D3.7 Ensemble Scenarios for Global Challenges

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List of Acronyms

Abbreviation / acronym	Description
AI	Artificial Intelligence
CKAN	Comprehensive Knowledge Archive Network
EC	European Commission
ECWMF-IFS	ECWMF Integrated Forecasting System
Dx.y	Deliverable number y belonging to WP x
HPDA	High Performance Data Analytics
MTW	Material Transport in Water
mUQSA	Multipurpose Uncertainty Quantification and Sensitivity Analysis Toolbox
PCE	Polynomial Chaos Expansion
RES	Renewable Energy Sources
SC	Stochastic Collocation
UQ	Uncertainty Quantification
SA	Sensitivity Analysis

UAP	Urban Air Project
UB	Urban Buildings
WP	Work Package

Executive Summary

This document, Deliverable D3.7 "Ensemble Scenarios for Global Challenges", outlines the role, methods, and applications of ensemble runs within the HiDALGO2 project. Ensemble runs involve executing multiple simulations or models, either in parallel or sequentially, and can be used for uncertainty quantification studies or to increase the predictive accuracy of models. Ensemble runs are categorized into two types:

- Parallel Independent Runs (Type 1): Multiple instances of the same model are run with varying input conditions or parameters to assess uncertainty.
- Coupled Simulations (Type 2): Different models are combined to better capture system complexity and interactions.

While similar to application coupling, ensemble runs differ in their focus on running multiple model versions under varying conditions to assess variability, rather than simply integrating models to simulate complex systems.

This document is part of Work Package 3 (WP3) and contributes to other tasks like WP4.3 (AI for Global Challenges) and WP4.6 (Uncertainty Quantification). The ensemble scenarios identified in this deliverable are key components for various project deliverables (D4.3 [7], D4.4 (future reference), D4.9 (future reference), and more).

The structure includes an introduction to ensemble runs, a detailed description of methods and technologies used, and an overview of how pilot use cases in HiDALGO2 are incorporating ensemble scenarios. The document concludes by summarizing key findings.

1 Introduction

Ensemble runs involve executing multiple simulations or models either in parallel or sequentially, often with varying input data, initial conditions, or model parameters. These ensemble scenarios can be categorized in two main ways:

- **Parallel Independent Runs** (Type 1): Executing several instances of the same model or simulation simultaneously, but with different input conditions or parameters. This approach is commonly used for uncertainty quantification [2]].
- **Coupled Simulations** (Type 2): Combining different types of models or simulations to better capture the complexity of a system by accounting for interactions between diverse computational processes [1]. This type of ensemble run was already mentioned in other deliverables (D4.1 [6] , section 3 - technologies; D5.3 [5] - use cases coupling).

Ensemble methods are crucial in areas where uncertainty quantification and predictive accuracy are essential. In complex simulations or AI workloads, single model outputs often fail to capture the full range of potential outcomes due to inherent uncertainties in input data, model parameters, or approximations. Ensemble runs address these limitations by providing a more comprehensive analysis through variance and sensitivity assessments, thereby improving confidence in the final results.

In uncertainty quantification, ensemble runs are fundamental because they enable the exploration of possible outcomes by incorporating variations in initial conditions and model parameters. This approach provides insights into how uncertainties influence the range of predicted results. For AI workloads, ensemble methods can be used to improve model robustness and predictive accuracy by averaging results from different models or simulations, such as in Bayesian model combination. In both contexts, ensemble runs yield a distribution of outcomes rather than a single deterministic result, allowing for more informed decision-making.

While both ensemble runs and application coupling involve the interaction of multiple models or simulations, their purposes differ significantly. Simple application coupling focuses on integrating different models to simulate complex systems as a whole, where interactions between components are essential to the outcome. Ensemble runs, on the other hand, emphasize running multiple versions of the same or similar models under varying conditions, often independently, to assess variability and uncertainty. Ensemble methods combine the results of these runs to extract additional insights, such as confidence intervals, sensitivity analyses, or refined predictions, which are not the primary focus in simple coupled simulations.

In summary, ensemble runs are powerful tools for uncertainty quantification and enhancing predictive accuracy, particularly in AI and simulation-based studies. They offer a systematic approach to account for uncertainties and variability, providing more robust and reliable results than single-run models or simple coupled simulations.

1.1 Purpose of the document

This Deliverable D3.7 "Ensemble Scenarios for Global Challenges" is prepared in the context of WP3 and provides information about the methods and technologies developed for the ensemble runs. Also, the ensemble scenarios identified for the different pilot test cases are described in this document.

1.2 Relation to other project work

The ensemble scenarios and the technology described in this deliverable are used in tasks T4.3 (Artificial Intelligence for Global Challenges) and T4.6 (Uncertainty Quantification). The results of the simulations using the ensemble scenarios are part of the deliverables D4.3, D4.4, D4.5 ("*Advances in HPDA and AI for Global Challenges*" in M16, M34 and M45, respectively), and D4.9, D4.10 (*Uncertainty Quantification*, M26 and M47, respectively).

1.3 Structure of the document

This document is structured in 3 major chapters and a conclusion.

The current **Chapter 1** introduces and defines ensemble runs and explains why HiDALGO2 needs them. **Chapter 2** delineates the methodological principles that will inform the formulation of ensemble scenarios within the defined frameworks. **Chapter 3** presents the methods and technologies used in the ensemble runs in HiDALGO2. **Chapter 4** presents how each HiDALGO2 pilot use case incorporates or is planning to incorporate ensemble scenarios. **Chapter 5** Roadmap, includes a description of the activities to be carried out in the coming months. Finally, the **Conclusion** summarizes the report.

2 Methodologies for ensemble scenarios

The main objective of this chapter is to outline the methodological principles that will guide the definition of ensemble scenarios within the established frameworks. The execution of ensemble scenarios is intricately linked to the areas of verification, validation, uncertainty quantification, and the evaluation of the sensitivity of simulation models. The methodologies enable the comprehensive capture of all potential outcomes and uncertainties inherent in complex simulations. The selection of a particular approach is contingent upon the research domain, the computational resources at hand, and the specific objectives of the simulation. The techniques employed in these processes ought to be integrated into the mechanisms offered by ensemble scenario tools.

