Performing Validation, Verification, and Sensitivity Analysis on Multiscale Fusion Plasma Simulations with the VECMA Toolkit

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To effectively simulate the dynamics of a fusion plasma, one must take into account the widely disparate phenomena happening in both space and time. Namely, the micro-instabilities developed in plasma turbulence can affect the overall transport and ultimately destroy confinement. Hence, a component based approach is used to couple various single-scale models together in a workflow. This multiscale fusion workflow MFW (see Figure 1) uses MUSCLE to connect the transport, equilibrium and turbulence models together with a module that converts fluxes into transport coefficients. While this workflow has provided insights into the overall plasma transport with turbulence taken into account [1], it needs to get verified, validated and its uncertainties quantified (e.g. analyze sensitivity) before any meaningful comparison between simulation results and experimental data can be carried out.

The VECMA toolkit [2] is utilized to study uncertainties in the workflow: it is composed of several components that aim to aid users in bringing Verification, Validation and Uncertainty Quantification (VVUQ) into their complex single-scale or multiscale models. For example, EasyVVUQ [4] is a python-based library that enables the VVUQ process in a simulation model. MUSCLE3 [5] helps couple single-scale models together to form a multiscale workflow and advanced UQ can be applied to the workflow as well. We use these components to guide us through the VV and sensitivity analysis (SA) processes in the MFW.

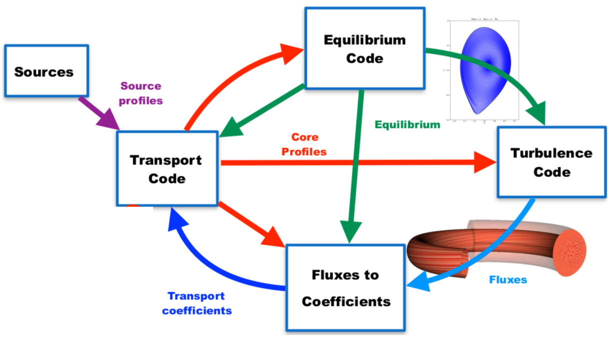

Figure 1: Multiscale fusion workflow.

To validate the results coming from MFW simulations, we quantitatively compared the electron and ion temperature, T_e and T_i respectively, distributions coming from simulations and experimental data of the ASDEX Upgrade tokamak[1]. The more well-known similarity measures such as Hellinger distance, Jensen-Shannon distance, and Wasserstein metric were utilized for

[1] https://www.ipp.mpg.de/16195/asdex

such task, and they are available in 2 components of the toolkit: FabSim3[2] and/or EasyVVUQ. The validation results using these metrics can be found in [3].

We derived a different measure: the compatibility measure can provide a quantitative comparison between distributions that places more emphasis on the lower moments. The measure produces a compatibility distance, or total weight w_{tot}, with a value between 0 and 1:

$$w_{tot} = (1-w)\frac{(\mu_2-\mu_1)^2}{2(\sigma_1^2+\sigma_2^2)+(\mu_2-\mu_1)^2} + w\frac{(\gamma_2-\gamma_1)^2}{2(\sigma_1^2+\sigma_2^2)+(\mu_2-\mu_1)^2+(|\gamma_1|+|\gamma_2|)^2}. \quad (1)$$

w is the weighting factor with a value also ranging between 0 and 1. μ, σ, and γ are the mean, standard deviation, and skewness of a distribution, respectively. The users of this metric can vary w accordingly. For example, we tested w = 0.05, 0.5, 0.95, and w_{tot} with $w = 0.05$ agrees with our intuition the most. We will use $w = 0.05$ in the rest of this paper. The initial validation results using both compatibility distance and Z-test can be found in [3] as well. These two measures will be implemented and become available in the VECMA toolkit in the near future.

