountered during the development of the models, and outlines the steps to be taken to achieve the final objectives of the project, even outstanding some innovative solutions to be addressed in the future.

Document name:	D5.7 lr	nplementation Repo	Page:	10 of 48			
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



# **1** Introduction

#### **1.1 Purpose of the document**

The purpose of this document is to provide a comprehensive overview of the status of the implementations of each task under Work Package 5 (WP5), reflects the challenges encountered during the development and sets out the work plan to complete the objectives of each of the project pilots. It also includes the status of implementation of the various couplings planned between the different pilots.

The final objective is to provide a detailed overview of the current state of implementation of each individual use cases in WP5 and the couplings under development, detailing the results achieved during the last months since the submission of deliverable D5.6 [33] and describing the technical developments foreseen until the end of the project.

#### **1.2 Relation to other project work**

This document although mainly related with WP5 activities is also closely related to the activities of other WPs of the project such as WP2 by collecting CI/CD mechanisms in pilots, WP3 in terms of scalability and assemblies and WP4 through the use of data transfer mechanisms AI or HPDA.

#### **1.3 Structure of the document**

This document is organized along the same pattern as D5.6 [33], the previous version of the HiDALGO2 implementation report. It is intended to present a clear and coherent flow of information, enabling a thorough grasp of the implementation processes and results of each HiDALGO2 pilot application. The pilot applications are detailed in their own section, with the Urban Air Project (UAP) in section 2, Renewable Energy Sources (RES) in section 3, Urban Buildings (UB) in section 4, Wildfires (WF) in section 5, and Material Transport in Water (MTW) in section 6.

This document is structured in 8 major chapters.

**Chapter 1**, **Introduction**, presents the overall purpose of the document, outlines the main goals and intended impact of the deliverable, and describes how the document relates to other project work. It concludes with a detailed explanation of how the document is organized to guide the reader through the content.

**Chapters 2 to 6, Pilot X implementation status,** review the pilot applications status. Each pilot section comprises two subsections. These subsections cover the pilot's

Document name:	D5.7 lr	nplementation Repo	Page:	11 of 48			
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



implementation status (subsection x.1), and an outlook on the expected technical advancements until the end of the project (subsection x.2).

**Chapter 7, Pilot couplings implementation status,** presents the advances in the connections and couplings between different pilots and their software packages.

**Chapter 8, Conclusions,** summarizes the main outcomes of the current work, discusses the expected impact on the pilot applications, and outlines the next steps for ongoing development.

Document name:	D5.7 lr	nplementation Repo	Page:	12 of 48			
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



# 2 Urban Air Project implementation status

As stated in HiDALGO2 D5.6 [33] deliverable, the aim of the Urban Air Project is to create a realistic model for microscale urban climate which enables modelling the spread of air pollution, and so assessing the air quality of a city on a microscale level. The several solvers used in the UAP pilot have undergone significant advances during the last year since the delivery of the previous version D5.6 [33].

### 2.1 Current status on software development and implementation

#### **UAP-FOAM**

The following features have been implemented since the last deliverable D5.6:

Support for thermal conduction. As part of the implementation for UAP-UBM coupling, temperature support had to be implemented into the UAP-FOAM workflow using the *buoyantBoussinesqPimpleFoam* solver [1].

*buoyantBoussinesqPimpleFoam* is a solver in OpenFOAM specifically tailored for transient, incompressible flow simulations incorporating buoyancy effects using the Boussinesq [21] approximation. It's commonly employed for heat transfer analysis and buoyancy-driven flows, like natural convection or mixed convection scenarios, where density variations are sufficiently small to be modelled linearly with temperature variations.

Under the Boussinesq approximation, density ( $\rho$ ) is expressed as:  $\rho = \rho_0 [1 - \beta(T - T_0)]$  where  $\rho_0$  is the reference density,  $\beta$  is the thermal expansion coefficient, and  $T_0$  is the reference temperature. This approximation assumes incompressible fluid dynamics with slight variations in density due to temperature gradients affecting buoyancy forces.

• Support for the newer OpenFOAM version v2412 [2], as reported in D3.2 [36]. Please, refer to this deliverable for further details on this implementation.

#### RedSim

In the period just ending, i.e. between M19 and M29, the RedSim code [3] has been developed very significantly. Beside implementing the full MPI+GPU functionality to RedSim, RedSim has been vectorised with SIMD. Several new functionalities have been implemented, too, namely a full Lua-API [22] and extensive development of the preprocessing tool has been done. The latter developments were induced by the requirements emerged from the application of RedSim to Stockholm city in a collaboration with SZE, ENCCS (the Swedish NCC for boosting supercomputing), and SLB-analys (the unit of Stockholm City responsible for monitoring and analysing air and noise pollution of the city).

• Lua API Rework. RedSIM's scripting Lua scripting API has been reworked from the ground up, in order to be as modular as possible, and now has the following features.

Document name:	D5.7 lr	nplementation Repo	Page:	13 of 48			
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



- Meshes and other resources can be created through the API, with a handle to the resource returned.
- The user can then combine all these different resource handles in order to define a simulation workflow. For example, it is possible to load multiple meshes, multiple solvers and boundary conditions, store their handles and launch different simulations with different resource combinations.
- MPI [23] Parallelization rework. RedSIM's parallelization strategy has been reworked from a centralized model (master-slave), to a purely democratic model (the only exception being the initial execution of the Lua script, which is done through a centralized model). Furthermore, thanks to MPI I/O, we now have well scaling file exports in Ensight GOLD [24] and VTK [25], which is crucial for scaling on a large number nodes.
- MPI + CUDA [26] Parallelization. Previously, RedSim was using MPI for the CPU version of the code, and CUDA for the GPU version without MPI. Although it was possible to simulate on 8 GPU-s on a single node, now that the code has been rewritten to use an OpenMPI + CUDA framework, it is possible to use as many GPU-s as desired, distributed on as many CPU nodes as desired
- Flux Vectorization in SIMD. All flux computations have been rewritten to utilize SIMD. This was really challenging, since it required a fundamental change in how we stored flux in our dataset (AoS vs. SoA).
- Optimization on pure tetrahedral meshes. Although RedSim works for arbitrary conform polyhedral meshes, often (e.g. Stockholm UAP application) simulate on tetrahedral-only meshes. A separate code path has been created, tetrahedral only, which is heavily optimized for only manipulating tetrahedra.
- A very thorough reimplementation of mesh generation for RedSim was done to fulfill the requirements for the Stockholm use case. Namely, the geometry input files can already be SHAPE files, terrain information has been incorporated to the 3D geometry of the airflow domain by creating a non-flat ground according to the isolines of the terrain, which are provided by the external user in a SHAPE file, Gmsh has been integrated and properly configured to the UAP applications.

## XYST

Since the reporting for D5.6, three new solvers have been implemented into Xyst: all of them targeting the simulation of low-speed fluid flows, suitable for atmospheric conditions. Solvers' correctness has been verified (comparing to known analytic solutions, and validated with experimental data). More details on these solvers can be found at the Xyst docs webpage [27] and on verification and validation at the Xyst V&V webpage [28].

Computational performance at large scales has been tested on one of the EuroHPC-JU [32] machines, Lumi, up to almost 200 thousand CPU cores, yielding good strong scalability for all solvers tested. Details can be found on the above link and at the HiDALGO2 Xyst description page [29].

Document name:	D5.7 Implementation Report on Pilot Applications						14 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



### 2.2 Challenges faced and future plans

#### UAP-FOAM

Excluding the above advances, coupling and integration, the following features are planned for UAP-FOAM: simulation and validation of chemical reactions between pollution species, and solar radiation. Further development and validation of our models on additional cities is also planned. Implementing UAP-FOAM with GPU based OpenFOAM implementations is among the next steps.

#### RedSim

In the just ended period many new functionalities were implemented to RedSim. In the next period the documentation, testing and application for external use cases will be the main tasks of the code. Also, the licensing is planned to change to be able to distribute it and create a user community, according to the KPIs of HiDALGO2.