The phases involved in the implementation of ensemble scenarios encompass several fundamental steps: the preparation of input parameters, the simultaneous execution of multiple simulations, the synthetic analysis of the results from these simulations, and the optional incorporation of feedback.

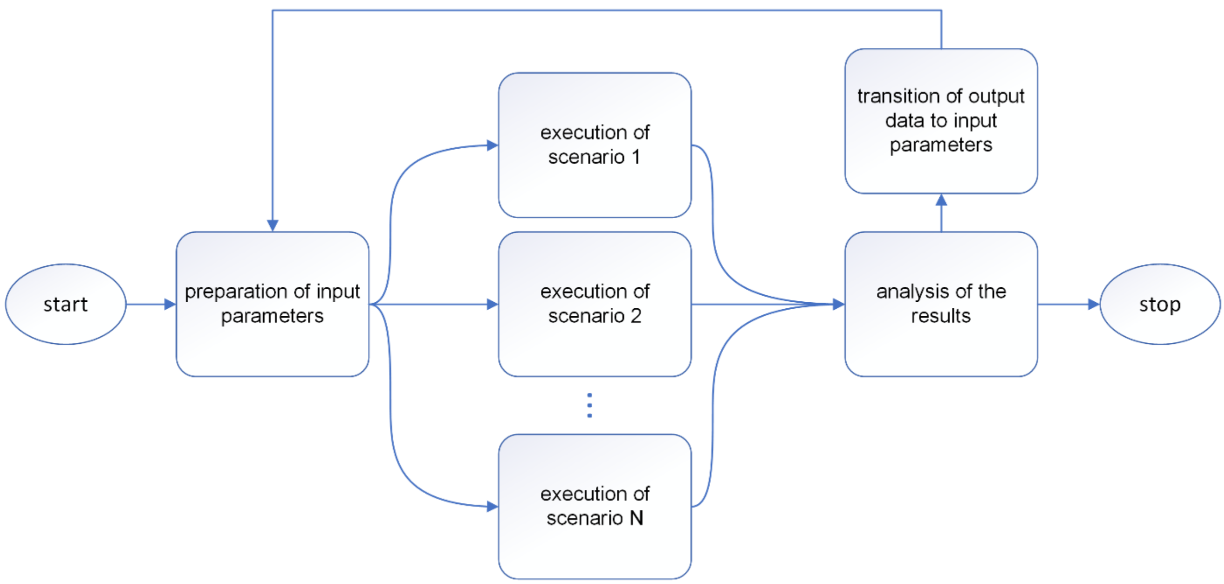

Figure 1. Key stages of implementing ensemble scenarios

Below are the various optimization techniques systematized. Systematization consisted in assigning a specific method to the category that best corresponded to the operations on which emphasis was placed. Methods that substantially cover all phases of the ensemble scenario implementation were placed in the last category.

2.1 Input parameters

Ensemble scenarios which based on **deterministic methods** [17] provide an approach that explore of the sensitivity and variability in systematic way under model predictions. This enables the consideration of variations in input data and how each set of conditions affects the model's behaviour. In addition, such techniques are used in situations where a more structured exploration of the parameter space is required or randomness is lacking. By including this type of determinism, we provide insight into the dynamics of the system and increase the robustness of the decision-making processes.

When it is necessary to analyses the influence of random variability or noise-generated interference, the **stochastic approach** [18] is used. It facilitates the assessment of the influence of random fluctuations on the result. It is particularly beneficial in systems characterized by unpredictability. In the preparation of data or input parameters, tools that generate values from a specified range or perturbators help.

In the **Monte Carlo ensemble** [19], model parameters are derived from probabilistic distributions, and numerous simulations are conducted to explore the range of potential outcomes. The initial step involves defining probability distributions for the uncertain input parameters. Following the execution of the simulation through random sampling, the ensemble produces probabilistic estimates of the results.

The systematic study of the parameter space is possible thanks to the **grid-based approach** [20]. This methodology facilitates the study of the influence of parameter values on the model results in different combinations. In the first step, a parameter grid is established. Each axis of this grid corresponds to a separate model parameter. Simulations are performed in two variants: for each grid point or selectively based on a specific algorithm. Post-processing analysis consists in assessing the relationship between changes in the input parameters, interpreted as movements along the grid, and the model-generated results.

2.2 Scenario execution

Multi-model ensembles consist of employing various models, each grounded in distinct formulations, to analyse the same phenomenon [21]. It employs various models to replicate the same phenomenon, rather than merely adjusting parameters within a single model. This approach is advantageous when a single model fails to encompass the entire complexity of the system. By integrating the outcomes of these models, one can examine a spectrum of deterministic results without the influence of random variability. It is crucial to choose simulation models that are intended to replicate the same process while utilizing different mathematical formulations, assumptions, or algorithms. This method uses closely related initial conditions or parameters which allow for comparison of the obtained results.

Scenario analysis involves defining divergent scenarios that are expected to lead to a wide range of outcomes that reflect the assumptions made [22]. This method is often used to examine “what if” scenarios. It takes into account changing hypotheses about future circumstances, such as analysing the impact of different policies or changing the boundary conditions of a given strategy. Typically, each of the scenarios analysed operates on deterministic principles, implementing changes in the relevant parameters.

Systematic parameter variation refers to the methodical alteration of one or more parameters within a predetermined range, allowing for the observation of resultant changes [23]. This process is executed in a structured and non-random fashion, frequently employing fixed intervals for the parameters involved. After identifying the parameters of interest, a specific range of values is established for potential modifications. Through the deliberate adjustment of these parameters, the model's sensitivity is evaluated based on the resulting output data.