Next we search for a systematic approach to interpret w_{tot} values, i.e. at what value of w_{tot} shall we consider 2 distributions as the same. After comparing various distributions, we classify the values into 4 categories: $0 \leq w_{tot} < 0.45$: same; $0.45 \leq w_{tot} < 0.6$: marginally the same; $0.6 \leq w_{tot} < 0.75$: significantly different; and, $0.75 \leq w_{tot} \leq 1$: highly significantly different.

Next we take the compatibility measure to compare two T distributions from simulation. The way we obtained distributions at every flux-tube is we take output T values from within one simulation second period, place them in a time bin, and then calculate μ, σ and γ. The resulting μ and $\mu \pm \sigma$ of the T distribution at every flux-tube, at each 1-s time bin are plotted in Figure 2). We then use the compatibility measure to determine when the plasma reaches a quasi-steady state by comparing distributions from two consecutive time bins n and $n-1$, starting with $n = 2$ (or 2-3s time bin). We found the distributions from 3-4s and 4-5s time bins at every flux-tube, for both T_e and T_i, are qualitatively the same based on the established categories. Therefore, we determine the plasma reaches a quasi-steady state at 5s, and use T distributions from 4-5s time bin to compare with experiment.

The ASDEX Upgrade experiments have certain restrictions and diagnostics that leads to further uncertainties involved in the measurements, in addition to the reported upper and lower values. This is especially so near the edge ($\hat{\rho}_{tor}$ near 1.0). First, we took the data and treated the distributions as a split-Gaussian. To account for the further uncertainties, we expand σ to include 10% of μ to broaden the spread of the temperature distributions. Therefore we define

[2]https://github.com/djgroen/FabSim3

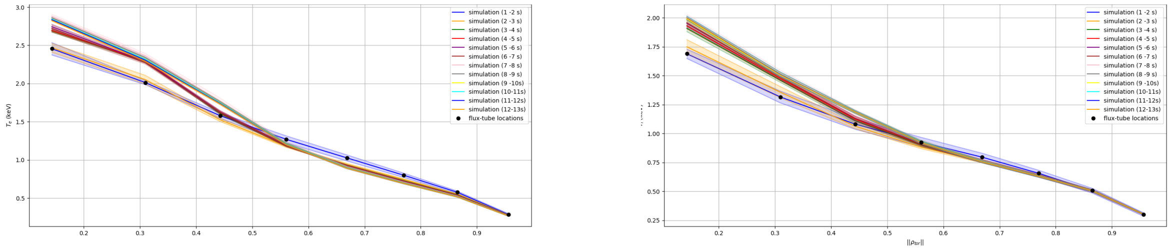

Figure 2: T_e (left) and T_i (right) profiles at every simulation second.

