ENABLING REAL-TIME ICRF HEATING PREDICTIONS VIA AN AUTOMATED SURROGATE MODEL GENERATOR SUITE

[1]A. Sanchez-Villar, [2]Z. Bai, [1]J. Berkery, [1]N. Bertelli, [3]E. W. Bethel, [4]J. Hillairet, [2]T. Perciano, [5]G. Pyeon, [1]S. Shiraiwa, [5]G. M. Wallace, and [5]J. C. Wright

[1]Princeton Plasma Physics Laboratory, Princeton, NJ 08540 Jersey, United States
[2]Lawrence Berkeley National Laboratory, Berkeley, CA 94720, United States
[3]San Francisco State University, San Francisco, CA 94132, United States
[4]CEA, IRFM, F-13108 Saint-Paul-Lez-Durance, France
[5]MIT Plasma Science and Fusion Center, Cambridge, MA 02139, United States

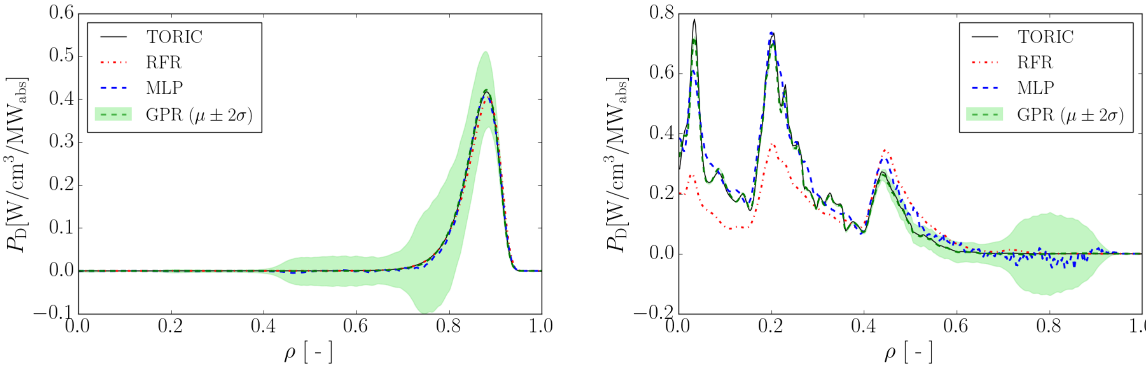
Email: asvillar@pppl.gov

An Automated Surrogate Model Generator Suite has been developed to achieve accurate and real-time capable predictions of 1D ion cyclotron range of frequencies (ICRF) heating. The suite is designed to provide an effective streamlined workflow to train, optimize, save and deploy surrogate models, leveraging open-source artificial intelligence and machine learning (AI/ML) frameworks such as PyTorch, TensorFlow, and Scikit-learn, along with Bayesian optimization for hyperparameter tuning. This work advances our efforts towards the development of a toolkit to deploy surrogate models which are effective for multiple scenarios. The suite is tested to develop surrogates that predict ICRF heating profiles for NSTX, where our previous models were trained and optimized using methodical scanning, randomized and gridded searches. The new methodology improves surrogate accuracy while simplifying implementation through an end-to-end framework based on various ML algorithms.

AI/ML methodologies present a potential opportunity to accelerate research in multiple areas relevant for fusion energy sciences [1] such as disruption prediction and control [2], experimental analysis [3], enhanced diagnostics [4], or model extraction and reduction via surrogate model development [5-7]. Surrogate models enable overcoming the large computational expenses of conventional modeling codes. A recent example is their application to accelerate predictions of radio-frequency heating and current drive, from the lower hybrid current drive at EAST [5], to the more recently shown real-time capable predictions of the ICRF heating of multiple plasma species for the high harmonic fast wave (HHFW) heating system at NSTX, and the ion cyclotron minority heating at WEST [7]. These surrogate models have been shown not only to accelerate predictions by six-to-seven orders of magnitude compared to the reference model, TORIC [8], but also to overcome other numerical code limitations such as numerical artifacts [9].

The Automated Surrogate Model Generator Suite presented here addresses several challenges identified previously, including hyperparameter optimization, model training, and uncertainty quantification. The models included in the suite are the Random Forest Regressor (RFR), the Multi-layer Perceptron (MLP), and the Gaussian Processes Regressor (GPR). The suite expands on the methods shown in [7] by implementing the MLP models using the PyTorch framework, and also adds GPR models via TensorFlow based libraries. Additionally, model hyperparameter tuning is carried out via Bayesian Optimization, which seeks for optimized model hyperparameters including surrogate architecture. In the case of the GPR model, the suite tests multiple kernels and optimizes its trainable variables. The inclusion of GPR-based models establishes verification, validation and uncertainty quantification (VVUQ) framework for ML/AI-based surrogates. The suite is tested on the HHFW heating database for NSTX described in [8]. The predictions are compared against those of the reference ICRF heating model (TORIC), via two regression accuracy metrics: (i) the mean squared error (MSE) and (ii) the coefficient of determination (R^2).