2.3 Assembling data

A noteworthy method employed in data assimilation (optimal combination of theory and observation) is **Ensemble Kalman Filtering** [24]. This technique involves the continuous updating of a model ensemble as new observational data becomes available. It is particularly useful in real-time simulations, where predictions are revised in response to incoming data. The process includes defining parameters for computational models utilizing observational data and statistical methods. Following each computational iteration, the state of the model is assessed.

Bayesian Ensemble Methods are capable of integrating uncertainty and prior knowledge into ensemble simulations [25]. These approaches utilize probabilistic inference to adjust beliefs regarding the state of a system, informed by both ensemble simulations and observed data. The methodology requires defining the distribution of model parameters and/or scenarios before performing calculations. Once data on the distribution of outcomes are available, Bayesian updating techniques are used to improve their accuracy.

In **ensemble averaging**, the final forecast is derived from the average or weighted mean of the results of multiple ensemble simulations [26]. This approach eliminates the uncertainty associated with the performance of a single individual model. Reaching consensus involves using different sets of initial conditions or models when performing different deterministic simulations.

2.4 Cross-sectional technique

The **parameter sensitivity analysis technique** involves systematically altering the model parameters within a predetermined range to evaluate the sensitivity of the model output to these parameters [27]. This approach is frequently employed to explore uncertainty in models where certain parameters are not accurately defined. After pinpointing the critical parameters that may significantly influence the results, a set of values for each parameter is established, followed by the execution of simulations. Upon obtaining the results, the influence of the parameters on each output value is analysed by comparing them to the theoretically anticipated values. This technique is often combined with a cyclical feedback approach.

The **adjoint sensitivity method** employs the conjugate (or inverse) formulation of the model to assess how minor changes in the inputs affect the results [28]. This deterministic technique is frequently utilized in optimization and sensitivity analyses, particularly in large-scale systems. By utilizing the adjoint model, one can compute the gradients or sensitivities of the system's response to input perturbations, thereby enabling the estimation of the impact of parameters or the data itself in relation to their most significant influence on the system.

2.5 Summary

Many techniques use a combination of the above methods (hybrid approaches), such as combining deterministic, stochastic, and multi-model approaches to obtain a more comprehensive understanding of the modelled system (e.g., stochastic multi-model ensemble). In such approaches, both the aggregation and analysis of results are performed using advanced statistical or machine learning methods.

The generation of perturbation methods for input data depends on the model used, the nature of the sensitivity analysis, and the specific research goals. Additive and multiplicative perturbations serve as simple but powerful tools for local sensitivity assessments [13], while global methodologies such as Latin Hypercube Sampling [14] and global sensitivity analysis [15] examine the entire spectrum of input data. In addition, scenario-based and adversarial perturbations [16] focus on realistic future scenarios or stress tests of models. Each technique allows researchers to methodically investigate the impact of input changes on model performance, thereby increasing its robustness and enhancing its reliability.

It should be emphasized that the final choice of the ensemble scenarios method and the related uncertainty quantification or sensitivity analysis will be up to the owners of the pilot applications and will depend on the defined methodological goals and the capabilities of the supporting tools used. The methodology for uncertainty quantification will be presented in detail in the next report D4.9 Uncertainty Quantification (M26).

3 Technologies for ensemble runs

Within the scope of HiDALGO2, ensemble simulations play a critical role in advancing the accuracy and reliability of computational models in environmental research and simulations. By executing multiple runs with varying input data, initial conditions, or model parameters, ensemble methods help address the inherent uncertainties often present in complex real-world scenarios, such as urban air quality, urban buildings, renewable energy systems, wildfire behaviour, and water pollution transport. These scenarios are present in the pilot use cases of HiDALGO2, namely Urban Air Project (UAP), Urban Buildings (UB), Renewable Energy Sources (RES), Wildfires (WF), and Material Transport in Water (MTW), described in the Deliverable D5.3 "*Research Advancements for the Pilots*" [5].

Ensemble simulations are crucial in addressing environmental challenges, where uncertainties and complexities are inherent. Environmental systems, such as urban air quality, renewable energy resources, wildfires, and water pollution, are inherently influenced by a wide range of dynamic factors, including weather conditions, human activities, and natural variability. These systems are difficult to model accurately using a single simulation, as the unpredictability of input parameters and the sensitivity of models to small changes can lead to a limited understanding of the full scope of potential outcomes.

Ensemble runs overcome this limitation by conducting multiple simulations, each with different initial conditions, inputs, or model parameters, allowing researchers to capture the broad range of possible scenarios. This is especially important in environmental problems, where accurate prediction and risk assessment are critical for effective decision-making. This is crucial for ensuring the robustness of the predictions especially in environmental problems. For AI-based models, ensemble methods also enhance predictive accuracy by combining insights from multiple models, leading to a more reliable output. Overall, ensemble simulations offer a powerful means of improving confidence in the results, contributing to more informed decision-making for addressing critical environmental challenges in the future.

3.1 General purpose tools

3.1.1 mUQSA

The mUQSA platform is developed by the Poznan Supercomputing and Networking Center with the main aim to comprehensively support Uncertainty Quantification and Sensitivity Analysis of computational models. Originally proposed in the PIONIER-Lab project for Polish stakeholders, it is now being adapted to meet the needs of European scientific communities and deployed at EuroHPC sites, all within the framework of the HiDALGO2 project. By the very nature of the offered UQ&SA algorithms based on non-intrusive evaluations, mUQSA is able to effectively support selected ensemble scenarios. From the user point of view, the particular advantage of mUQSA is its user-friendly graphical interface for both scenario definition and results analysis, as well as the full automation of ensemble execution on HPC resources.

Internally, the mUQSA platform has been grounded in several existing software components that provide required underline functionality, including:

- **QCG-Portal** - which provides a graphical web interface that facilitates remote access to computing resources and can be adjusted towards specific application needs.
- **QCG-PilotJob** - which allows for efficient and flexible execution of a large number of tasks (e.g. ensembles) on computing resources.
- **EasyVVUQ** - which delivers core algorithmic capabilities for UQ & SA.

