PSFC/JA-23-2

Towards Fast, Accurate Predictions of RF Simulations via Data-driven Modeling: Forward and Lateral Models

G.M. Wallace,[1] Z. Bai,[2] N. Bertelli,[3] E.W. Bethel,[4]
T. Perciano,[2] S. Shiraiwa,[3] and J.C. Wright[1]

[1)] *MIT Plasma Science and Fusion Center, Cambridge, MA, USA 02139*
[2)] *Lawrence Berkeley National Laboratory, Berkeley, CA, USA 94720*
[3)] *Princeton Plasma Physics Laboratory, Princeton, NJ, USA 08540*
[4)] *San Francisco State University, San Francisco, CA, USA 94132*

February 2023

Plasma Science and Fusion Center
Massachusetts Institute of Technology
Cambridge MA 02139 USA

This work was supported by the Director, Office of Science, Office of Fusion Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231, through the grant "Accelerating Radio Frequency Modeling Using Machine Learning". This research used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility located at Lawrence Berkeley National Lab- oratory, operated under Contract No. DE-AC02-05CH11231. This research used the resources of Princeton Plasma Physics Laboratory operated under Contract No. DE-AC02-09CH11466. The simulations presented in this paper were performed on the MIT-PSFC partition of the Engaging cluster at the MGHPCC facility (www.mghpcc.org) which was funded by DoE grant number DE-FG02-91-ER54109.

Submitted to *AIP Conference Proceedings*

Towards Fast, Accurate Predictions of RF Simulations via Data-driven Modeling: Forward and Lateral Models

G.M. Wallace,[1, a)] Z. Bai,[2] N. Bertelli,[3] E.W. Bethel,[4] T. Perciano,[2] S. Shiraiwa,[3] and J.C. Wright[1]

[1)] *MIT Plasma Science and Fusion Center, Cambridge, MA, USA 02139*
[2)] *Lawrence Berkeley National Laboratory, Berkeley, CA, USA 94720*
[3)] *Princeton Plasma Physics Laboratory, Princeton, NJ, USA 08540*
[4)] *San Francisco State University, San Francisco, CA, USA 94132*

[a)] *Corresponding author: wallaceg@mit.edu*

Abstract. Three machine learning techniques (multilayer perceptron, random forest, and Gaussian process) provide fast surrogate models for lower hybrid current drive (LHCD) simulations. A single GENRAY/CQL3D simulation without radial diffusion of fast electrons requires several minutes of wall-clock time to complete, which is acceptable for many purposes, but too slow for integrated modeling and real-time control applications. More accurate simulations with fast electron diffusion are even slower, requiring multiple hours of run time with parallel processing. The machine learning models use a database of 16,000+ GENRAY/CQL3D simulations for training, validation, and testing. Latin hypercube sampling methods implemented in πScope ensure that the database covers the range of 9 input parameters ($n_{e0}, T_{e0}, I_p, B_t, R_0, n_{||}, Z_{eff}, V_{loop}, P_{LHCD}$) with sufficient density in all regions of parameter space. The surrogate models reduce the computation time from minutes-hours to ms with high accuracy across the input parameter space. Data-driven surrogate models also allow for solving inverse and "lateral" problems. A surrogate model for the inverse problem maps from a desired current drive or power deposition profile to a set of input parameters that would result in such a profile, while a surrogate model for the lateral problem maps from a measured experimental quantity such as hard x-ray emission to a current drive or power deposition profile. The πScope database creation workflow is flexible and applicable to other RF simulation codes such as TORIC.

INTRODUCTION

Most tokamak fusion reactor designs feature radio frequency (RF) heating and current drive (H&CD) actuators to supplement the self-generated fusion heating and bootstrap current [1, 2, 3]. Simulation models to calculate the power deposition and current drive profiles such as the ray tracing/Fokker-Planck solver suite GENRAY [4]/CQL3D [5] are relatively mature and can yield results on timescales of minutes to hours, which for many applications is sufficiently fast. However some applications, for example time-dependent integrated modeling and real-time control, require results in milliseconds. Previous work [6] showed that it is possible to predict the output of GENRAY/CQL3D using machine learning (ML) based methods with high speed and accuracy. This paper will focus on refinement of the previous work including the effects of radial diffusion of the fast electrons, as well as application of ML tools to the "lateral" problem. Figure 1 illustrates the forward, inverse, and lateral problems as they relate to GENRAY/CQL3D.