The Automated Surrogate Model Generator Suite is used to develop three ML-based surrogate models for accurate and real-time capable predictions of ICRF heating profiles for electrons and deuterium species in the HHFW system of NSTX. For the electron-based predictions, these models achieve excellent regression accuracies with MSE values of 1.67e-5, 1.85e-5, 2.07e-6 and R^2 scores of 0.965, 0.977 ,0.993, for the RFR, MLP, and GPR models, respectively. Similarly, for the deuterium database, the achieved MSE values are 1.14e-4, 3.5e-5, 8.6e-6 and the R^2 scores are 0.934, 0.982, and 0.996. As observed, in terms of regression accuracy, the GPR outperforms the other two architectures, while the RFR, though the least accurate, still provides excellent regression scores. RFRs typically feature the simplest and fastest implementation, and it shows marginal accuracy enhancement due to hyperparameter optimization, and features fast training times. However, in order to achieve further refined ML-surrogates, we demonstrate that the suite provides workflows for deploying two alternative and more accurate algorithms for surrogate implementation.



(a) Single-pass absorption (b) Multi-pass absorption

Figure 1: Machine learning based deuterium power absorption predictions from the RFR (red dash-dotted), MLP (blue dashed), and GPR (green) models obtained with the Automated Surrogate Model Generator Suite are shown in (a) strong single-pass and (b) multi-pass absorption scenarios in NSTX, and compared to the reference computational model TORIC (black solid). For the GPR we show the mean prediction (μ, green dashed) and the 95% confidence interval based on the estimated standard deviation (σ, green shadow).

Figure 1 shows ML-based predictions of (a) a strong single-pass absorption (b) a multi-pass absorption scenarios of deuterium power absorption (P_D) for the RFR (red dash-dotted), MLP (blue dashed) and GPR (green dash-shadowed) surrogates compared to the reference prediction obtained by TORIC (black solid). Figure 1(a) illustrates an example of a strong single pass absorption scenario where the fast wave is deposited in the lower field side region of the plasma, yielding a profile dominated by a singly-peaked feature corresponding to a harmonic resonance. This is the most frequent type of pattern in the NSTX-P_D database, and matches the type of profiles that all surrogates can capture accurately. Figure 1 (b) depicts the P_D prediction with the lowest surrogates' regression accuracy, featuring a more complex deuterium power deposition pattern corresponding to multi-pass absorption scenario. In these, while the RFR can reproduce the heating characteristics, only the MLP and particularly the GPR model accurately capture the deuterium power absorption profile. Additionally, the GPR model prediction also provides a standard deviation (σ), shown as a 95% confidence interval (green shaded area) in Figure 1. This interval denotes the estimated uncertainty in the prediction, and is inhomogeneous along the radial direction and specific to each case. The estimated uncertainty is a result of a combination of factors including the inherent data variability, data scarcity near specific data points, and the model's limitations in entirely capturing the underlying physical function. GPR models thus allow an estimate of the prediction confidence in different plasma regions for each parametric combination.

Overall, this work introduces an Automated Surrogate Model Generator Suite that streamlines model hyperparameter optimization, training and evaluation, while incorporating uncertainty quantification through GPR-models. The framework, demonstrated on ICRF heating predictions, is a versatile, VVUQ-based surrogate modeling implementation tool applicable to a wide range of fusion-relevant datasets.

ACKNOWLEDGEMENTS

This work was supported by the U.S. Department of Energy under contract number DE-AC02-09CH1146.

References

[1] HUMPHREYS, D., et al. *Journal of Fusion Energy* **39** (2020) 123.
[2] SEO, J., et al. *Nature* **626** (2024) 8000.
[3] CHOUCHENE, S., et al. *Phys. Rev. E* **109** (2024) 045201.
[4] JALALVAND, A., et al. "Enhancing Temporal Resolution in Fusion Diagnostics through Multimodal Neural Networks", *Bulletin of the American Physical Society* (2024).
[5] WALLACE, G. M. et al. *J. Plasma Phys.* **88** (2022) 895880401.
[6] SHOUSHA, R., et al. *Nucl. Fusion* **64** (2023) 026006.
[7] SANCHEZ-VILLAR, A., et al. *Nucl. Fusion* **64** (2024) 096039.
[8] BRAMBILLA, M., *Plasma Phys. Control. Fusion* **41** (1999) 1.
[9] SANCHEZ-VILLAR, A. et al. "On the development of robust realtime capable ICRF heating models", *Bulletin of the American Physical Society* (2024).