The mUQSA user can easily configure and execute UQ & SA scenarios for the majority of types of computational models. Depending on a use-case, it can select from a few offered methods:

- **Basic** - the method allows for a basic ensemble analysis by means of multiple evaluations of the model with the same input parameters. Thus it is particularly useful for measuring internal variability of the model.
- **Parameter sweep** - the method performs a summary analysis of the model based on evaluations fed by the parameters drawn from precisely defined ranges. Due to its universal and predictable behaviour, the technique can be quite widely used.
- **Monte Carlo** - this popular approach allows obtaining statistical moments and sensitivity indices based on the executions of a model with random samples generated according to selected probability distributions.
- **PCE** - this method makes use of polynomial chaos expansion to approximate the behaviour of a system that contains random variables. For scenarios with a low number of input parameters and smooth response, the method requires significantly less model evaluations than MC to produce reliable UQ and SA statistics.
- **SC** - the stochastic collocation is another technique that uses polynomials to approximate the model behaviour, but in this case, the polynomials are constructed based on the model evaluation in specifically selected collocation points. The convergence rate is similar to PCE, but the method can be more suitable to perform UQ and SA for non-continuous and non-smooth systems.

3.1.2 QCG-PilotJob

Execution of a large number of model evaluations that are necessary for the effective UQ or ensemble analysis is challenging and limited by diverse and natural restrictions present on HPC computing sites. Simply speaking, due to efficiency reasons it is not directly possible to dynamically run a large number of jobs through a classical scheduling system interface. In order to overcome this issue, mUQSA employs the mechanism of QCC-PilotJob, and the dedicated QCG-PilotJob Executor class that has been embedded in the EasyVVUQ library. With the usage of QCG-PilotJob, multiple model evaluations can be run inside a single regular job launched in a queuing system, ensuring high flexibility and scalability of the solution.

The mUQSA platform will be described in more detail in the forthcoming deliverable D4.9.

3.1.3 OpenTURNS

OpenTURNS (Open-source Treatment of Uncertainties, Risks, and Statistics) [8] is a powerful open-source Python library designed to address the challenges posed by uncertainty in modelling, simulations, and decision-making processes. It is commonly used for uncertainty quantification (UQ), reliability analysis, sensitivity analysis, and probabilistic modelling across various industries, such as engineering, finance, and science.

OpenTURNS is written in C++ and provides Python wrappers, enabling the full extent of the library.

One of the core features of OpenTURNS is its ability to manage forward propagation of uncertainties and perform sensitivity analysis, which helps in understanding the impact of uncertainties in inputs on model outputs. The former feature provides a framework to run Ensemble Runs from programming point of view as well as advanced analysis tools for the associated results.

3.2 Pilot purpose tools

3.2.1 Urban Air Project

While there is no unified tool in use for ensemble scenarios in the UAP Pilot, all UAP applications have inherent support for running simulations with various parameters at once.

RedSIM

The parametrisation of RedSIM can be facilitated by Lua [12]. The tool's Lua API provides a fully functional scripting language to control import, export, initial conditions, and solution. A range of parameters can be freely generated within LUA and then seamlessly passed to the highly optimized application itself. Post processing these singular values is done in a similar manner.

Xyst

Using Lua input files, Xyst simulations can be parameterized to perform independent ensemble simulations, useful for parameter studies and uncertainty quantification. Initial and boundary conditions as well as physics and model parameters can be varied within given ranges, producing multi-dimensional sweeps of ensemble simulation input parameters, which can then be run controlled from a script. Such parameterized ensemble simulations are one of future use-case scenarios while designing Xyst's input, relying on the simplicity and power of scriptable text-based input files.

UAP-FOAM

The OpenFOAM based tool supports simulation variants with the parameter file `variants.cfg`. For simple simulations, within the simulation folder, input files reside in the input folder, configuration parameters are set within `uap_foam.cfg`. The utility `uapFoamSetup.sh` creates an OpenFOAM case directory based on the inputs and configuration file – without doing any processing yet. Afterwards, the `submit.sh` tool will do the actual execution or the submission to the HPC queue.

For creating cases with several parameters, the `variants.cfg` file is created in a tab separated table form. Each simulation variant will use a separate row, with the simulation ID in the first column. Columns are used for different parameters, having the parameter name in the first row, and appropriate parameter values inside the table itself. Parameter names must match the appropriate parameter within `uap_foam.cfg`.

A separate case directory is created for each variant using the uapFoamSetup.sh -v command, which are submitted to the cluster with submit.sh. Inherent support for post processing is not present yet.

3.2.2 Urban Building

Feel++ Overview

Feel++, stands for Finite Element Embedded Language in C++, is an open-source C++ library designed for solving partial differential equations (PDEs) using the finite element method (FEM). It provides a domain-specific embedded language that allows users to express mathematical formulations in code that closely mirrors their mathematical notation. This approach enables researchers and engineers to implement complex simulations efficiently and accurately within a high-performance computing framework. Feel++ is the core framework for Ktirio Urban Building.

Feel++ emphasizes: (i) Expressive Syntax: Allows users to write code that closely resembles the mathematical expressions of their models. (ii) Modularity and Extensibility: Provides reusable components and the ability to extend the library with custom elements, functions, and solvers. (iii) High Performance: Optimized for parallel computing architectures, making it suitable for large-scale simulations in engineering and scientific computing.

Ensemble Runs in Feel++

The Ensemble Runs feature in Feel++ enables users to execute multiple simulations with varying parameters within a single computational framework. This capability is primarily used for scenario testing, allowing users to explore how different parameter values or initial conditions affect simulation outcomes.

Execution Using MPI Communicators and Groups

Feel++ leverages MPI (Message Passing Interface) communicators and groups to manage and execute ensemble runs. Each simulation within the ensemble is assigned to its own MPI communicator group, which allows for efficient parallel execution without relying on external schedulers for resource management. This approach enables multiple simulations to run simultaneously while facilitating organized communication and data management across the ensemble.