FORWARD MODEL

A forward model predicts certain quantities of interested based on a set of causal factors used as inputs to calculation. In the case of RF models, the quantities of interest are typically current drive and power deposition profiles across the minor radius, while the causal factors are quantities related to the plasma (n_e, T_e, Z_{eff}, magnetic equilibrium, etc). The forward surrogate model published in [6] uses a database of 16,384 simulations sampled over a set of nine 0-D input parameters sampled with a Latin hypercube algorithm [7] using the πScope [8] framework. Each simulation requires about ten minutes of wall-clock time to complete, with the entire database requiring several weeks on the MIT Engaging cluster.

ML tools using multi-layer perceptron (MLP), random forest regression (RFR), and Gaussian process regression (GPR) techniques can predict the results of GENRAY/CQL3D with high accuracy (mean squared error « 1) and high speed (inference time ~ 1 ms). Although the ML surrogate models accurately predict the results of GENRAY/CQL3D for a given set of inputs, the ML surrogate models are only as good as the simulations in the training database. The simulations in the initial study do not include radial diffusion of the fast electrons in CQL3D, however Garofalo *et al* show that radial diffusion is necessary to accurately reproduce the experimental current density profiles in EAST [9].

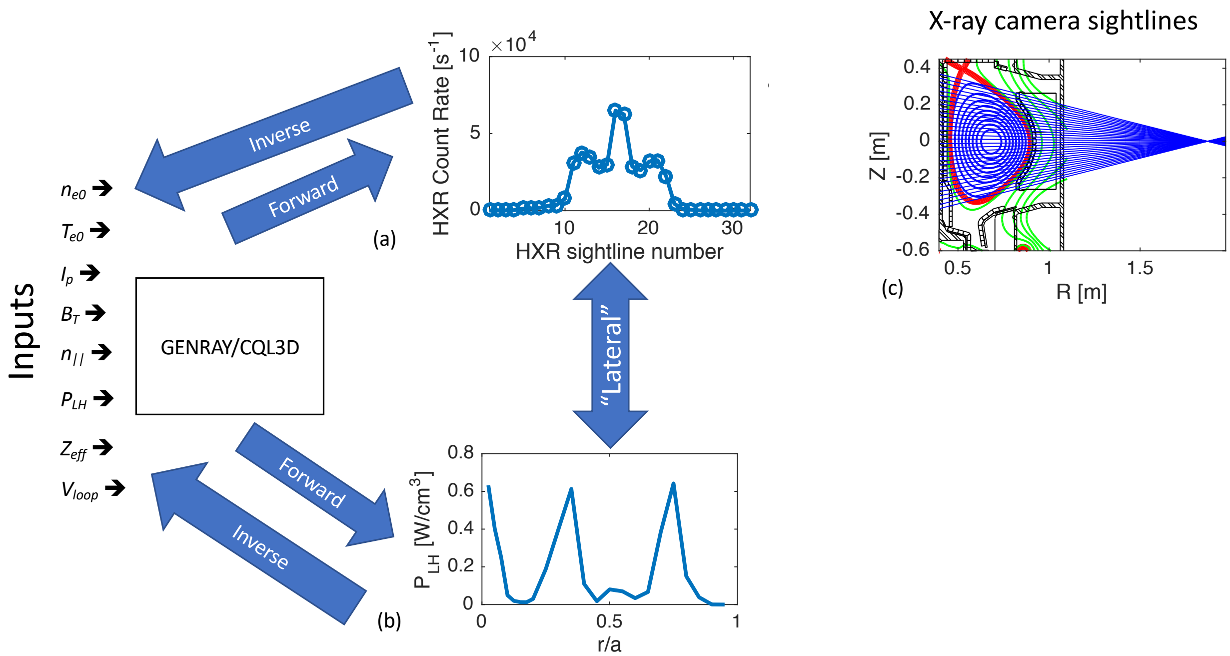

FIGURE 1. Schematic illustration of the forward, inverse, and "lateral" problems. (a) Example hard x-ray profile calculated by CQL3D. (b) Corresponding power deposition profile calculated by CQL3D. (c) Hard x-ray camera sightlines for Alcator C-Mod.