#### XYST

Future work in Xyst is useful in the following different directions:

- Scalar transport: Constant-density solvers need scalar-transport implemented and tested.
- 200k-core runs: Scalability of some of the solvers need to be tested in the 200k-CPU range.
- Atmospheric boundary conditions need to be implemented, reading inhomogeneous user-specified fields on wind data on domain boundaries.
- Beside point source, line source also need to be implemented as a source of UAP-FOAM

Document name:	D5.7 lr	nplementation Repo	Page:	15 of 48			
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



# **3 Urban Building Model implementation status**

#### 3.1 Current status on software development and implementation

The Ktirio [4] Urban Building pilot has been considerably developed during the last year. Developments have occurred in all components to streamline and automatise the pilot application deployment and data management.

In Figure 1, the Ktirio Urban Building (UBM) workflow integrates multiple components of the HiDALGO2 ecosystem to enable scalable, high-resolution urban simulation. Input data—ranging from weather forecasts and GIS layers to simulation scenarios— is managed through standardized platforms such as CKAN, Girder, and Zenodo. These inputs are accessed by tools like Modelica, the Ktirio GUI, and Feel++ Benchmarking, which are used to generate simulation configurations or trigger execution workflows.

Workflow orchestration is handled by services including MathSO, QCG, and KUB-CD, with GitHub and GitLab supporting source control and continuous integration. These tools deploy simulation workflows onto the Ktirio execution core, composed of the DB Shell and the Urban Building engine, which orchestrate the data lifecycle and compute tasks. Simulations can be executed on EuroHPC systems (e.g., LUMI, Karolina, Vega), other supercomputers, or cloud infrastructure.

Outputs—including 3D meshes, fields, logs, and reports—are pushed back to the data management layer and made accessible through output tools such as ParaView [5], the Ktirio GUI, and web-based platforms for benchmarking and case review. The workflow supports both desktop and web deployment, with some modules running as WebAssembly [6] for lightweight execution. This cohesive system enables end-to-end simulation, visualization, and benchmarking for urban-scale building models, facilitating climate-resilient design and high-performance urban planning.

Document name:	D5.7 Implementation Report on Pilot Applications						16 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



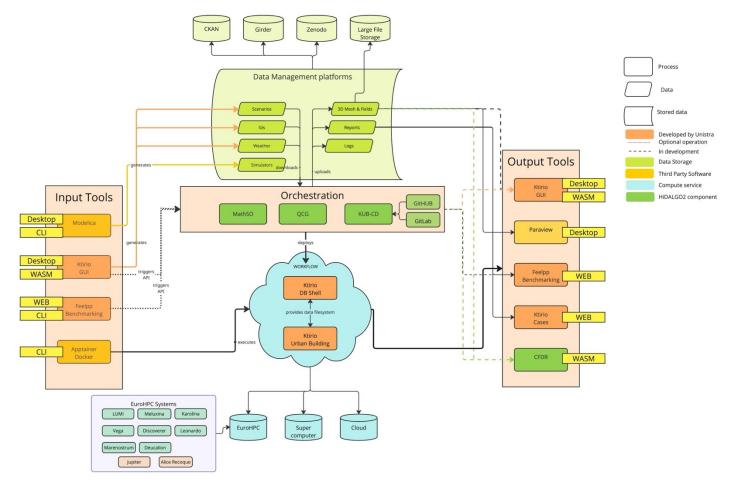


Figure 1. Workflow of the Ktirio Urban Building from inputs (left) to outputs (right), orchestration (middle top), data management (top) and the actual application (middle).

Document name:	D5.7 Implementation Report on Pilot Applications						17 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final





#### **Building Modelling Enhancements**

Recent simulation upgrades have boosted stability, efficiency, and adaptability by dynamically sizing the boiler, heat pump, pump flow rate, and fan speed in C++ using the 30-year minimum temperature. Each floor's radiator and the air-water heat pump now run on optimized PI control loops—mixing boiler output and recirculated water or regulating outflow temperature—to ensure precise, stable thermal regulation. Wall temperatures are initialized via a preliminary steady-state solution, improving spin-up and realism. We've also implemented BVH-based solar mask computations with MPI parallelization (including vegetation shading), enhanced energy- and mass-flow meter handling, and enabled true multi-storey building support. Together, these changes deliver a robust, scalable model capable of accurate performance across varied building sizes. The models are tested against standards in the building energy simulation domain.

### **HPDA** Developments

We've implemented city-scale data aggregation to compute key energy metrics and export them as JSON—enabling dynamic generation of web dashboards or detailed reports on urban energy behaviour, checkout Ktirio web page [30] and Figure 2. Additionally, these datasets have been provided to the HPDA Team from ICCS in HiDALGO2 to integrate and extend the HPDA workflows for solar-cell placement optimization across urban areas.

Document name:	D5.7 lr	D5.7 Implementation Report on Pilot Applications					18 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



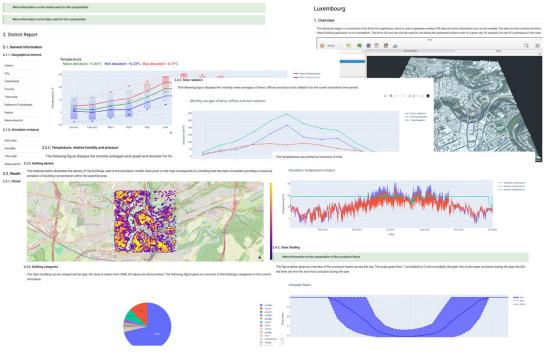


Figure 2. Screenshots of the report for the city of Luxembourg on cases.ktirio.fr

#### Al Integration

We have supplied geospatial and energy-model assets to the AI Team from ICCS to support AI-driven analyses of urban form changes—specifically to evaluate the energetic impact of adding or removing buildings within a city. This enables data-driven decision-making for urban development scenarios.

#### Ensemble & Uncertainty Quantification (UQ)

We have begun architecting our Ensemble & UQ framework to integrate seamlessly into standard district-scale energy simulations. Rather than relying solely on deterministic runs, our stochastic ensemble approach will sample key input uncertainties—such as weather, occupancy, and material properties—to generate probability distributions of performance metrics. This will equip decision-makers with statistically robust insights into expected energy behaviour and risk profiles.

#### **Computing Environment Enhancements**

On the computing environment front, we've upgraded data management to produce watertight meshes—including vegetation and meter geometries—and now integrate Girder and CKAN as our DMP backends. Our CI/CD pipelines have been streamlined

Document name:	D5.7 lr	nplementation Repo	Page:	19 of 48			
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



to automatically build and publish Apptainer [13] containers, and we've embedded FEEL++ benchmarking into the workflow for end-to-end automated performance tests, checkout <u>bench.ktirio.fr</u>.

### **Application Deployment**

The simulation has now been deployed across several cities (Strasbourg, Athens, Luxembourg, Stuttgart, Poznan, Madrid, Gyor, Erlangen), including all partner municipalities and several additional urban areas, to support a wide range of case studies and comparative analyses. You can explore live examples and results at <u>cases.ktirio.fr</u>.

In **Error! Reference source not found.**, a screenshot of a large scale simulation using K tirio Urban Building including vegetation of Paris and suburbs with more than 160K buildings.

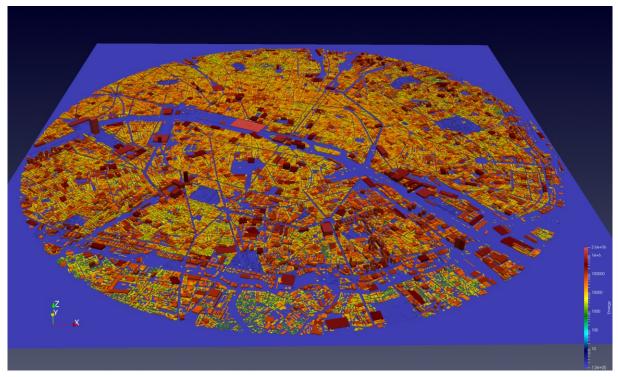


Figure 3. Visualisation of Ktirio Urban Building simulation of Paris and suburbs. The colour shows the useful energy.