Gathering Results and Analysis

Within this MPI-based framework, Feel++ can collect and aggregate results from all simulations in the ensemble. While advanced statistical analyses for uncertainty quantification or sensitivity analysis are not currently implemented, users can manually compare and analyse the outcomes to gain insights into the system's behaviour under various scenarios. This setup provides a solid foundation for effective scenario testing.

Future Extensions

Extensions to incorporate Uncertainty Quantification (UQ), Sensitivity Analysis (SA), and Optimization are being considered for future development. These enhancements aim to provide built-in tools for: (i) Uncertainty Quantification (UQ): Enabling probabilistic analysis by running simulations over distributions of input parameters and computing statistical metrics. (ii) Sensitivity Analysis (SA): Assessing the impact of varying parameters on simulation outcomes to identify which variables most significantly affect the results. (iii) Optimization: Facilitating automated searches for optimal parameter values that meet specific performance criteria or objectives.

These future developments will expand the capabilities of the Ensemble Runs feature, making it a more powerful tool for simulation studies and in particular the Ktirio Urban Building pilot.

3.2.3 Wildfires

The application of uncertainty quantification tools to forest fires in the Wildfires pilot requires the use of spatial data and raster images analysis functions to study how the fire may spread under different atmospheric conditions compatible with the observations. This analysis functionality is not currently available in mUQSA (potential tool for implementation WF ensemble scenarios), so it will be necessary to define and develop it with CDO type tools that allow the calculation of specialized statistics to facilitate a better understanding of the possible impact and evolution of the fire from the set of simulations obtained. It is foreseen to define such tools during this next year in order to apply them to the ensembles of simulations obtained using QCG-PilotJob.

4 Ensemble scenarios for Global Challenges

This chapter presents how each HiDALGO2 pilot use case incorporates or is planning to incorporate ensemble scenarios.

Where it is relevant, the two types of ensemble scenarios are highlighted: type 1 (running a number of simultaneous simulations in parallel e.g. with different input data) or type 2 (running coupled simulations of different kinds).

4.1 Urban Air Project

Current ensemble scenarios within the UAP pilot run the same simulations with different input data (type 1). The following scenarios are considered and run currently.

Using ensemble data for boundary conditions.

To quantify uncertainty for weather conditions, ensemble parameters from ECMWF data is acquired and used for simulation. A total of 51 variants are investigated including one normal, and 50 ensemble variants. All 51 simulations are run, where ensemble variants may be run with a lower resolution to conserve core-hour usage. Afterwards, statistics are generated for the ensembles and compared to the normal run. These may include point sample values, surface samples, or any other derived metrics.

Using ensembles to map parameter space for reduced order model generation.

While the number of freedom for high resolution meshes may seem enormous, the actual simulation results occupy just a fraction of this space. The singular value decomposition method can be used to determine those states, using the linear combination of which states can highly accurately reconstruct actual simulation results. To create a proper reduced model, a large number of base simulations must be run traversing the appropriate parameter space. These simulations can be run separately, in an ensemble run.

4.2 Urban Building

The Urban Building Model (UBM) pilot application [4], developed by Cemosis within the HiDALGO2 project, aims to improve building energy efficiency and indoor air quality through advanced simulation tools at both the building and urban scales. Given that approximately 75% of the EU building stock is energy inefficient and buildings contribute to 36% of EU greenhouse gas emissions, enhancing our understanding and control of energy consumption is crucial for meeting the objectives of the European Green Deal.

Type of Ensemble Scenario: Type 1

In the context of the UBM use case, the ensemble scenario corresponds to Type 1: running a number of simulations in parallel with different input data. This approach involves executing multiple simulations simultaneously, each with variations in parameters such as geometrical and meteorological inputs, modelling parameter choices, building heat sources, temperature settings, and building usage scenarios like occupancy and utilization patterns.

Importance of Ensemble Runs in UBM

The UBM relies on numerous assumptions due to incomplete or inaccurate data available in online databases. Ensemble runs are critical for several reasons: (i) Assessing uncertainties—by varying uncertain parameters, ensemble runs help quantify the impact of these uncertainties on energy consumption and air quality predictions at the city scale; (ii) Scenario testing—they allow for extensive scenario testing to understand how different conditions affect building performance, aiding in identifying defects and abnormalities in urban design and building usage; (iii) Improving model accuracy—ensemble runs enable the calibration and validation of models by comparing simulation outputs against observed data across a range of scenarios; (iv) Supporting decision-making—the insights gained from ensemble simulations inform building stock managers and policymakers in making evidence-based decisions to enhance energy efficiency and indoor comfort.

Implementation Strategy

Although ensemble scenarios are in the implementation stage in the pilot, the final integration would involve several steps: (i) Parameter variation—defining a range of values for each uncertain parameter based on available data and expert knowledge; (ii) Parallel execution—utilizing Feel++'s ensemble runs feature, leveraging MPI communicators and groups to manage and execute simulations in parallel without external schedulers, allowing for efficient computation and resource utilization; (iii) Data collection and analysis—gathering results from all simulations to perform statistical analyses, identify trends, and evaluate the influence of different parameters on the outcomes.

Benefits of Type 1 Ensemble Runs

Implementing Type 1 ensemble runs offers multiple benefits: (i) Efficiency—running multiple simulations in parallel reduces overall computation time, enabling timely analysis and feedback; (ii) Comprehensive exploration—it facilitates a thorough examination of the parameter space, finding potential interactions and nonlinear effects that might be missed in single-run simulations; (iii) Risk mitigation—it helps in identifying worst-case scenarios and assessing the robustness of building designs and urban planning strategies under varying conditions.

Future Extensions

Implementing Type 1 ensemble runs is an important component for future enhancements in the UBM use case, such as: (i) Uncertainty Quantification (UQ)—extending the ensemble runs to perform probabilistic analyses, quantifying the confidence in simulation results; (ii) Sensitivity Analysis (SA)—identifying key parameters that significantly affect outcomes, which is essential for optimizing building designs and retrofitting strategies; (iii) Optimization studies—utilizing ensemble data to find optimal solutions that balance energy efficiency, indoor comfort, and air quality. Currently, we are working on scenario modelling and integrating relevant parametrization of the overall simulation workflow.