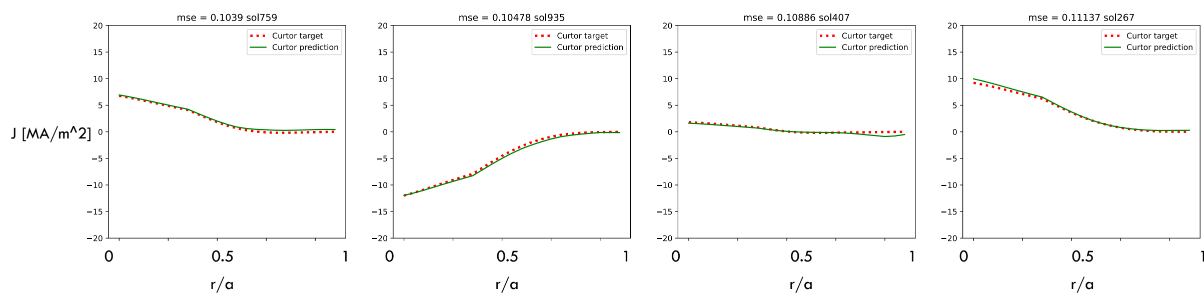

FIGURE 2. Four typical "average" cases comparing the ground truth GENRAY/CQL3D current profile (red dotted curve) with the GPR surrogate model (solid green curve).

RADIAL DIFFUSION

Including radial diffusion of the fast electrons increases the computation time for a single CQL3D simulation from a few minutes to 12 hours. The significant increase in computation time is a result of implicit versus explicit time steps used when radial diffusion is disabled or enabled, respectively. This represents both a challenge and an opportunity for the ML surrogate models. The challenge is that producing the training data requires 50$\times$ more computational effort, while the opportunity is that a ML surrogate model may produce even greater increases in speed relative to the "ground truth" model.

Furthermore, we hypothesize that the inherent smoothness of the profiles that result from calculations with radial diffusion of the fast electrons enabled should be easier for the ML model to predict, given that there will be fewer instances of radically differing profiles between nearby points in the 9-dimensional parameter space. To test this hypothesis, we created a new database of 1,000 GENRAY/CQL3D simulations with a radial diffusion coefficient, D_r, of 1.0 m^{2}s^{-1}. This much smaller database required three times the computational resources as the original 16,384 simulation database because of the radial diffusion calculation.

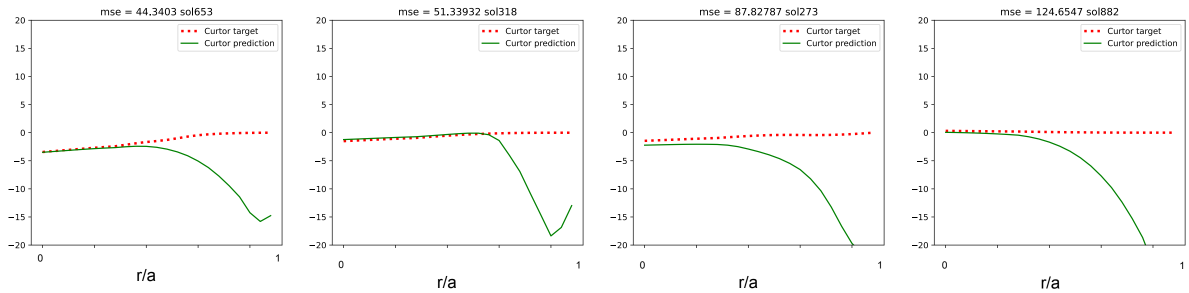

FIGURE 3. The four least accurate cases from the testing data set for the GPR surrogate model including radial diffusion.

