FUMEplot: a Prototype Tool for Automated Visualisation of Uncertainties in Ensemble Modelling Outputs

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Abstract. Here we present FUMEplot (Facilitated visualisation of Uncertainty in Model Ensemble outputs using plots), a general-purpose library which facilitates the automated visualisation of ensemble modelling outputs. We demonstrate the tool by applying it to three existing agent-based modelling tools, showcasing its ease of (automated) use and potential for wider application. We also describe how visualisations with FUMEplot can be generated automatically with minimal user configuration effort through its integration with the FabSim3 automation framework.

Keywords: Model Visualisation · Agent-based modelling · Output coupling.

1 Introduction

Whenever we measure aspects in the physical world or capture its dynamics in a model abstraction, we introduce uncertainties [2]. Specifically in simulation, increased uncertainty can emerge from its inputs (epistemic uncertainty) or from inherent variability within the simulation algorithm (aleatoric uncertainty) [19]. Likewise, observational records are subject to uncertainty, for instance due to accuracy limitations of the observational instrument or due to limitations in the fidelity of the record-keeping approach. One common approach to quantify uncertainty in simulation output data is to allow for the execution of multiple simulations instances. Such instances may be replicated (with each run having identical inputs) to quantify aleatoric uncertainty, and/or be aggregated into an ensemble (with each run having different inputs) to quantify predefined types of epistemic uncertainty, using specialized tools [9; 7; 1].

Visualizing uncertainty across different simulation runs, when it is done at all [21], is normally done using ad-hoc visualisation scripts, application-specific visualisation tools and/or more general purpose but proprietary visualisation tools. Within our own research domain we have seen dozens of visualisation scripts and tools emerge with the aim of visualising uncertainty. Although each

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modelling tool may have unique input and output formats, we find that in many cases, the modelling results describe phenomena of a similar nature and structure. Moreover, many application-specific visualisation tools may lose functionality over time due to insufficient community effort available to maintain them through updates of libraries, licenses or cloud-based services. This particularly happens as libraries get updated, licenses expire or cloud-based services get modified or removed.

Within this paper we propose a generic approach towards ensemble model visualisation which aims to provide paper-ready visualisations for a range of different applications in an automated way. We argue that by establishing a single tool applicable across domains we can share the maintenance cost for the visualisation software across application communities, and lighten the maintenance burden for each of these. This may lead to greater uptake of numerical uncertainty visualisation, which is considered to be a best practice in comparison with textual descriptions [21], and a more consistent use of it across disciplines. Our tool, named *Facilitated visualisation of Uncertainty in Model Ensemble outputs using plots*, or FUMEplot, reduces the need for users to construct bespoke visualisation infrastructure by applying the concept of "sensible defaults" or the "rule of least surprise" [18], and by providing a single visualisation representation which is established by decoding relevant parts of the model output. To showcase the reusable nature of our tool, we will present three application exemplars in human migration, epidemiology and disaster evacuation management.

2 Related Work

The field of information visualisation is extensively researched, with a range of advanced approaches available for a wide range of use cases, including those for ensemble data (see e.g. [20; 22; 11; 23; 17; 10]). In our proof-of-concept implementation, we have chosen to prioritize tool integration and user convenience over visualisation quality, but we note the presence of these advancements as an obvious direction for future improvement.

In terms of automation and convenience, we have chosen to build on the FabSim3 automation toolkit, which streamlines the access of remote compute resources and allows users to define custom and customizable workflows using a flexible plugin system [8]. FabSim3 is not the only automation toolkit in use by the scientific community, with notable alternatives being Aiida for instance [16], Apache Airflow https://airflow.apache.org/, Pegasus [3], NextFlow (widely used in bioinformatics [4]) or the A/OMUSE suite of research integration programs [15]. To our knowledge, the visualisation tools within these alternative automation environments are geared towards specific applications only, and tend to stay close to the functionalities provided by the underlying libraries (e.g. matplotlib). But perhaps more importantly, the work presented here is exclusively dedicated to visualising the results of ensemble simulations, not that of single runs.

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3 Conceptual Overview

FUMEplot is an open-source, open development tool that publicly available via GitHub [1]. It can be used either as a stand-alone Python program (or library) or as a closely integrated plugin for the FabSim3 automation environment. Within this section we will focus on the workings of FUMEplot within the wider automation environment, but all visualisation features are equally accessible when it is used as a standalone tool.