4.3 Renewable Energy Sources

Ensembles play a crucial role in the Renewable Energy Sources (RES) pilot, which consists of an application coupling two weather prediction models at different scales. Ensembles can be applied to each model independently, and their purpose varies based on the use case. This section outlines the work done using ensembles and explores their potential for future applications. QCG-PilotJob and mUQSA, detailed in Section 2, were used to orchestrate ensemble generation and execution in an HPC environment. Further details can be found in [3].

Ensembles to solve the problem

RES-damages is a tool designed to predict the probability of damage to wind farms, photovoltaic systems, or overhead electrical networks. Ensembles, consisting of multiple simulations with varying input parameters, are used to assess this probability for existing installations.

As an example, consider the risk of damage to overhead electrical networks due to excessive wind speed and gusts. A study was conducted in a Polish city, focusing on these factors and utilizing three nested domains with varying resolution – from 3.6km to 100m. A detailed overhead electrical network was created to simulate meteorological conditions for individual components.

Ensembles were generated to simulate diverse wind conditions (direction, speed, and gusts) and assess damage probabilities. Five electrical lines were analysed, and wind sectors were divided into eight directions. For each direction, wind speeds ranging from 1 to 20 m/s were applied as boundary conditions.

Figure 2 illustrates example results, showing how wind speed varies for each overhead line. The x-axis represents the five electrical lines under study, while the y-axis indicates wind speed in meters per second. The red line denotes the average wind speed across all ensembles, while the lighter and darker blue lines represent the 10th and 90th percentiles, respectively. The 90th percentile means that in 90% of ensembles, the wind speed hitting the electrical line is equal to or less than the dark blue line. In other words, the dark blue line indicates the maximum wind speed for 90% of the generated conditions. The average wind speed is relatively low, especially for two sites, suggesting that their location makes them less susceptible to wind conditions. However, the remaining three sites may face a greater impact on electrical line safety due to wind speed and direction.

Moreover, sensitivity analysis was conducted to identify lines vulnerable to wind speed or direction, depicted in Figure 3. While wind speed is generally the most influential factor for all five sites, the analysis reveals variations in its dominance. At certain sites, e.g. site number 3, wind direction is nearly as impactful as wind speed. However, at other sites, such as site number 5, wind direction has a minimal or negligible effect on the probability of damage. Further details can be found in [3].