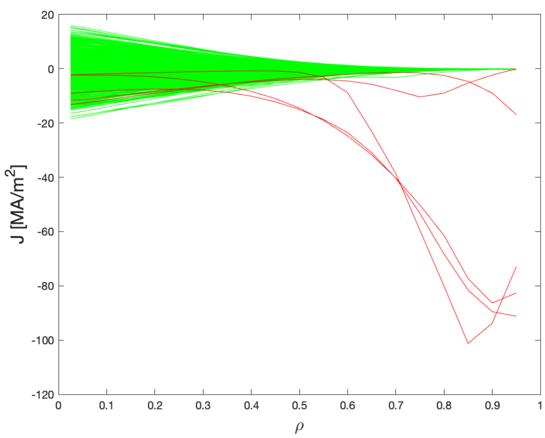

FIGURE 4. Current profiles for all 1,000 GENRAY/CQL3D simulations in the database with radial diffusion of fast electrons turned on. The five "outlier" profiles highlighted in red (representing only 0.05% of the database) are responsible for the large errors present in 15% of the GPR test cases as shown in Fig. 3

Figure 2 illustrates four average (as defined by mean squared error (MSE)) GPR current profiles with their corresponding ground truth GENRAY/CQL3D profiles. These current profiles are considerably smoother than those published in [6], but still retain identifiable structure in the profiles representing off-axis current drive. The MLP surrogate model provides a highly accurate prediction of the ground-truth CQL3D results for nearly every one of the 200 simulations held back in the testing dataset, even when simulations in the "slide-away" regime (where the force of the DC electric field exceeds the collisional drag on the fast electrons at $v = c/n_{||}$) are included in the training database. On the other hand, the GPR surrogate model introduces large errors near the edge of the plasma in about 15% of the 200 test cases when the slide-away regime is included in the training database. Previous work [6] justifies excluding the slide-away regime simulations from the database.

Figure 3 illustrates the four worst cases for the GPR surrogate model with radial diffusion when the slide-away regime is included in the database. The large errors near the edge of the plasma are driven by a very small number of simulations in the slide-away regime ($N = 5$) with large values of current for $\rho > 0.5$ (Fig. 4). Excluding these slide-away simulations from the database eliminates the spurious edge peak entirely (see Fig. 5. This illustrates the importance of carefully examining the data that feeds into the machine learning models.

LATERAL MODEL

We define the "lateral" model as a surrogate model that creates a mapping between correlated outputs of the underlying physical model. In this example, the correlated outputs are the line-integrated hard x-ray emission (Fig. 1a) and the RF power deposition profile (Fig. 1b) or current profile. These two outputs are related through the electron distribution

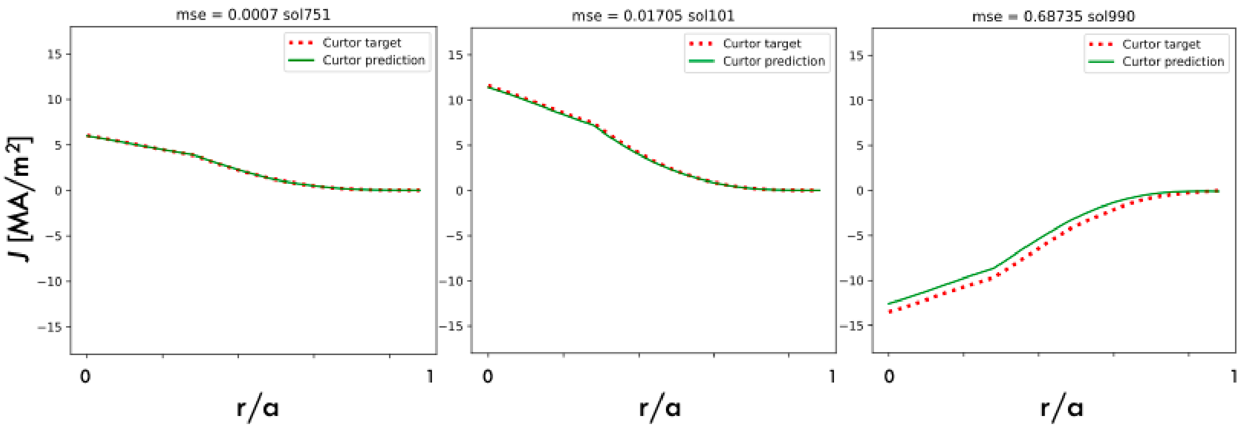

FIGURE 5. Representative best (left), average (center), and worst (right) cases for the GPR surrogate model including radial diffusion but with outliers filtered from the training database.