Useful energy, shown in <u>Figure 3</u>, refers to the portion of energy that is effectively used to meet the desired indoor conditions, such as heating, cooling, lighting, and ventilation. It represents the energy demand at the point of use, before considering system losses or inefficiencies. Useful energy helps quantify the intrinsic performance of a building design (insulation, orientation, windows, etc.) independent of the technical system. The unit is usually in kilowatt-hour.

Document name:	D5.7 Implementation Report on Pilot Applications						20 of 48
Reference:	rence: D5.7 Dissemination: PU Version: 1.0					Status:	Final





## 3.2 Challenges faced and future plans

## Challenges Encountered

We faced significant hurdles in securing high-quality input data for meteorology, urban vegetation, and city-scale contexts, which directly affected the fidelity of our simulations. As our physical models became ever more sophisticated, I/O routines emerged as a critical performance bottleneck, forcing us to optimize data pipelines and solver workflows extensively to recover lost efficiency. Ensuring solver robustness across complex, multi-physics configurations also demanded considerable effort, as we needed to tune parameters continuously to prevent intermittent slowdowns and numerical instabilities.

## Future Plans

Support for description Levels 1 and 2, the level of geometric accuracy of the building description, will be added to capture finer details of building systems and usage patterns. To accelerate solar-mask computations, we plan to implement advanced spatial pre-processing and hierarchical data structures, and our topography module will be overhauled to handle terrain relief with greater accuracy and efficiency. The stochastic ensemble and UQ framework we have designed will be fully implemented, delivering probabilistic performance metrics that empower decision-makers with statistically robust insights. Finally, we will expand our modelling capabilities to include detailed indoor-air-quality simulations coupled with outdoor air quality—leveraging both meteorological datasets and WRF [7] outputs—and integrate these with our UAP coupling to provide end-to-end air-quality forecasting from the city scale down to individual building zones.

To provide a comprehensive understanding of the couplings with Urban Building Model (UBM), it's essential to contextualize this integration within a multi-scale modelling framework. This framework encompasses three tiers of atmospheric data sources, each varying in spatial resolution and complexity, and each serving distinct roles in urban climate simulations.

## Multi-Scale Atmospheric Modelling Framework

- Point-Based Meteorological Data (e.g., OpenMeteo, Station Observations)
  - **Resolution**: Single-point measurements
  - **Characteristics**: These datasets provide time series of meteorological variables such as temperature, humidity, and wind speed at specific locations. They are readily accessible and useful for general assessments but lack spatial granularity.
- WRF–UBM Coupling
  - **Resolution**: Approximately 1 km<sup>2</sup> grid cells

Document name:	D5.7 Implementation Report on Pilot Applications						21 of 48
Reference:	Reference: D5.7 Dissemination: PU Version: 1.0					Status:	Final



- **Functionality**: The WRF model offers mesoscale atmospheric simulations, capturing regional weather patterns and urban effects through parameterizations like the Urban Canopy Model (UCM). When coupled with UBM, WRF provides spatially distributed meteorological inputs, enhancing the realism of building energy simulations.

#### • UAP–UBM Coupling

- **Resolution**: 1–5 meters spatially; minute-level temporally
- Capabilities: The Urban Air Project (UAP) utilizes computational fluid dynamics (CFD) to simulate urban airflow at a micro-scale, resolving individual building geometries and street canyons. This high-resolution modelling enables detailed analysis of microclimatic conditions and supports bidirectional coupling with UBM, allowing for dynamic feedback between building energy use and local airflow patterns.

A comparison of the characteristics of the different coupling scenarios described is shown in <u>Table 1</u>.

Coupling Approach	Spatial Resolution	Temporal Resolution	Coupling Direction	Key Applications
Point-Based Data	N/A	Hourly/Daily	One-way	Basic energy modelling, general assessments
WRF–UBM	~1 km²	Hourly	One-way	Regional climate studies, urban planning
UAP-UBM	1–5 meters	Minutes	Bidirectional	Microclimate analysis, detailed energy modelling

#### Table 1. Comparative overview of coupling approaches

#### Integration and Application

This tiered modelling approach allows for flexibility in urban climate studies:

- **Baseline Assessments**: Utilizing point-based meteorological data for preliminary evaluations or in data-scarce regions.
- **Regional Analysis**: Employing WRF–UBM coupling to understand broader urban climate dynamics and inform policy decisions.
- **Detailed Design**: Applying UAP–UBM coupling for high-fidelity simulations necessary in architectural design, urban redevelopment, and resilience planning.

By integrating these models, researchers and planners can achieve an understanding of urban microclimates, facilitating informed decision-making in urban development and sustainability initiatives.

Document name:	D5.7 Implementation Report on Pilot Applications						22 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



## 4 Renewable Energy Sources implementation status

Renewable Energy Sources (RES) pilot is tailored towards modelling renewable energy sources such as wind farms and photovoltaic systems to provide energy production forecast. Details on pilot can be found in deliverables D5.3 [35] and D5.6.

#### 4.1 Current status on software development and implementation

#### **RES-runner**

Several implementations and enhancements were realised. New input flags were added to the framework for more versatility in its deployment and execution on multiple sites and to improve the pipeline's flexibility when using partially processed data files. Moreover, a dedicated RES configuration was prepared for the newly installed HPC resources at PSNC, 'Proxima' partition, including not only new servers but also new operating system and environment. Also, in order to speed up the development and debugging process of computationally demanding EULAG component of RES-runner, a lightweight, and quick to resolve additional debugging execution option was implemented. The automatic pictures generation at postprocessing stage was also improved for non-default simulation time regime. Apart from implementing new functionalities, several bugs in the code were identified and fixed.

A significant enhancement has streamlined the simulation domain preparation. Instead of depending on building data from local municipalities, the system now utilises OpenStreetMap<sup>1</sup> data, greatly increasing its applicability across diverse locations. Furthermore, the manual conversion of this data into the structured grid format required by the EULAG model [8,9] is now automated directly upon retrieval from OpenStreetMap.

#### **RES-wind/PV scenario**

The Renewable Energy Sources (RES) pilot leverages the EULAG model, a versatile all-scale geophysical flow solver, adept at tackling a wide array of complex phenomena. Each RES scenario necessitates a tailored model setup, including specific parametrisation schemes, domain configuration, and supplementary mesh data.

For RES-damages, RES-PV, and RES-wind applications outside urban areas, a dedicated EULAG configuration incorporates orography, with physics optimised for such terrain-driven flows. In contrast, urban environments utilise a distinct model configuration that accounts for intricate building structures through immersed boundary methods.

<sup>&</sup>lt;sup>1</sup> OpenStreetMap data https://www.openstreetmap.org

Document name:	D5.7 Implementation Report on Pilot Applications						23 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



Crucially, RES now features an integrated vertical wind profile capability, enabling wind condition predictions at any height of interest. This enhancement is applicable to both urban and non-urban model setups. It proves invaluable for RES-damages scenarios, facilitating the assessment of damage probability to overhead networks, and for RES-wind scenarios, enabling detailed wind condition forecasting. While less critical, RES-PV also benefits from this vertical wind profile, as wind is a contributing factor to photovoltaic system efficiency.

### Wind and solar energy modules

Accurate energy production forecasting is crucial for the RES workflow. Given PSNC's existing photovoltaic systems, our initial focus is on PV forecasting. We are leveraging AI in the form of predictive models that analyse sequential (time series) data to identify correlations between weather conditions and energy generation, enabling more effective forecasting. The AI model training is currently being finalised using publicly available sensor data and forecasts from sources like OpenMeteo. Once trained, the model will be integrated with daily RES weather forecasts for operational use.

#### CKAN

Following the successful integration of RES with CKAN, all intermediate and final outputs from daily processes are now automatically archived within CKAN. This includes forecast data and basic visualisations, ensuring their availability for subsequent reanalysis, HPDA, ensemble generation, and AI model development.