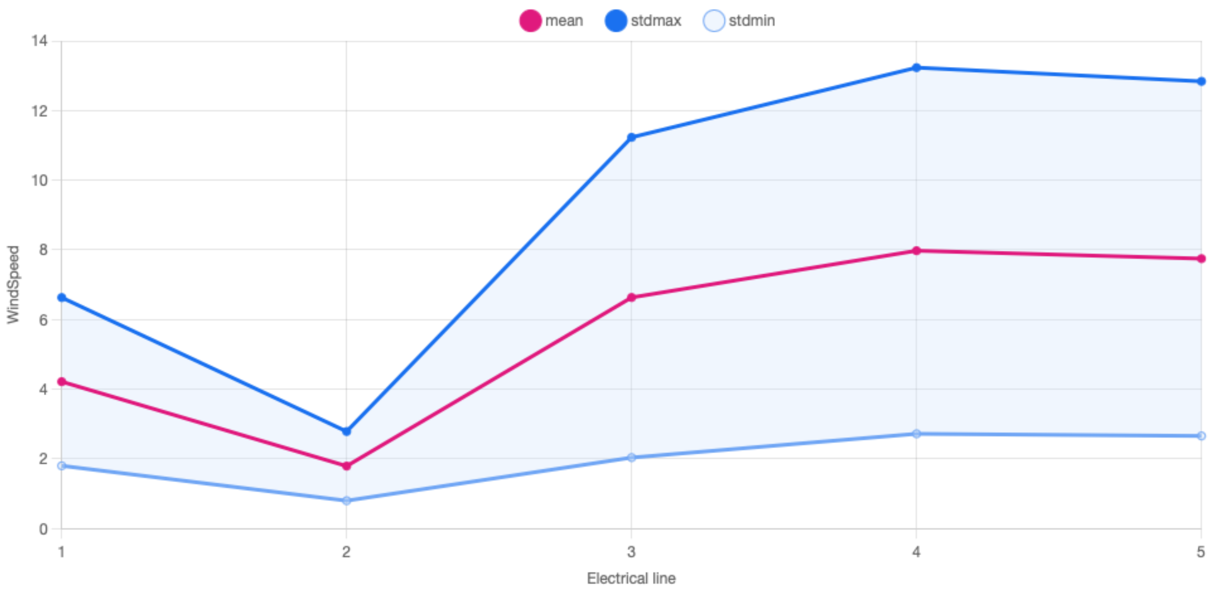

Figure 2. Mean wind speed at different electrical lines

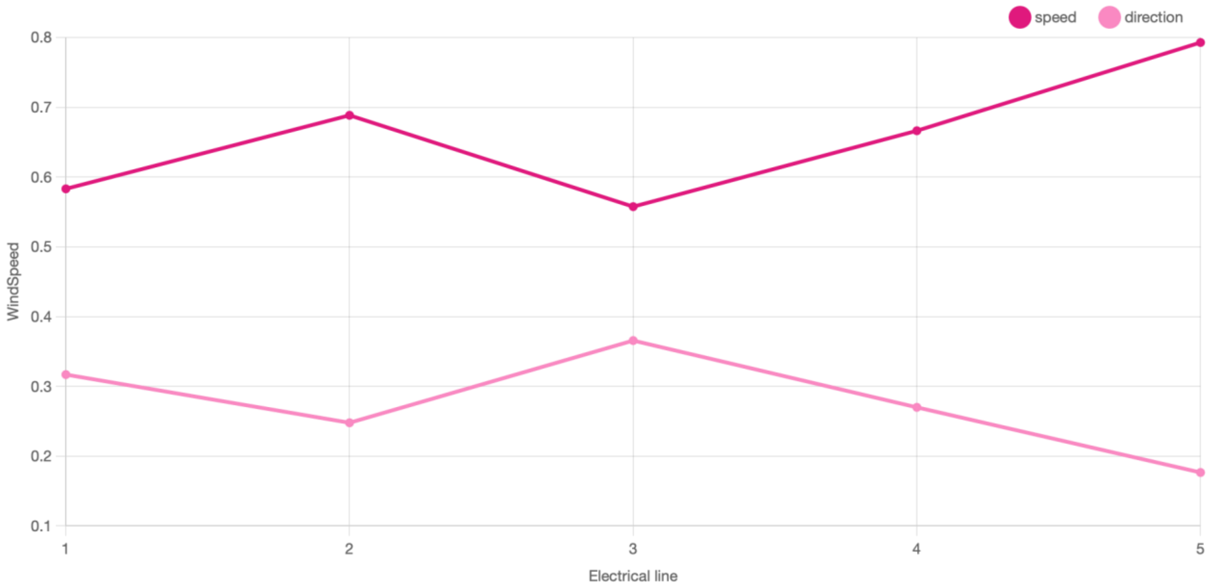

Figure 3. Electrical line sensitivity to wind speed and direction

Ensembles for uncertainty quantification, sensitivity analysis, AI and HPDA

Ensembles can also be used to account for input uncertainties and model parameterisation variations. RES relies on initial data from larger scale models, such as the Global Forecasting System. However, other prediction systems, like IFS from ECWMF [9] or ICON [10], can also be incorporated.

By generating more ensembles, we can explore different model parameterisation schemes within each RES model. This allows us to address uncertainties arising from varying inputs and minimise their impact on final results. Additionally, sensitivity analysis helps identify parameters with negligible influence on the final results, enabling us to reduce the number of required ensembles and improve computational efficiency.

The ultimate goal is to enhance the credibility of the simulation. Ensemble results will be processed using HPDA techniques to provide mean values of forecast parameters across the entire ensemble set. The RES-damages case is already operational, generating results and uploading them to CKAN [11] for further processing.

Ensemble results can also be used to train AI models and discover interesting correlations between input and output. These correlations can be translated into surrogate models that mimic the simulation but provide results more quickly. This could lead to more efficient and accurate simulations in the future.

Another aspect of using ensemble scenarios is to study the influence of mesh resolution and time step on result quality and gain a deeper understanding of the complex physical phenomena being modelled.

4.4 Wildfires

Regarding uncertainty quantification in wildfire simulation, this is an area as interesting as it is relatively under-researched. Nevertheless, after several years of providing operational simulation services to wildfire firefighters, we have clearly identified the sources of uncertainty.

Uncertainty associated with weather prediction

This uncertainty has two possible sources:

- As the prediction time increases (i.e., predictions further into the future), the reliability of the results decreases. For this reason, we use ensembles of predictions with several models to identify trends and probabilities.
- High-precision prediction models based on downscaling processes lose reliability as more nested domains are coupled to achieve high resolutions. This is a specific issue in high-resolution predictions with mesoscale models like WRF, which we use in the HiDALGO2 wildfire pilot.

Uncertainty associated with data and data structure

Other uncertainties are associated with the idealized representation of reality, particularly regarding vegetation structure, which is linked to limited catalogues of uniform forest fuel models. These models often hide or distort the effect of real-world forest fuels. For example, in crown fires, one of the parameters considered regarding vegetation structure is the height of the crown base, which influences the process of fire transitioning from surface to crown fire. However, in the real world, this is a probabilistic process, never deterministic: a fire has a probability of transitioning to a crown fire, but it's difficult to know exactly where this will occur, and whether this transition coincides with a critical point that could lead to more violent fire development.

Additionally, in simulations, vegetation moisture is often assumed to be uniform across space and, in many cases, constant over time, particularly regarding the moisture content of live (green) vegetation. In reality, this is much more complex, as there can be areas within the vegetation canopy where moisture is locally higher or lower, especially in critical locations like ravine knots, saddles, or ridges, where it can alter fire behaviour. Likewise, categorical deterministic rules are applied to estimate moisture content rather than probability functions, which adds uncertainty to the simulations.

Uncertainty associated with fire spread models.

We focus here on the uncertainty inherent in fire spread models: their deterministic nature. Specifically, cellular automata models used for fire spread assume a continuous propagation, where the fire always spreads from one cell to the next. In reality, this is not always the case, particularly when non-combustible areas or breaks in vegetation continuity (such as roads, firebreaks, and other prevention structures) are present. It's also important to consider that the raster cell size used can be a source of uncertainty: if the cells are too large, they may mask particularities not captured in the final map; if they are too small, they may not reflect the uniformity of fuel models. Both situations can lead to a vegetation model that deviates from what happens in the real world.

The deterministic nature of fire spread modelling has the added problem of error accumulation as the simulation progresses. Indeed, the spread of a flame front is based on its previous position, which, if simulated, can accumulate errors and deviate significantly from reality. This source of uncertainty is partially mitigated by incorporating the observed flame front position from the real world into the simulation, providing updated boundary conditions that reflect reality and allow for adjustments in the simulation, particularly regarding the estimation of spread rate at each point. Data assimilation, i.e., the incorporation of observations during the progression of the simulation, partially mitigates uncertainty, especially for simulations that project fire behaviour many hours into the future.

As can be seen, it is important to conduct a sensitivity analysis of the landscape to all these factors to determine the extent to which they contribute to simulation uncertainty. This is addressed in the HPDA analysis proposed for the wildfire pilot.

Uncertainty associated to wildfires phenomena.

