Pyvale: An Open-Source Python Package for Image-Based Simulation Validation

L. Fletcher[1a], J. Charlton[1], J. Hirst[1], J. Horne-Jones [1], A. Marsh[1], M. Sampson[1], L. Sibson[1], A. Tayeb[1], A. Harte[1], and C. Hamelin[1]

[1]UK Atomic Energy Authority, Culham Campus, Abingdon, OX14 3DB, United Kingdom

[a]lloyd.fletcher@ukaea.uk

Abstract. Qualifying components for service inside the extreme environment of a fusion power reactor is a significant engineering challenge. Fusion reactor components are subjected to significant thermal (10's MW/m^2), mechanical (MN range) and electromagnetic loads (several Tesla) making experimental validation under these conditions expensive and time consuming. Here we develop a sensor simulation and data analysis toolbox called `pyvale` (python validation engine) which is designed to reduce experimental effort required for simulation validation. `pyvale` is open-source and the code is available here: [1]. A key application of `pyvale` is the analysis of simulation validation metrics for image-based data. We demonstrate this capability for digital image correlation data used for validation analysis of a probabilistic multi-physics simulation.

Possible Sessions

1. Model Validation, 18. Nuclear Applications: Fusion, 6. Data-Driven Testing

Introduction

Nuclear fusion is a promising source of clean energy but there are significant engineering challenges that must be overcome to make it commercially viable. One key challenge for fusion is maintaining the structural integrity of components inside the vacuum vessel that are exposed to the extreme environment of the plasma. These in-vessel components are subjected to high heat fluxes, significant mechanical loads, electromagnetic body forces from several Tesla magnetic fields, and neutron irradiation damage. The cost of performing large-scale validation tests on complex in-vessel components will be on the order of £M's. Therefore, significant cost and risk reduction can be achieved by maximising the information obtained from an optimised set of targeted experiments. Time and cost constraints make it impossible to perform thousands of meter scale component experiments, but it is possible to perform significant numbers of simulations on the latest generation of supercomputing clusters that have thousands of chips with hundreds of thousands of cores. To bridge this gap between experiments and simulations we are building a software engine that can simulate realistic sensor data from a simulation with a focus on multi-physics scenarios and image-based sensors. A key application of our software is the calculation and analysis of simulation validation metrics that can be applied to: image-based data, multi-physics scenarios and probabilistic simulations.

We take inspiration from the experimental mechanics community in which synthetic image deformation has been developed for predicting uncertainties for digital image correlation [2]. We extend this idea to simulating uncertainties for arrays of sensors applied to multi-physics scenarios. We have called our sensor simulation, experiment design and simulation validation platform the python validation engine, `pyvale`. `pyvale` is provided with an open-source MIT license allowing commercial use and the code is freely available here [1]. In this work we focus on the use of `pyvale` for the calculation of validation metrics for image-based data.

Application of the `pyvale` for Validation Metric Calculations

Simulation and experimental datasets. The component we analysed is a mock-up heatsink component machined from stainless steel 316L. The geometry consisted of a central rectangular solid block (50 L x 37 W x 35 H mm) with a 12 mm internal diameter water-cooling pipe passing through the bottom half of the block. Induction heating was applied to the top of the block imposing a temperature gradient with the highest temperature at the top of the block decreasing towards the cooling pipe near the base of the block. A probabilistic coupled electro-magnetic, thermal and mechanical simulation was performed using COMSOL Multiphysics outputting 100 simulations sampling different combinations of the input parameters using SmartUQ. The experimental dataset consisted of digital image correlation (DIC) from a stereo DIC system imaging the front face of block experiencing the temperature gradient (i.e. the face on the side of the block parallel to the cooling pipe axis). For the simulation the displacement fields were output on a regular grid of 0.5mm pitch on the same face that was imaged by the DIC system. For the experiment the steady state portion of the experiment was used. This was identified from the stability of thermocouple traces to be between frames 300 and 650. The DIC data consisted of the 3-displacement components sampled at 47,566 points over the 350 steady state time steps. We corrected both datasets for rigid body motion by subtracting the mean of the displacement field for each simulation of experimental data frame.

Validation Metric Analysis. We transformed both datasets to consistent coordinate systems by shifting the origin of each coordinate system to its centroid and then using singular value decomposition to extract the principal axes for the transformation. The experimental dataset was significantly denser than the simulation, so we linearly interpolated it onto the regular grid of the simulation output. We then averaged each dataset and compared the mean displacements fields as shown in Fig. 1 below. We then used the 100 probabilistic simulations and the 350 steady state experimental time steps to calculate the Modified Area Validation Metric (MAVM) from [3] to account for sources of uncertainty in the simulation and experimental data.