#### HPDA SA

Performing High-Performance Data Analytics Sensitivity Analysis (HPDA SA) on the EULAG model aims to analyse the sensitivity of output results to input parameters. The primary focus of this analysis is wind velocity, a crucial parameter for wind turbine energy production forecasting. However, the analysis also encompasses wind direction, temperature, and pressure. To achieve this, the RES runner tool has been integrated with the mUQSA toolkit [37][38] through the development of custom data converters, encoders, decoders, and integration scripts. The analysis results are stored in a NetCDF4 file, with topographical layers representing individual parameters such as descriptive statistics and Sobol' indices. Currently, an issue with insufficient Sobol' index values necessitates further investigation. More details regarding the RES HPDA Sensitivity Analysis will be provided in the WP4 deliverable dedicated to HPDA.

Document name:	D5.7 Implementation Report on Pilot Applications						24 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



## 4.2 Challenges faced and future plans

Currently, the primary challenges revolve around deploying a containerised version of RES. Many of the issues encountered during the RES-UBM integration are proving relevant here, and the solutions developed for that integration will be applied to RES to address these current challenges.

Another challenge involves acquiring real-world energy production data from wind farms. Discussions are underway with a Distribution System Operator in Poland to potentially share this data for model validation purposes. As an alternative, synthetic data can be utilised to develop and propose the RES-AI module for wind farms, with the understanding that the module's capabilities will be further refined once actual measurements become accessible.

The immediate next step is the integration of a RES-AI module into the workflow, with the goal of forecasting energy production from renewable sources. Another key priority is enhancing the integration of RES with QCG [37][38]. While basic integration exists, improvements are needed to offer users greater flexibility in defining boundary conditions, particularly the region of interest. Furthermore, while rudimentary forecast visualisation is in place, the integration with CFD is planned to provide a more insightful and scientific representation of the results.

Document name:	D5.7 Implementation Report on Pilot Applications						25 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



# 5 Wildfires implementation status

As described in the HiDALGO2 deliverable D5.6, two different use cases have been defined within the WF Pilot. A first use case using WRF-SFIRE focused in atmosphere and wildfire interactions at **landscape scale**, this is several km of fire spread in the wildland area; and a second use focusing on the fire behaviour around houses in the **WUI scale** (wildland-urban interface), using OpenFOAM [2] and specific solvers for the modelling of pyrolysis and combustion of vegetation and other fuels.

## 5.1 Current status on software development and implementation

### Landscape scenario

In response to the portability and scalability challenges detected described in HiDALGO2 D3.2 deliverable [36], mainly related to the difficulty of the installation process on different machines and the reduced scalability of the tests performed up to month 19 of the project, the WF pilot undertook during this reporting period a series of corrective actions. In particular:

- A hybrid implementation of WRF-SFIRE [10] using MPI and OpenMP has been installed in several Euro-HPC machines,
- With the support from the EPICURE project [16] co-design task, the pilot's build system and execution environment have been refactored to ease the deployment on new EuroHPC systems, reducing hard dependencies and improving modularity.

In addition to solving WRF [7] bottlenecks, MTG is adapting its wildfire simulation engine (FSE) for CPU and GPU execution on HPC systems. The GPU version is being prepared to support large-scale sensitivity analysis and uncertainty quantification campaigns. These activities, carried out jointly with other HiDALGO2 partners (namely ICCS, Eviden and PSNC), leverage HPDA techniques to process the outputs of thousands of simulation runs for territory vulnerability assessment and are helping in defining AI solutions applied to fire behaviour.

The CPU version is intended to be used for a quick evaluation of uncertainty quantification (UQ) to be compared with a more resource-demanding assessment using WRF-SFIRE. In both cases, up to 50 different equi-probable boundary conditions from the ECMWF ensemble model are used. The new version is currently being installed in Meluxina and the scripts are being prepared to run the simulations in parallel.

The WF pipeline needs to use meteorological and weather data from external providers. For this purpose, it will be using functionality developed within the HiDALGO2 Data Management tasks (T4.1). Currently, the data can be requested to the providers, stored locally or in CKAN, and used within the pipeline for simulation as boundary conditions. As of the writing of this document, the external provider available

Document name:	D5.7 Implementation Report on Pilot Applications						26 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



data available to be included in the pipeline is NOAA but new developments are in progress to add data from the ECMWF.

#### Wildland-Urban scenario

At the property scale (i.e., the house and its immediate surroundings), the computational domain is considered to be on the order of a few dozen meters. The objective is to simulate fire behaviour and its impact on building components, particularly the façade, roofing, and glazing.

In the implementation of the considered thermo-fluid dynamic models, the computational domain is designed as an equivalent to a wind tunnel, in which both the building and surrounding vegetation are inserted. The combustion of vegetation is the main source of heat.

Two levels of increasing complexity have been considered:

- Simulation of the **effect of a heat source** located 2 meters from the south façade of a simplified single-family house model. The heat source represents the combustion of a green hedge that is 1 meter deep, 1 meter high, and extends along the entire length of the south façade (a total of 7 meters).
- Simulation of the effect of **combined combustion** of hedges, ornamental plants, and trees in the surroundings of the house. For this, detailed 3D models of the vegetation are used, along with estimates of the biomass involved in combustion and the porosity factor.

The goal of the simulations is to assess the incident heat flux  $(kW/m^2)$  on each building component and determine whether it exceeds established thresholds for structural survival. Advances in HPC simulation during this period have focused primarily on the first level of complexity, considering a constant heat source  $(CH_4 \text{ burner})$ , for which **two cases** have been developed.

#### Case 1: simplified single-family house

The first case simulation domain is a rectangular enclosure measuring 27x10x17 meters, Figure 4. A clearance of 5 meters was maintained along the Z-axis on both sides of the building to avoid boundary effects from the lateral walls. Similarly, the building was placed 10 meters away along the X-axis to allow for proper stabilization of the airflow at the inlet (X=0) and outlet (X=27). The vertical limit of the domain was set at 10 meters to capture most of the local convective effects near the building. The distance between the top edge of the building's roof and the upper boundary of the domain is 6.7 meters.

As for the building used in the initial simulations, it is a simplified model of a singlefamily home. This building has six façades, a roof, a porch, two wooden doors, and glazing throughout its envelope. The materials considered are: brick and cement for

Document name:	D5.7 Implementation Report on Pilot Applications						27 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



the façades, clay tile for the roofing, solid pine wood for the doors, and glass for the glazing.

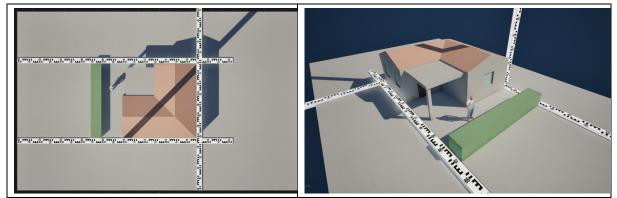


Figure 4. Visualisation of the domain used in the first case of the wildland-urban scenario.

As for the approach and solvers selected:

- In the first simulation, a constant heat source is considered—specifically, a 7x1 meter methane burner representing the surface area covered by the green hedge which combustion is thermally equivalent. For these simulations, the *fireFoam* [17] solver within the OpenFOAM simulation framework has been used.
- In the second simulation, the vegetation is assumed to be a reactive porous medium; therefore, the use of the *porousGasificationFoam* [18, 19] solver within the OpenFOAM simulation environment is proposed.

In both cases, simulations were carried out with zero wind and with a 2 m/s wind aligned exactly with the X-axis (the main flow direction). This allows assessment of the advection effect on the heat source and its impact on the building, <u>Figure 5</u>.

#### Simulation resolution, meshing and parallel partitioning

To evaluate the scalability of the solutions, simulations are proposed at different base cell resolutions of 10 cm, 5 cm, and 2 cm, respectively. Additionally, the base mesh has been refined through castellation and snapping processes with snappyHexMesh tool, especially on the surfaces and edges that define the geometry of the house. This significantly increases the cell count and requires finer timesteps.