In recent years, we have witnessed extreme wildfire events with pronounced fire-atmosphere interaction, generating phenomena such as area-wide combustions, fire whirls, eruptive fire behaviour, and pyrocumulus clouds. These phenomena, their appearance, and development are difficult to predict and even harder to locate geographically, making them the most significant source of uncertainty for firefighting operations, both in terms of effectiveness and safety. It is important to remember that many accidents and entrapments with fatal outcomes are associated with these unpredictable and surprising behaviours, making this a crucial area of research in fire simulation.

We also know that for certain types of wildfires, particularly crown fires, flying embers are generated and dispersed, potentially causing new spot fires ahead of the main fire front. This alters both the overall spread rate and the fire's behaviour. Current literature demonstrates the probabilistic nature of spot fire generation, which, if landing in critical locations, can lead to significant changes in fire behaviour, making it more violent.

Ensemble scenarios we foreseen to address these issues are of type 1:

- Ensemble of scenarios to address the quantification of uncertainties associated with the operational simulation of forest fires, for this we will evaluate the possibility of launching several simulations based on the ensemble of atmospheric models generated by the ECMWF also including stochastic processes of generation of sparks and jump to crown fire.
- Uncertainties associated with topographic conditions, fuel type and humidity, generation of secondary fires associated with sparks or crown fires. The strategy proposed in this case is the use of a program generated from the MeteoGrid propagator that allows launching a set of simulations under different boundary conditions to subsequently perform two types of analysis: 1) of the shape/size indicators of a fire; 2) of the passage of the fire through the territory.

4.5 Material Transport in Water

In the scope of the current pilot, several scenarios are planned on being adopted for the ensemble runs. The data is based on running the simulations in parallel by varying input parameters such as particle shapes and sizes and other physical properties.

Ensemble Scenarios in the Context of Scalar Transport in Particle-laden Flows

In fluid dynamics, the transport of scalar species and the interaction with solid particles often involve uncertainties arising from factors like initial and boundary conditions or material properties. To address these uncertainties, multiple scenarios are run in parallel with varying key input parameters. The focus is on scalar transport in water, both coupled with fully resolved solid particles and containing no particles. Goals are to explore the spread of pollution under impact of varying particle shapes and sizes. By varying particle parameters, we can investigate how changes in particle geometry influence key fluid and scalar dynamics.

We aim to better understand how these variations influence scalar transport and fluid-particle interactions. In real-world systems such as riverbeds, coastal regions, or industrial processes, heterogeneous mixtures of particles are common. The behaviour of these particles affects patterns of deposition, erosion, and transport efficiency.

Ensemble scenarios can provide a broader perspective on these interactions, capturing the inherent uncertainties and the complexity of natural environments.

AI and ensemble scenarios

The data generated from the simulations will be used to train surrogate models, improving AI's ability to predict particle-fluid-scalar interactions for complex-shaped particles. Surrogate modelling offers a faster and computationally efficient way to simulate these systems, facilitating better prediction and analysis for future research. For ensemble scenarios, we will use different classifiers to improve the predictions. In our case this means that we plan to combine the results of different AI models like pure data-based and operator-based learning into hybrid approaches. In this way we are able to obtain improved results compared to relying only on a single classifier.

Advantages of Ensemble Scenarios

Realistic Modelling: Ensemble scenarios allow us to better represent the variability in particle shapes and sizes, making the simulation results more applicable to real-world systems.

Improved Insights into Particle Dynamics: By exploring how different particle geometries interact with the scalar and fluid, we gain a deeper understanding of their coupled behaviour.

Complexity Analysis: Varying particle shapes adds layers of complexity to the system. Ensemble scenarios help us analyse these complexities, leading to more robust and accurate models.

5 Roadmap

Table 1 presents a summary of the planned activities from each pilot for the next project period. These activities will be part of the upcoming report, “D3.8 Ensemble Scenarios for Global Challenges,” scheduled for release in M41.

Table 1. Roadmap for the next project period.

HiDALGO2 pilot	Planned activities
Urban Air Project	Ensemble runs with parameter variation for boundary conditions
	Use ensemble runs to map parameter space for reduced order model generation
Urban Building	Ensembles runs with parameter variation based on available data and expert knowledge
	Parallel execution of ensemble runs utilizing Feel++'s ensemble runs feature
	Data collection and analysis to perform statistical analyses, identify trends, and evaluate the influence of different parameters on the outcomes
Renewable Energy Sources	Ensembles runs to assess the probability of damage to wind farms, photovoltaic systems, or overhead electrical networks
	Ensembles to account for input uncertainties and model parameterisation variations
Wildfires	Ensemble of scenarios to address the quantification of uncertainties associated with the operational simulation of forest fires
	Uncertainties associated with topographic conditions, fuel type and humidity, generation of secondary fires associated with sparks or crown fires
Material Transport in Water	Ensemble of multiple scenarios with varying particle geometries and sizes
	Train surrogate models using the data generated from ensemble simulations

6 Conclusions

This deliverable defines ensemble runs in HiDALGO2 and highlights the importance of ensemble runs in addressing global challenges, their importance for uncertainty quantification and predictive accuracy. By incorporating ensemble methods, HiDALGO2 enhances its capability to model complex systems and explore variability, providing a more comprehensive analysis than single-run models or simple coupled simulations. The methodologies outlined in this document demonstrate the project's commitment to advancing AI and simulation-based studies, particularly in the context of uncertainty and sensitivity assessments. Also numerous tools used in HiDALGO2 to manage ensemble runs have been presented.

The deliverable also illustrates how ensemble scenarios are integrated into HiDALGO2's various pilot use cases, reflecting their crucial role in improving the reliability and robustness of predictions. Moving forward, the project's continued focus on ensemble runs, as outlined in its roadmap, will be pivotal in delivering impactful results for uncertainty quantification and AI-driven insights in high-performance computing applications for global challenges.

This work will be further developed and expanded upon in the upcoming report, “D3.8 Ensemble Scenarios for Global Challenges,” scheduled for release in M41.

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