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Towards scalable large-scale model validation with data science

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Computationally costly models, with a selection of uncertain input parameters, are ubiquitous in science, including magnetic confinement fusion research (MCF) [1 – 4]. Due to the input uncertainties, multiple forward passes are typically required in model validation to quantify the input parameter distributions that best reproduce the experimental observations [5]. This inverse uncertainty quantification need represents one of the key challenges in model validation and must be done algorithmically in large-scale validation workflows.

Simulation-based inference (SBI) is a rapidly developing field aiming to address these inference challenges related to complex, high-fidelity simulators in science [6]. While data-efficient inverse inference workflows have been demonstrated in model validation applications within MCF [5, 7 – 9], a large-scale adoption of these methods in model validation activities in MCF has not emerged yet. One of the key entry barriers is the software infrastructure that is needed for large-scale applications. In addition to the SBI algorithms, a large-scale workflow requires solutions for overall task orchestration on high-performance computing (HPC) platforms, management of the simulation database, and for processing failed simulations automatically within the workflow. However, these requirements align with those needed for data generation for general machine learning surrogate model development for computationally demanding models [10 – 12]. Therefore, it is foreseen that developing fast surrogate models for a very broad range of applications and large-scale validation of computational models can be established within a unified, holistic workflow that advances both objectives simultaneously. To proceed towards this vision, a scalable SBI framework is being developed, building on top of *Enchanted-surrogates*, originally designed for simulation data generation for surrogate models [13].

The developed framework is applied for parameter inference of runaway electron (RE) transport simulations of JET Pulse Number (JPN) 95135 with argon induced disruption and RE beam. The study is initialized by simulating the current quench and early RE plateau with DREAM assuming no radial RE transport with background electron temperature, argon assimilation fraction, and RE seed magnitude optimized with Bayesian Optimization (BO) to reproduce the experimentally measured plasma current, similar to [5]. At the end of this initialization simulation, the synthetic synchrotron image, obtained with SOFT [14], is qualitatively in agreement with experimental observations. Starting from this initialization simulation, RE plateau is simulated allowing radial diffusion via the Rechester-Rosenbluth model [15]. The transport is parameterized through magnetic field fluctuation magnitude (δB/B) and radial variation through α and β as $r^{\alpha-1}e^{-\beta r}$ [15]. The established workflow is able to sample through several hundred kinetic DREAM simulations, post-processed with SOFT, while using BO to efficiently find a solution that aligns significantly better with the experimentally observed synchrotron image at the end of the simulated time window than a simulation without RE transport would. Further application of the framework in model validation and future perspectives of enabling large-scale SBI in MCF studies will be discussed.

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