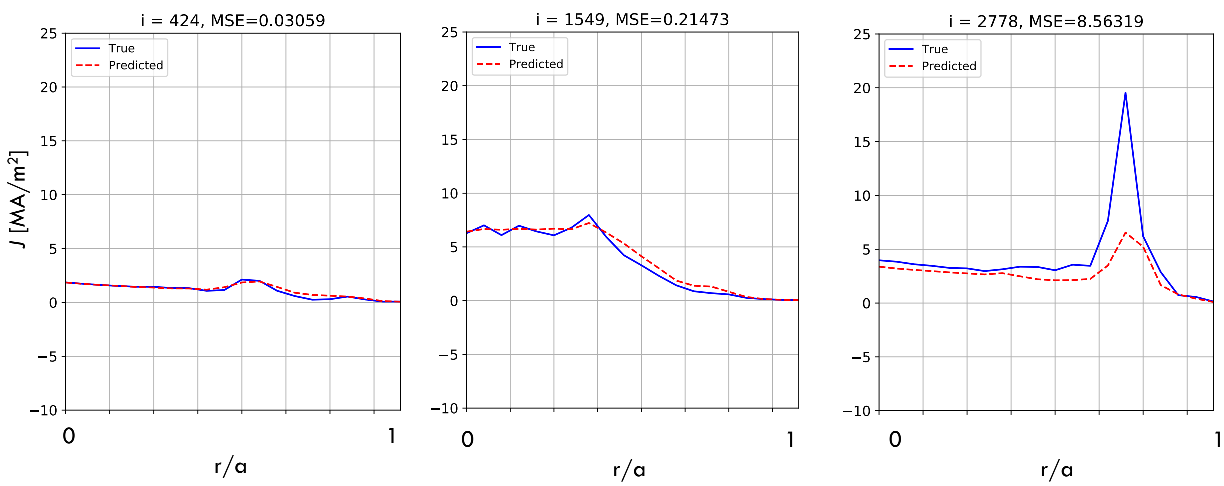

FIGURE 6. Examples of the best (left), average (center), and worst (right) predictions of the random forest regression (RFR) surrogate lateral model mapping from the hard x-rays $+n_{e0}+T_{e0}+V_{loop}$ to current density profile.

function, but a quantitative calculation relating one to the other is infeasible due to the complicated differential cross sections for fast electron bremsstrahlung with respect to electron energy, photon energy, and geometry. Still, the hard x-ray emission is well correlated enough with the quantities of interest (power deposition and current density) to make qualitative inferences; for example a broader hard x-ray profile indicates a broader power deposition profile.

Figure 6 shows typical best, average, and worst predictions of the current density profile for a random forest regression (RFR) based lateral model using line-integrated hard x-ray in combination with central electron density, temperature, and loop voltage as inputs to the lateral model.

In all three cases, the model correctly identifies the location of the off-axis current peak. The best and average cases provide excellent quantitative agreement between the ground truth and surrogate lateral model prediction. In the worst case, the magnitude of the off-axis peak is too low by a factor of 3 however the shape of the profile is remarkably similar to the ground truth CQL3D current profile.

Figure 7 contains the results from a similar RFR based lateral model using only the hard x-rays and loop voltage as inputs. The best and average results are very similar to the more complete surrogate model in Figure 6, however the difference between the ground truth and the surrogate model in the worst case is significantly larger across the entire profile. This is due to the fact that without including information on the plasma density and temperature, the RFR