Indeed, given the reactive and turbulent nature of fire simulations, the initial advection velocity (2 m/s) is accelerated in many areas of the computational domain (up to 14 m/s), making it necessary to control the Courant number using very small timesteps (on the order of 0.002 s). To solve this, the simulations include automatic timestep adaptation with a target Courant number of 0.9, which ensures the numerical stability of the simulations. This fine time discretization results in more frequent pauses in MPI-

Document name:	D5.7 Implementation Report on Pilot Applications						28 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



based simulations for processor synchronization and can become a bottleneck in the total computation time, particularly using larger number of cores.

Domain partitioning has been used for parallel computation from 1 to up to 2000 cores using scotch scheme.

#### Simulation of heat emission from a burner

The basic configuration parameters for OpenFOAM / fireFoam in this case are:

**Burner Definition** 

- Ground area from (7, 0, 5) to (8, 0, 12)
- Surface area: 1 m × 7 m
- Defined as a faceset (patch) for fuel/energy injection
- Uses topoSetDict and createPatch tools
- fvOptions is used to inject energy or a fuel mixture (CH<sub>4</sub>)

Inlet / Outlet / Boundaries

- X=0: fixedValue for U = (2 0 0) m/s
- X=27: outlet with zeroGradient
- Side walls and ground: wall
- Top: pressureInletOutletVelocity (open)
- Burner: flow (+Y) of methane, varies from 0.1306 m/s, for the simulation of a 4220 kW/m fire (3 m flame length), to 0.5 m/s, for the simulation of a fire of 21500 kW/m (flame length of 10.7 m, as in Figure 5).

Combustion and Reactions

- Methane-air mixture
- A singleStepReactingMixture reaction model is used
- Methane heat of reaction: ≈ 50 MJ/kg
- fvOptions is used to inject methane as a mass or energy source into the burner.

#### Case 2: detailed house architecture

A new simulation has been carried out using a much more detailed 3D model of a wooden building that incorporates all the architectural elements of the envelope. In this case, the geometry description process has been more demanding, as well as the meshing and refinement process. In this case, a general wind of 2 m/s along the X-axis has also been considered, blowing towards the south façade of the building, with a green hedge located 6 meters in front of it. The combustion of this hedge is considered the main heat source.

Document name:	D5.7 Implementation Report on Pilot Applications						29 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



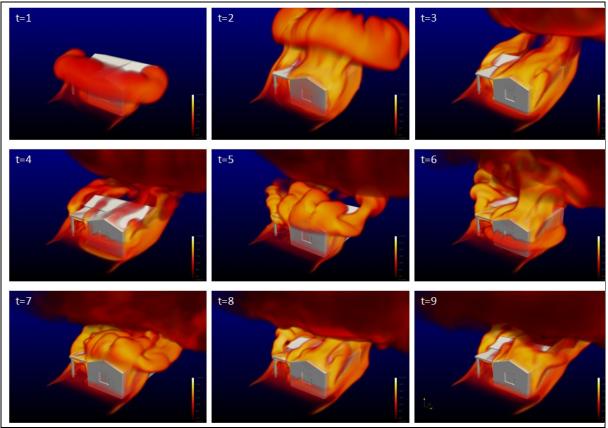


Figure 5. Results of the simulation of flame advection around a house in different time steps (in seconds) in the first case of WUI scenario using fireFoam solver. Visible flame temperature threshold is 723 °K.

#### Simulation resolution, meshing and parallel partitioning

A computational domain of  $47 \times 15 \times 27$  m has been defined with a base resolution of 10 cm. Subsequent refinement has been applied to the building's surfaces (level 1 = 5 cm) and edges (level 2 = 2.5 cm) to capture the details of smaller elements, especially the porch railing. In this case, the Courant number has also been controlled (Co = 0.9) using automatic timestep adaptation. This aspect has been particularly important given the fineness of the 3D model and the turbulent and reactive nature of the flow.

#### Simulation of heat emission from a burner

The basic configuration parameters for OpenFOAM / fireFoam in this case are: Burner Definition

- Ground area from (10, 0, 7) to (12, 0, 20)
- Surface area: 2 m × 13 m
- Defined as a faceset (patch) for fuel/energy injection
- Uses topoSetDict and createPatch tools
- fvOptions is used to inject energy or a fuel mixture (CH<sub>4</sub>)

Document name:	D5.7 Implementation Report on Pilot Applications						30 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



Inlet / Outlet / Boundaries

- X=0: fixedValue for U = (2 0 0) m/s
- X=41: outlet with zeroGradient
- Side walls and ground: wall
- Top: pressureInletOutletVelocity (open)
- Burner: flow (+Y) of methane of 0.1306 m/s, for the simulation of an 8567 kW/m fire (6.2 m flame length as in <u>Figure 4</u>).

**Combustion and Reactions** 

- Methane-air mixture
- A singleStepReactingMixture reaction model is used
- Methane heat of reaction: ≈ 50 MJ/kg
- fvOptions is used to inject methane as a mass or energy source into the burner.

Special attention has been given to the areas of the building with flame impingement, as these are the regions where the highest temperatures are observed. Thermally thin elements are particularly vulnerable, as they exhibit less pronounced temperature gradients, <u>Figure 6</u>.

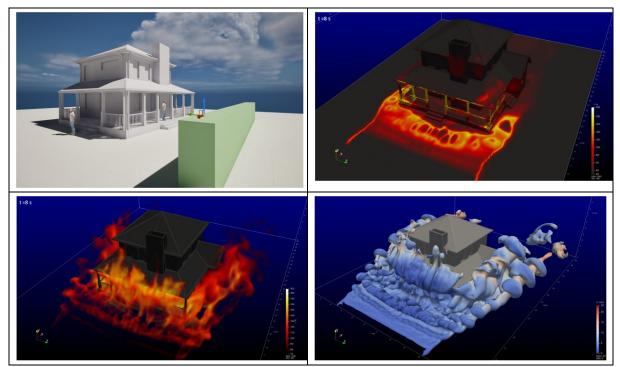


Figure 6. Top left: detailed architectural model of a single-family house. Top right: surface temperatures of the building in °K at timestep 8 s. Bottom left: visible flame surrounding the house (723 °K). Bottom right: visible flame boundary coloured by velocity magnitude. Note the acceleration within the vortices.

Document name:	D5.7 Implementation Report on Pilot Applications						31 of 48
Reference:	D5.7 Dissemination: PU Version: 1.0					Status:	Final



## 5.2 Challenges faced and future plans

## **Challenges Encountered**

A big challenge encountered in the last year has been the installation and deployment of the project code versions on the different HPC-JU machines. Different solutions have been defined for the different applications of the pilot.

The solution proposed for WRF-SFIRE thanks to the support received from EPICURE is the use of EESSI [11]. The main objective of EESSI is to build a scientific software stack for HPCs or any other system (cloud, local, etc.). This facilitates the installation of any existing software in the EESSI software repository that can be then installed on any system on which EESSI has been previously deployed, making use of EasyBuild. EESSI is currently available on several of the HPCs in the Euro-HPC network (Karolina, Vega, Deukalion and MareNostrum5) but the ultimate goal is to make it available on all of them. A contribution to the EESSI software repository, with a WRF-SFIRE EasyBuild recipe [12] is currently under development in the pilot, in order to have a reliable and replicable solution for installation on all HPCs.

The solution adopted for FSE is Apptainer [13] which integrates with Git and allows a fully automated deployment. Within the project, a course on Containerisation, CI/CD, and Benchmarking solutions for HPC was held to present the different solutions available in terms of container technology and their integration with Gitlab or Github. The Apptainer containerisation has been already tested on Meluxina.