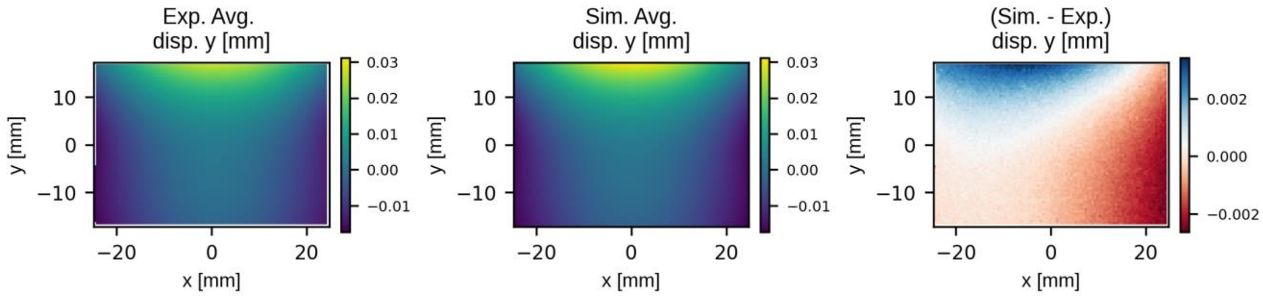

Figure 1: Comparison of the average vertical displacement fields for the experiment (averaged over the steady state region) and the simulation (averaged over all probabilistic simulation runs).

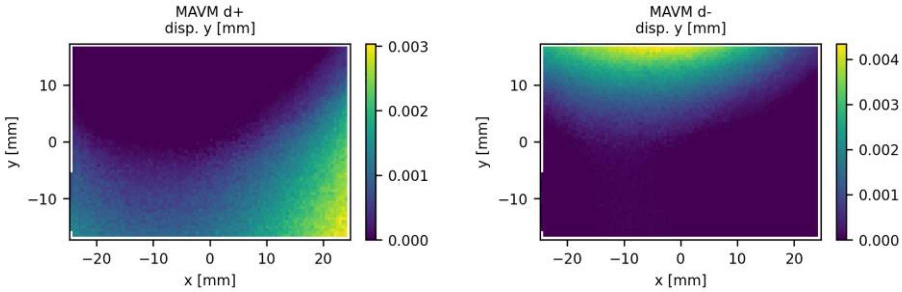

Figure 2: Modified area validation metric (MAVM) bounds between the probabilistic simulation and the image-based experimental data showing the upper (d+) and lower (d+) bounds of the simulation uncertainty.

Analysis of Figs. 1 and 2 shows: 1) the overall shape of the field is similar between the experiment and simulation; and 2) the simulation over predicts the displacement magnitude by ~10%. Given the main source of deformation is thermal expansion and that the field shapes are similar we suspect that the thermal expansion coefficient is the source of the difference. As we also have thermal data for this experiment, we will investigate and implement simulation calibration procedures in `pyvale` that will isolate the difference in temperature fields and aid us in confirming the difference in thermal expansion coefficient.

Conclusion & Future Work

In this work we have demonstrated the use of the `pyvale` python package for calculating a validation metric for a probabilistic multi-physics simulation with image-based data. In the future we will integrate the validation functionality of `pyvale` with our image simulation and digital image correlation toolbox as well as including additional validation metrics. To ensure scalability and performance of `pyvale` we are implementing the underlying algorithms in Cython, C and/or GPU code while providing a Python interface to allow ease of use. Our goal is to have a single open-source Python package for simulating and analysing data from imaging sensors that can be deployed at scale on supercomputing clusters without the license restrictions of commercial software.

Acknowledgements. We would like to acknowledge the support of UKRI through the Future Leaders Fellowship of Dr Lloyd Fletcher, grant number MR/Y015916/1. We would also like to acknowledge support from the EPSRC energy programme through grant number EP/W006839/1.

References

[1] L. Fletcher, et al., *pyvale*, https://github.com/Computer-Aided-Validation-Laboratory/pyvale, 2025

[2] P. Lava, et al., Validation of finite-element models using full-field experimental data: Levelling finite-element analysis data through a digital image correlation engine, Strain 56/4 e12350.

[3] Whiting et al., Assessment of Model Validation, Calibration and Prediction Approaches in the Presence of Uncertainty, Journal of Verification, Validation and Uncertainty Quantification 8 (2023),