We present the FUMEplot architecture in Figure 1, an architecture which consists of three main concepts: (i) (ensemble) simulation output representations, (ii) FUMEplot representations and (iii) visualisation definitions. First, simulation output representations can vary depending on the codebase used, the type of output file generated and the structure of the ensemble simulation used (ensemble, replicated or ensemble with replicas). Here, FUMEplot usess FabSim3 internal variables and environmental characteristics to automatically detect the simulation output representations available for the selected use case: all the user needs to do is specify the name of the results folder that it needs to visualise. Second, FUMEplot representations indicate the kind of visualisations that are supported by the tool, featuring a visualisation kernel for each representation type. These representations may vary in spatial structure (free coordinates, gridded coordinates or named locations), object representation (stock counts or singular representation) and time representation (time-aggregated metrics, time step indicated or date/time indicated). Third, the visualisation definition component auto-detects the ensemble output representation, reads in a visualisation configuration information (using codebase-specific defaults stored in a YAML format) and incorporates user visualisation preferences to define the visualisations it needs to generate. Through the use of these components, FUMEplot allows users to use the typical FabSim-style one-line commands to generate visual outputs that fit their needs.

4 Implementation Overview and Status

In this paper, we present a prototype version of FUMEplot, which was first established during the SEAVEA Hackathon [2] on 7 February 2025. Given the tight development time frame, we opted not to provide a complete reference implementation yet. Instead, our prototype serves to demonstrate how automated visualisation can deliver a meaningful benefit in real-world research use cases.

Our prototype is fully integrated with FabSim3 as a plugin (named "FUMEplot") and can be installed easily within FabSim3 using the command "`fabsim localhost install_plugin:FUMEplot`". It can also be run easily using the oneliner "`fabsim localhost fplot:<results_dir>`" command, with "`results_dir`" specifying the directory where the ensemble simulation output is stored.

[1] URL: https://github.com/djgroen/FUMEplot

[2] for more information, see: https://dorahacks.io/hackathon/seavea

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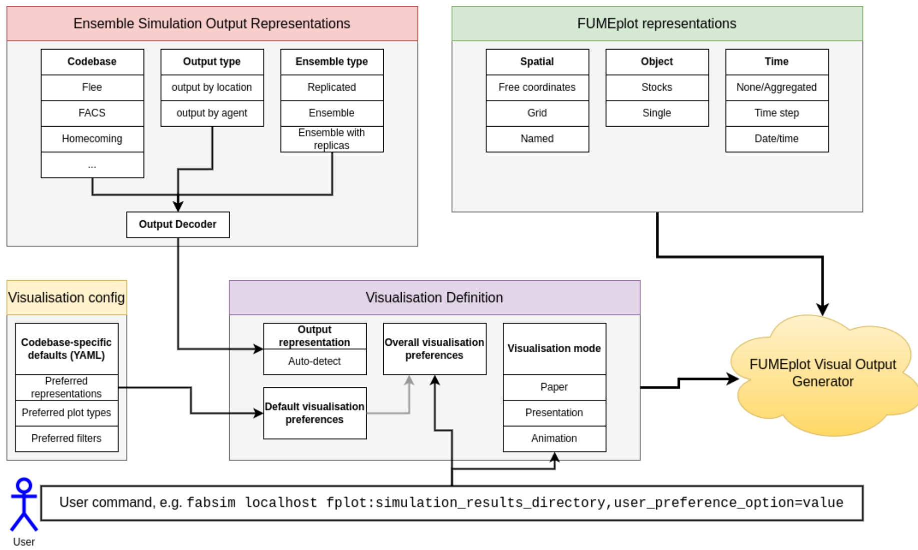

Fig. 1. Architectural overview of FUMEplot. Visual outputs are generated by combining the ensemble simulation outputs with predefined Visualisation Definitions and flexible representation functions from the FUMEplot library.

At time of writing, FUMEplot features two example FUMEplot representations ("named stocks by time step" and "named single by time step") applied to three example code bases (Flee, FACS and Homecoming), supporting all output types and ensemble types for these code bases. In terms of user preferences, our implementation currently supports graphs in "paper" mode, with the other modes still to be developed.

5 Example applications

To illustrate the capabilities of FUMEplot, we present several exemplary visualisations. The visualisations are generated using outputs from three different code bases: (i) Flee 3, an open source agent-based migration model [5], (ii) the Flu And Coronavirus Simulatios (FACS), an open source community disease transmission model [13], and Homecoming, which is a proprietary agent-based returnee modelling tool commissioned by UNHCR.

For example stock representations we present the number of susceptible persons over time in an ensemble FACS simulation, along with their uncertainty statistics (Fig. 2 (top)) and a screenshot of a histogram animation that shows the change of distribution over time (Fig. 2 (bottom left)). Furthermore we show a violin animation for ensemble output data of a Flee simulation (Fig. 2 (bottom right)) and a boxplot showing the ensemble results of migrations of a greatly simplified Homecoming simulation, grouped by source location (Fig. 3).