After carrying out several tests and analyses of mUQSA [14] and EasyVVUQ [15], the approach that seems the most appropriate one to carry out a UQ study with WRF-SFIRE, given the complexity of the study, is the use of ensembles that allow the incorporation of a controlled set of parameters, and the analysis of the results obtained in this way. This is intended to provide an analysis of the uncertainty associated with the weather situation, by simulating in parallel with different equiprobable initial conditions from the ECMWF ensemble.

An analysis, also modifying other initial variables such as the forest fuel moisture and the distribution, or the location of initial sources, will be carried out with the recently developed version of FSE.

In wildfire simulation and vegetation combustion around buildings in the WUI, several challenges have been identified. On one hand, as it is a reactive turbulent diffusion phenomenon, fluid accelerations require detailed control of the Courant number to ensure numerical stability—especially for more detailed architectural models. This requires a significant reduction of the timestep, which in turn leads to more frequent MPI synchronization stops. Dividing the domain into many subdomains for parallelization (more than 1000) further exacerbates scalability issues in such cases. It is therefore a challenge to find a solution that both ensures the numerical stability of the simulations and improves the scalability of the parallel process.

Document name:	D5.7 Implementation Report on Pilot Applications						32 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



Regarding the use of specialized solvers for reactive porous media, one of the main challenges lies in defining transfer functions capable of capturing the biomass distribution and, more importantly, the porosity of vegetation structures found in forested areas and the WUI. Furthermore, the suitability of the solver porousGasificationFoam still needs to be tested in more complex vegetation structures, with varying degrees of moisture, for estimating combustion and smoke production under partial oxidation conditions.

### **Future Plans**

The implementation of the WF pilot has been planned in different steps, for which the first ones have been completed. However, in light of the new challenges formulated along the pilot development, the future plans also include:

- Integrate a smoke dispersion model in FSE and compare the results between WRF-SFIRE and FSE in different meteorological conditions by further analysing the fire-atmosphere interaction and its implications on the development of fire spread.
- Integration of 3D biomass distributions (i.e., solid phase fraction) and porosity factor derived from complex vegetation structures. A uniform porous medium is considered, with wood as the solid phase (<u>Figure 7</u>).
- It is proposed to assess the suitability of the selected solvers for combustion simulation (fireFoam, porousGasificationFoam) through a comparative study, including their scalability, in order to identify the workflow that both provides results closest to reality and is sufficiently practical for use in real-case scenarios.
- The use of specialized solvers for simulating fire spread over more complex vegetation structures—such as wildfireFoam—will also be explored, and their suitability for application in WUI scenarios will be evaluated. As with the previously mentioned solvers, a comparative study of both the simulation results and scalability in parallel computing environments will be conducted.
- The simulations will be extended to larger domains including multiple houses and complex vegetation patterns in specific case studies: Győr, Strasbourg, and Luxembourg. LiDAR data sources have been identified for this purpose.

Document name:	D5.7 Implementation Report on Pilot Applications						33 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final





Figure 7. An example of a 3D distribution of biomass around houses.

Document name:	D5.7 Implementation Report on Pilot Applications						34 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



## 6 Material Transport in Water implementation status

### 6.1 Current status on software development and implementation

Significant progress has been achieved in the modelling of material transport in water, particularly in the area of multi-physics coupling. During the year 2024, efforts were focused on establishing a robust two-way coupling between the fluid and temperature fields. This coupling was successfully developed and rigorously validated using benchmark test cases.

Building upon this foundation, the next step—planned towards the end of 2024—was to incorporate temperature-particle coupling. While the coupling between fluid and particles had already been implemented using the Partially Saturated Cells Method (PSM), the integration of particles with the temperature field remained a key missing component.

The established fluid–particle coupling, based on PSM, was implemented using the lbmpy code generation framework. This framework takes a high-level Python script as input and produces optimized C++ kernels for Lattice Boltzmann Method (LBM) [31] operations. These include the LBM sweep, ghost-layer communication, boundary condition enforcement, and initialization procedures. Kernel generation is architecture-aware, supporting both CPU and GPU execution. Particle dynamics, on the other hand, are managed via kernel calls within the mesa-pd library.

PSM implicitly enforces the no-slip boundary condition on particle surfaces during fluid–particle interactions. A similar methodology was adopted for the thermal coupling, herein referred to as thermal PSM. This approach ensures that particles maintain a uniform temperature throughout their volume at all times. All the associated thermal PSM kernels - for communication, boundary handling, and temperature sweep—are likewise generated using lbmpy.

At present, the model assumes a constant particle temperature, although it is conceptually expendable to incorporate energy balance equations for time-dependent particle temperature evolution. A critical feature of the current implementation is the absence of internal temperature gradients within the particles.

The thermal PSM framework has been validated against a benchmark case from the literature: the vertical motion of a single, thermally uniform spherical particle in a fluid at constant temperature, <u>Figure 8</u>. In this setup, the particle accelerates under gravity until it reaches a terminal velocity. The validation results confirm the accuracy and physical consistency of the implemented model.

Document name:	D5.7 Implementation Report on Pilot Applications						35 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



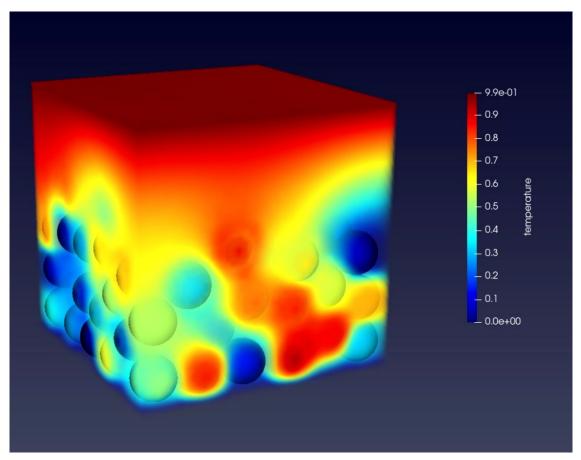


Figure 8. Figure demonstrating the temperature distribution in domain with fluid, particles and temperature effects.

#### 6.2 Challenges faced and future plans

No major challenges were encountered during the current phase of the implementation. The development up to the case of particles with constant and uniform temperature, including validation through the particle settling benchmark, was relatively straightforward.

Looking ahead, the next planned enhancement involves the implementation of Neumann boundary conditions at the particle surface. This boundary condition assumes zero diffusive flux into the particle, effectively modelling the particle as a thermal insulator. Such a feature would enable the simulation of scenarios where particles do not exchange heat with the surrounding fluid.

Following the implementation, thorough validation will be essential. This will involve benchmarking against reference data available in the scientific literature to ensure the physical accuracy and robustness of the new model.

Document name:	D5.7 Implementation Report on Pilot Applications						36 of 48
Reference:	eference: D5.7 Dissemination: PU Version: 1.0					Status:	Final



# 7 Pilot couplings implementation status

### 7.1 Current status on UAP-UBM coupling

Integrating Urban Building Models (UBM) with Urban Airflow Prediction (UAP) systems is pivotal for accurately simulating urban microclimates. This coupling enables an understanding of the interactions between building energy dynamics and urban atmospheric conditions, which is essential for urban planning, sustainability assessments, and improving residents' comfort.

### Motivation for Coupling UBM and UAP

Urban environments are complex systems where buildings and atmospheric conditions are interdependent. Buildings influence and are influenced by urban airflow patterns, temperature distributions, and pollutant dispersion. A coupled UBM-UAP system allows for:

- **Enhanced Accuracy**: Capturing the bidirectional interactions between buildings and the urban atmosphere leads to more precise simulations.
- **Dynamic Feedback**: Real-time exchange of data ensures that changes in one system (e.g., building heat emissions) are reflected in the other (e.g., local airflow patterns).
- **Informed Decision-Making**: Urban planners and policymakers can make better decisions regarding building designs, energy policies, and environmental regulations.

### **Coupling Strategies**

- Bidirectional OpenFOAM Transfer:
  - *UBM* → *UAP*: The UBM exports surface temperatures, heat fluxes, and related boundary conditions in a standardized format that OpenFOAM ingests to drive airflow simulations.
  - UAP → UBM: OpenFOAM returns airflow velocities, outdoor temperature fields, and air-quality indicators, which the UBM reads back in to update thermal loads and indoor comfort metrics.