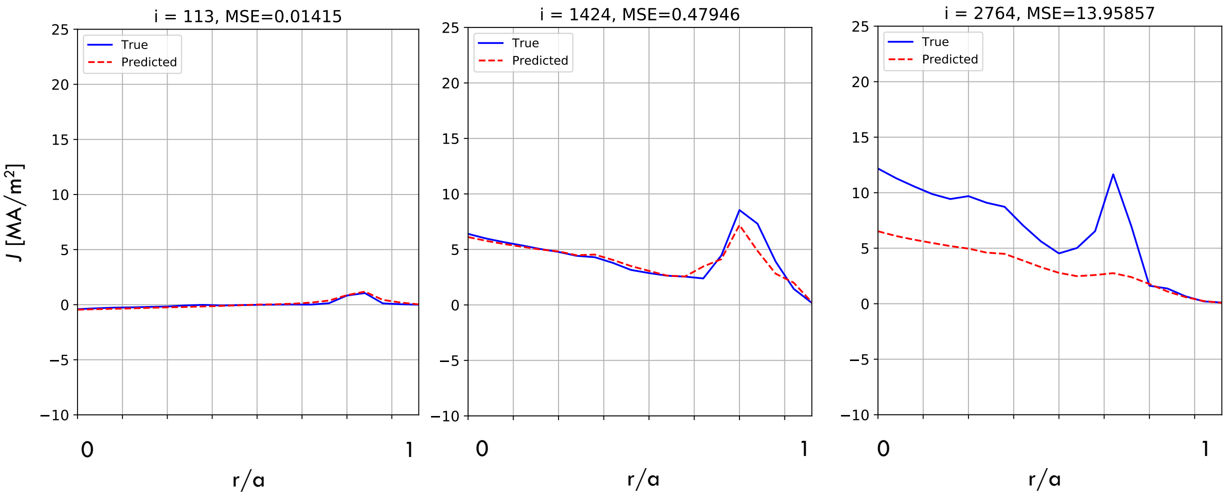

FIGURE 7. Examples of the best (left), average (center), and worst (right) predictions of the random forest regression (RFR) surrogate lateral model mapping from the hard x-rays $+V_{loop}$ to current density profile.

lateral model cannot accurately predict the Ohmic current profile. When the loop voltage (and the Ohmic current) is small this source of error disappears.

The lateral model is particularly interesting for experimental application because the hard x-ray profile is a straightforward measurement on tokamaks, while extracting the current density profile requires a very difficult measurement of the internal magnetic field profile (either by motional Stark effect or Faraday rotation polarimetry) combined with an equilibrium reconstruction constrained with the internal magnetic field data. Combined with the very fast inference time ($\sim$ 1 ms) of the RFR surrogate model, it is possible to have a real-time inference of the current profile based solely on a small number of experimental parameters. In the small loop voltage regime, which is common for current drive experiments, it is possible to infer the current profile from only the x-ray measurements as in Figure 7.

CONCLUSION AND FUTURE WORK

Machine learning based surrogate models can accurately replicate complex RF simulation tools such as GENRAY/CQL3D. Including the effects of radial diffusion for fast electrons in CQL3D dramatically increases the simulation run time for CQL3D, thus further increasing the speed gains of the ML-based surrogate model relative to the underlying model. The training databases used with radial diffusion of fast electrons can be smaller than those without radial diffusion due to the increased smoothness of the results with radial diffusion. Both the MLP and GPR based surrogate models generate accurate predictions of the power and current profiles when the training database excludes a small number of "outlier" simulations. Finally, an ML-based lateral model can predict current profiles based on the line-integrated hard x-ray profile combined with a small number of plasma parameters ($n_{e0}+T_{e0}+V_{loop}$).

Future work will focus on improving the GPR surrogate model with radial diffusion. The GPR model is particularly sensitive to "outlier" data points which can dramatically swing the predictions away from the ground truth in certain regions of parameter space. This behavior can be mitigated through introducing uncertainty in the data used in the training process of the GPR model, however quantifying the uncertainty in a deterministic simulation is not straightforward. A specific class of GPR models, the Student-t model, is known to be less sensitive to outliers [10]. We will investigate the use of Student-t regression models for comparison with GPR. We will also apply the ML-based surrogate modeling workflow to more advanced "ground truth" models including the effects of scattering from density fluctuations in the plasma edge [11, 12].