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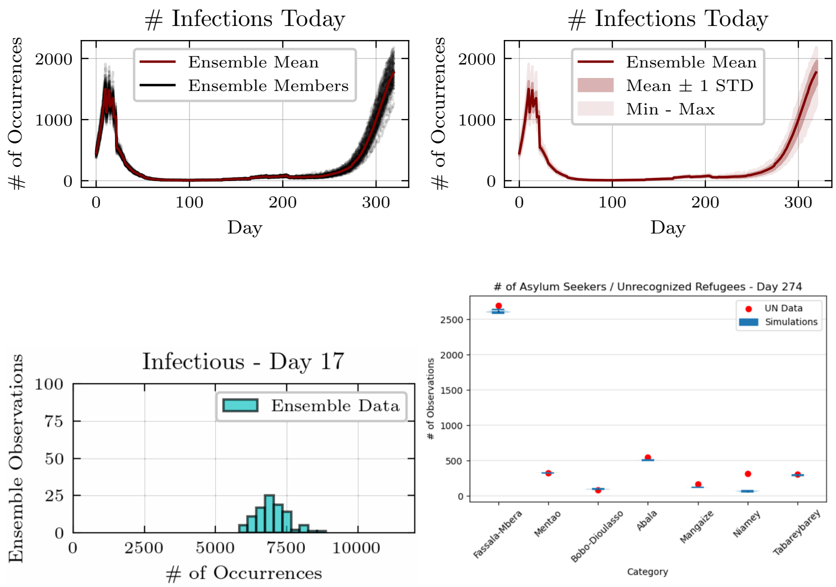

Fig. 2. FUMEplot visualisation examples: time-dependent simulation of a disease spread using FACS, with uncertainty captured by displaying trajectories of individual simulations in an ensemble (top left), and a calculated standard deviation across an ensemble and absolute range of values (top right). Animation stills of a histogram of ensemble data for a single subpopulation in a FACS simulation (bottom left) and a changing population sizes in camp locations in a Flee simulation ensemble, along with their uncertainties as a violin plot (bottom right), where the median value, extrema values, and Kernel Density Estimate fits of data PDF are shown. Animations are used to represent dynamics of ensemble uncertainty progressing over timesteps as a movie.

6 Evaluation and Discussion

To our knowledge, we are the first to present an automated tool exclusive dedicated to visualise uncertainties in ensemble simulations of population modelling. The tool as presented here was established in a short time span (6 weeks), and mainly serves to showcase how effective, lightweight, convenient and maintainable the concept can be. A main benefit of FUMEplot to users of Flee, FACS and Homecoming is that their ensemble runs can be configured such that the relevant metrics are automatically plotted, and that it is no longer required to maintain separate visualisation infrastructure for each separate code base. This work also fits within a larger effort to expand the FabSim3 automation approach (FabGuard [14] is another such example), allowing researchers to benefit from an automation approach that is more robust and reproducible than those currently provided by LLMs.

As future research we would like to incorporate the automated calculation and visualisation of advanced UQ metrics such as Sobol indices and generalize

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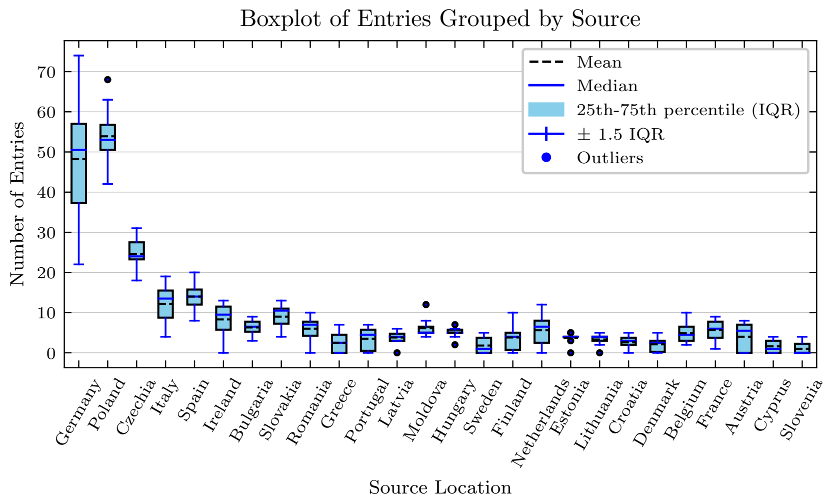

Fig. 3. A boxplot for each location involved in a Homecoming simulation ensemble created by FUMEplot. Here blue lines indicate mean values, dashed black lines indicate median values, shaded areas indicate 25% and 75% percentiles, whiskers indicate 1.5 distance between 25% and 75%, and dots indicate outliers.

FUMEplot to ensemble simulations in other fields such as computational physics, molecular dynamics and climate research. For simulations where a number of uncertain scalars evolving with time might be quantities of interest, most of the basic plots provided by FUMEplot should be applicable. To systematically represent ensemble outputs from a wide range of application domains, we will need to extend the design of FUMEplot representations and implement new representations (see [12] for diverse examples of uncertainty visualisation). In addition, some uncertainties are not (easily) quantifiable [6], and pose a specific challenge in being represented accurately.

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