This two-way data exchange via OpenFOAM has been designed for simplicity and extensibility. Initial tests have successfully validated the UBM  $\rightarrow$  UAP workflow.

#### MPI-Based Runtime Exchange:

This approach involves a lightweight MPI framework that exchanges data directly on the building's surface mesh during simulation. By synchronizing mesh partitions and buffers, it supports fully coupled, concurrent execution of UBM and UAP, allowing for real-time interaction between the models.

Document name:	D5.7 lr	nplementation Repo	Page:	37 of 48			
Reference:	nce: D5.7 Dissemination: PU Version: 1.0						Final



### Data Exchanged Between UBM and UAP

- From UBM to UAP:
  - Surface temperatures
  - Heat fluxes
  - Boundary conditions
  - Indoor air-quality indicators (under development)
- From UAP to UBM:
  - Airflow velocities
  - Outdoor temperature fields
  - Air-quality indicators

These data exchanges ensure that both models are informed by the most current and relevant information, leading to more accurate and responsive simulations.

#### **Next Steps**

Having validated the OpenFOAM unidirectional workflow, the next phase involves implementing a seamless two-way coupling and benchmarking its performance. Subsequently, the focus will shift to developing and integrating the MPI-based approach to enhance real-time simulation capabilities.

For visual insights, screenshots of the Lingolheim dataset with OpenFOAM results are provided in <u>Figure 9</u> to illustrate the practical applications of these coupling strategies.

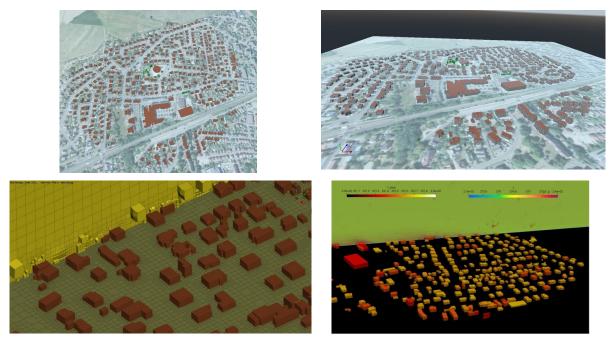


Figure 2. First one way coupling between UAP and UBM. Top panels represent the initial data from Ktirio Urban Building, bottom left panel displays the mesh and bottom right the temperatures in the air and at the walls of the buildings.

Document name:	D5.7 Implementation Report on Pilot Applications						38 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



### 7.2 Current status on UBM-RES coupling

The goal for UBM-RES coupling is weather forecast prediction for renewable energy sources like photovoltaic system in urban zones. After analysis of inputs and outputs of both solvers, it was found that direct coupling without changes in the program code would be impossible. Also the different types of meshes in solvers (structured vs unstructured) is a challenge.

**RES** Input:

- Quad mesh (based on GPS data)
- Output from WRF (weather data)
- Building height based on OSM (Open Street Maps)

**RES** Output:

- Wind velocity at 2m heigh
- Wind velocity at 10m height
- Temperature
- Pressure

UBM Input

- GIS file
- OSM (Open Street Map) mesh msh file (unstructured)
- Weather data csv file base on OpenMeteo data
- cloud cover
- diffuse radiation
- Direct radiation
- Relative humidity\_2m
- Surface pressure

#### UBM Output

- Solar Shading coef.
- Temp exterior
- Temp interior
- Temp ambience
- Ideal Qfloq cooling
- Ideal Qflow heating

The decision was made to use the output data from both solvers as the input for further HPDA analysis as complementary data. HPDA analysis is based on AI algorithms. The aim of the AI algorithm is to find correlation between forecasts and the energy production. This coupling with UB will complement solar data required to achieve greater accuracy of the aforementioned correlation.

Document name:	D5.7 lr	nplementation Repo	Page:	39 of 48			
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



The current status is preparing the data from both solvers to store them and use them in HPDA analysis. Both solvers were run on the Leonardo (Cineca) and Altair (PSNC) clusters. The UBM solver is running as the container using singularity. Some issues related with user rights in containerisation and version compatibility were solved. Additionally, tools to prepare the input data for the RES based on Open Street Maps (OSM) were used. Currently both solvers used the same source to prepare meshes and input data. The next step is preparing the workflow to store the output data using CKAN. The data will be used for further analysis.

## 7.3 Current status on UAP-WF coupling

In order to couple simulations between the UAP and the WF pilots, a residential area near a forested zone in the city of Győr, Hungary, has been selected. In this location, two aspects will be simulated: 1) the effect of smoke and flying embers on the urban area, and 2) the local combustion of vegetation around the buildings. The simulations will utilize existing LiDAR data from the national geographic service and vegetation data from the forest service have been obtained. To that end, MTG is designing transfer functions that convert complex vegetation models into 3D distributions of the parameters required by the porousGasificationFoam solver, particularly those related to the solid phase:

- Porosity [porosityF]
- Initial porosity [porosityF0]
- Viscous resistance tensor [Df]
- Solid temperature [Ts]
- Solid species mass fraction (biomass) [Ywood]
- Default solid species mass fraction field [YsDefault]
- Anisotropy of heat conductivity (optional) [anisotropyK]

At present, MTG is simulating the combustion of individual vegetation elements and will subsequently simulate vegetation populations with more complex layered structures using this methodology, applied to wildland-urban interface areas.

The outputs of these models in terms of meteorological variables as well as smoke and pollutants generated by combustion will serve as boundary conditions for the urban pollution simulation model.

### 7.4 Current status on UBM-WRF coupling

Integrating the Weather Research and Forecasting (WRF) model with the Urban Building Model (UBM) is essential for accurately simulating urban microclimates. This coupling provides detailed meteorological inputs to the UBM, enhancing the realism of

Document name:	D5.7 lr	nplementation Repo	Page:	40 of 48			
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



building energy simulations and aiding in urban planning and climate resilience strategies.

### **Context and Motivation**

Urban environments are characterized by complex interactions between buildings and atmospheric conditions. The WRF model offers high-resolution meteorological data, which, when integrated with the UBM, allows for:

- **Improved Accuracy**: Capturing localized weather patterns enhances the precision of building energy simulations.
- **Dynamic Feedback**: Real-time meteorological inputs enable the UBM to respond to changing weather conditions, improving the assessment of thermal comfort and energy demand.
- **Informed Urban Planning**: Detailed simulations support decision-making in urban design, energy policy, and climate adaptation measures.

### **One-Way Coupling Implementation: WRF to UBM**

The current implementation focuses on a one-way coupling from WRF to UBM, involving the following steps:

- **Structured Grid Overlay**: A georeferenced grid is generated over the urban area to map WRF outputs to building façades and roofs.
- **Data Interpolation**: WRF fields are interpolated onto each building's boundary conditions, supplying dynamic meteorological inputs for thermal and airflow simulations.
- **Initial Tests**: Early WRF runs for Strasbourg produced invalid values, prompting refinements in preprocessing and quality checks.
- **Status**: Coupling code is under development, with corrected WRF datasets expected for upcoming validation.

### Data Exchanged from WRF to UBM

The coupling facilitates the transfer of the following meteorological data from WRF to UBM:

- Air temperature
- Relative humidity
- Wind speed and direction
- Solar radiation
- Longwave radiation
- Surface pressure
- Precipitation rates

These data are crucial for accurately modelling building energy consumption and indoor environmental conditions.

Document name:	D5.7 lr	nplementation Repo	Page:	41 of 48			
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



#### **Initial Results**

WRF has been used to simulate regional climate over Strasbourg area with a 1km square resolution. <u>Figure 10</u> displays the temperature over the area which is then interpolated to provide outdoor temperature to buildings models.