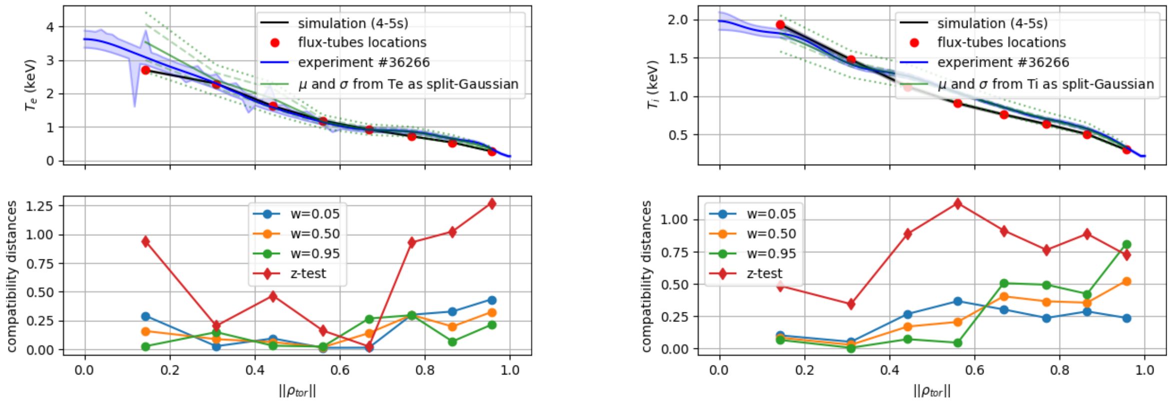

Figure 3: T_e (left) and T_i (right) distributions from simulation and ASDEX Upgrade shot #36266 (top), and their compatibility distance and Z-score (bottom). The solid, dashed and dotted green lines at the top panels represent μ, $\mu \pm \sigma$, and $\mu \pm \sigma_{eff}$ of split Gaussian (experiment) distribution, respectively.

an effective standard deviation: $\sigma_{eff} = \sigma + 0.1\mu$.

We take the distributions obtained from 4-5s time bin in simulation and compare that to the experiment, in particular shot #36266. The compatibility measure is shown in Figure 3, and it indicates the two distributions are qualitatively the same ($0 \leq w_{tot} < 0.45$) at every flux-tube. We also compare the simulation results with shot #36297, and it yields the same outcome.

An issue we encountered is that, as shown in Figure 2, T_e profile changes shape starting at the 7-8 s time bin. We compared T distributions at this time bin to the experiment's, and the compatibility measure shows the two distributions are qualitatively the same. If we used the compatibility measure to determine plasma's quasi-steady state like we stated earlier, then we would terminate the simulation too early (at 5s). We wouldn't be able to capture any interesting physics going on starting at 7s. Therefore, we will need to refine our method in the future.

The verification process to the workflow can be achieved via level of refinement on model parameters until quantities of interest (QoI) display asymptotic behavior. This approach has been applied to a simple fusion workflow that simulates a cylindrical plasma with fixed density, and it is available in the VECMA Toolkit[3] tutorial. UQ using polynomial chaos expansion

[3]https://www.vecma-toolkit.eu/

(PCE) method was performed to this workflow with the help of EasyVVUQ. We varied 5 input parameters and sought level of refinement to μ and σ of T_e distribution and 1st Sobol indices by scanning the value of PCE polynomial order, from 1 to 6. This test showed polynomial order of 3 is sufficient to get converged results. [6]

Finally, the turbulence model is computationally the most expensive single-scale model within the workflow. We want to apply SA to the model in the future to help reduce the number of varied inputs and therefore cut down the sample size and cost. In the meantime, Sobol SA was performed on the same UQ example from earlier. The 1st Sobol indices across the radial profile show that, at the sixth PCE order, T_e variance is most sensitive to the width of the heat source function, transport coefficient across the radial profile, and the edge T_e value. [6]

In conclusion, MFW uses component based approach and MUSCLE is to couple the single-scale models together into a workflow. We have made progress towards validation of the ASDEX Upgrade tokamak simulations . We used EasyVVUQ and MUSCLE3 from the VECMA toolkit to guide us in the VVUQ process. We quantitatively compared two T distributions from simulation and/or experiment using various similarity metrics, particularly compatibility distance. Comparison between distributions from two consecutive time bins shows that the distributions from 3-4s and 4-5s time bins were qualitatively the same at every flux-tube, for both T_e and T_i. The experimental data have additional uncertainties, therefore we broadened the spread of the split-Gaussian distribution by adding 10% of μ to σ while maintaining the overall trend of the distribution. By comparing simulation distribution at 4-5s time interval with data from shot #36266 or #36297, we found the two distributions are quantitatively the same. However, we also learned that the simulation T_e profile at 7-8s looked different from the one at 4-5s. If we utilized compatibility distance as described to determine a quasi-steady state (e.g. at 5 s), then we might terminate the simulation too early and therefore we need to develop a more sensible metric. While verification of and SA to MFW are work in progress, level of refinement and Sobol SA are applied to a simple fusion model to show 3rd order PCE is sufficient for converged results and T_e variance is most sensitive to 3 out of 5 varied inputs. This result can contribute toward dimension reduction of the model.

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