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Science, Office of Fusion Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231, through the grant "Accelerating Radio Frequency Modeling Using Machine Learning". This research used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility located at Lawrence Berkeley National Laboratory, operated under Contract No. DE-AC02-05CH11231. This research used the resources of Princeton Plasma Physics Laboratory operated under Contract No. DE-AC02-09CH11466. The simulations presented in this paper were performed on the MIT-PSFC partition of the Engaging cluster at the MGHPCC facility (www.mghpcc.org) which was funded by DoE grant number DE-FG02-91-ER54109.

REFERENCES

1. J. Galambos, L. Perkins, S. Haney, and J. Mandrekas, "Commercial tokamak reactor potential with advanced tokamak operation," Nuclear Fusion **35**, 551 (1995).
2. F. Najmabadi, A. Abdou, L. Bromberg, T. Brown, V. Chan, M. Chu, F. Dahlgren, L. El-Guebaly, P. Heitzenroeder, D. Henderson, H. S. John, C. Kessel, L. Lao, G. Longhurst, S. Malang, T. Mau, B. Merrill, R. Miller, E. Mogahed, R. Moore, T. Petrie, D. Petti, P. Politzer, A. Raffray, D. Steiner, I. Sviatoslavsky, P. Synder, G. Syaebler, A. Turnbull, M. Tillack, L. Waganer, X. Wang, P. West, and P. Wilson, "The ARIES-AT advanced tokamak, advanced technology fusion power plant," Fusion Engineering and Design **80**, 3 – 23 (2006), ARIES - AT Special Issue.
3. T. C. Luce, "Realizing steady-state tokamak operation for fusion energy," Physics of Plasmas (1994-present) **18**, 030501 (2011).
4. A. P. Smirnov and R. Harvey, "A general ray tracing code GENRAY," Bull. Am. Phys. Soc. **40**, 1837 (1995).
5. R. W. Harvey and M. McCoy, "The CQL3D Fokker-Planck Code," Proceedings of the IAEA Technical Committee Meeting on Simulation and Modeling of Thermonuclear Plasmas , 489–526 (1992).
6. G. M. Wallace, Z. Bai, R. Sadre, T. Perciano, N. Bertelli, S. Shiraiwa, E. W. Bethel, and J. C. Wright, "Towards fast and accurate predictions of radio frequency power deposition and current profile via data-driven modelling: applications to lower hybrid current drive," Journal of Plasma Physics **88**, 895880401 (2022).
7. M. D. McKay, W. Conover, and D. E. Whiteman, "Report on the application of statistical techniques to the analysis of computer codes," Tech. Rep. (Los Alamos Scientific Lab., N. Mex.(USA), 1976).
8. S. Shiraiwa, T. Fredian, J. Hillairet, and J. Stillerman, "πscope: Python based scientific workbench with mdsplus data visualization tool," Fusion Engineering and Design **112**, 835 – 838 (2016).
9. A. Garofalo, X. Gong, J. Qian, J. Chen, G. Li, K. Li, M. Li, X. Zhai, P. Bonoli, D. Brower, L. Cao, L. Cui, S. Ding, W. Ding, W. Guo, C. Holcomb, J. Huang, A. Hyatt, M. Lanctot, L. Lao, H. Liu, B. Lyu, J. McClenaghan, Y. Peysson, Q. Ren, S. Shiraiwa, W. Solomon, Q. Zang, and B. Wan, "Development of high poloidal beta, steady-state scenario with ITER-like tungsten divertor on EAST," Nuclear Fusion **57**, 076037 (2017).
10. J. Vanhatalo, P. Jylänki, and A. Vehtari, "Gaussian process regression with student-t likelihood," Advances in neural information processing systems **22** (2009).
11. B. Biswas, S. Shiraiwa, S.-G. Baek, P. Bonoli, A. Ram, and A. E. White, "A hybrid full-wave markov chain approach to calculating radio-frequency wave scattering from scrape-off layer filaments," Journal of Plasma Physics **87** (2021).
12. B. Biswas, P. Bonoli, A. Ram, and A. White, "Spectral broadening from turbulence in multiscale lower hybrid current drive simulations," Nuclear Fusion **63**, 016029 (2022).