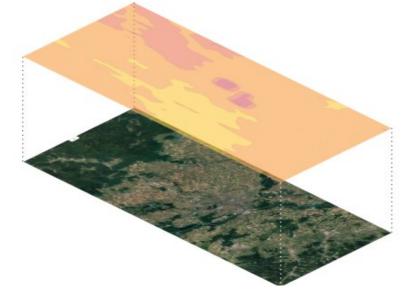


Figure 10. Strasbourg greater area overlaid by temperature field computed by WRF.

#### **Next Steps**

To enhance the coupling between WRF and UBM, the following steps are planned:

- **Data Validation**: Refine preprocessing routines and quality control measures to ensure the reliability of WRF outputs.
- **Code Development**: Complete the development of coupling code to facilitate seamless data exchange.
- **Performance Benchmarking**: Assess the impact of WRF-derived meteorological inputs on UBM simulations to evaluate improvements in accuracy and computational efficiency.
- Future Enhancements (not planned in HiDALGO2): Explore the potential for two-way coupling, allowing feedback from UBM to influence WRF simulations, thereby capturing the dynamic interactions between urban structures and atmospheric conditions.

By advancing the integration of WRF and UBM, we aim to develop a robust modelling framework that supports sustainable urban development and climate resilience initiatives.

Document name:	D5.7 lr	nplementation Repo	Page:	42 of 48			
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



DDLGOZ

The RES-runner, already described in detail in D5.3, is a framework allowing coupling of WRF and EULAG models and the whole pipeline automation. It takes advantage of both models in order to simulate weather predictions in mutiscale approach. As WRF is already a component of RES-runner, it is planned to integrate the framework with WRF provided by MeteoGrid, as mentioned in D5.6. The development of RES-runner made so far since D5.6 was focused on two goals: first, making it compatible with mUQSA toolkit and planned HPDA studies, second, implementing preliminary enhancements in order to improve the framework's maturity, pipeline's flexibility and debugging options before final coupling with WRF from MeteoGrid. RES will benefit from greater resolution this version of WRF is providing, while the integration should be straightforward as the coupling relies on data exchange via files. WRF and EULAG can be executed via RES-runner in sequence, or the data can be exchanged via CKAN – after WRF(MG) execution the output data is upload to CKAN to be processed by EULAG (RES) at later time.

### 7.6 Current status on MTW-WF coupling

Wildfires have several effects on the hydrological response of watersheds. Among them, the most notable are the partial or total removal of vegetation and the hydrophobic effect that the heat from combustion has on certain soils. In addition, wildfires are tremendous generators of ash. All these phenomena alter both the pattern and intensity of the hydrological response to post-fire rainfall, especially in the case of torrential rain, which can lead to significant erosion of the soil's surface layers.

MTW and wildfires use case partners have discussed on a possible collaboration to try to simulate these effects. The general idea of the coupling is: in real life scenarios, after the wildfires have destroyed the vegetations/forests, there is a lot of ash particles which are eroded by rains. This pilot coupling proposes an initial approach that links wildfire propagation simulation with the production and transport of ash and sediment through the river network. To this end, HIDALGO2 wildfires pilot will provide an input of ash and other particles into a specific section of the drainage network, based on simulations of fire propagation, vegetation type, etc. The distribution and quantity of particles (classified by diameter), entry location, density, and temperature will be specified. This input will be collected by MTW pilot team, which is responsible for solid transport simulation in water, and used to initialize the particles in the fluid domain and hence carry out simulations involving particle-particle and fluid-particle interactions.

Document name:	D5.7 Implementation Report on Pilot Applications						43 of 48
Reference:	D5.7 Dissemination: PU Version: 1.0					Status:	Final



# 8 Conclusions

In conclusion, D5.7 states the actual status of development and implementation of the HiDALGO2 Pilots and the couplings between models up to month 29. The report evaluates the implementation status of the pilots and the foreseen application couplings providing a comprehensive overview of the capabilities, challenges and planned next steps for each pilot application.

During this period, the applications modelling key processes in each of the pilot cases have evolved significantly in terms of functionality, scalability, and improvements in installation procedures.

Regarding the Urban Air Project (UAP) pilot, remarkable advances have been made in all the codes used (UAP-FOAM, Redsim and Xyst), with those made in Redsim being the most important. In addition to implementing all MPI+GPU functionality to RedSim, RedSim has been vectorized with SIMD and several new functionalities have been added during this period.

Regarding the Urban Building (UB) pilot, significant progress has been made with the Ktirio model, which has been considerably enhanced over the past year. Developments have taken place across all components to streamline and automate pilot deployment and data management. Recent simulation upgrades have improved stability, efficiency, and adaptability, and the system has now been deployed in multiple cities (Strasbourg, Athens, Luxembourg, Stuttgart, Poznan, Madrid, Gyor, Erlangen). The Ktirio Urban Building Model (UBM) workflow integrates multiple components of the HiDALGO2 ecosystem to enable scalable, high-resolution urban simulations, including CKAN, Girder, Zenodo, MathSO, QCG, and KUB-CD, with GitHub and GitLab supporting source control and continuous integration.

Regarding the Renewable Energies (RES) pilot, several enhancements have been implemented in the model, improving its functionality through the integration of a vertical wind profile feature and increasing deployment and execution versatility across multiple sites. The pipeline has also been made more flexible when using partially preprocessed data. To accelerate development and debugging, a lightweight and fast-resolving debugging mode was added. A significant enhancement was the streamlined preparation of simulation domains using OpenStreetMap data, greatly expanding the model's applicability across diverse locations.

Regarding the Wildfires (WF) pilot, advances have been made in both target scenarios. At the landscape scale, improvements are being made in installation processes with the aid of EPICURE, as well as in the scalability of the WRF-SFIRE model. Progress is also underway in uncertainty quantification (UQ) through ensemble simulations. In this context, the MeteoGrid FSE (Fire Spread Engine) solution has been implemented on GPUs. This approach is computationally less demanding and enables HPDA and UQ workflows.

Document name:	D5.7 lr	nplementation Repo	Page:	44 of 48			
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



At the WUI scale, notable results have been achieved in environmental description and data preparation workflow standardization, especially concerning the threedimensional distribution of biomass. Several solvers have been tested for combustion simulation around buildings, and a suitability analysis has begun for each. Simulations of increasing complexity have been carried out, including classic CFD simulations to estimate airflow around structures, methane burner simulations assessing wind-driven flame behaviour, and biomass combustion modelling based on its spatial distribution around buildings.

Regarding the Modelling of Material Transport in Water (MTW) pilot, substantial progress has been made, particularly in multi-physics coupling and in incorporating temperature-particle interactions, thus significantly improving the physical representation of the solution for a deeper insight into the complex process of pollution transport in rivers.

Another major area of development during this period has been the coupling between models, with notable progress in the UAP-UB coupling where [...], as well as in the UB-WRF integration. For the UB-RES coupling, it was decided to use the output data from both solvers as input for further HPDA analysis, treating them as complementary datasets. In this case, the HPDA analysis is based on AI algorithms. The progress made in the 3D characterization of vegetation as a porous medium will enable its use in urban settings, facilitating UAP-WF integration, which involves coupling WRF-SFIRE, a WUI combustion solver, and a UAP pollutant dispersion solver. Finally, detailed solutions have been defined for other potential couplings to be addressed in the remaining duration of the project—for instance, the WF-MTW coupling. For this, discussions have focused on the injection of ashes and other materials resulting from WF-modelled wildfires into drainage networks and waterways, with their subsequent transport simulated in the MTW model.

Moving forward, the work and lines of research already initiated during this period and which will consolidate the progress already made are detailed in the different sections above.

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Document name:	D5.7 Implementation Report on Pilot Applications						45 of 48
Reference:	D5.7 Dissemination: PU Version: 1.0					Status:	Final



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Document name:	D5.7 lr	nplementation Repo	Page:	46 of 48			
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



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Document name:	D5.7 Implementation Report on Pilot Applications						47 of 48
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final



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Document name:	D5.7 lr	nplementation Repo	Page:	48 of 48			
Reference:	D5.7	Dissemination:	PU	Version:	1.0	Status:	Final