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Insights into Machine Learning Predictions of Time-of-Flight Benchmarks

Antonio Huerta and Michael E. Rising

MCNP User Symposium

August 26, 2026

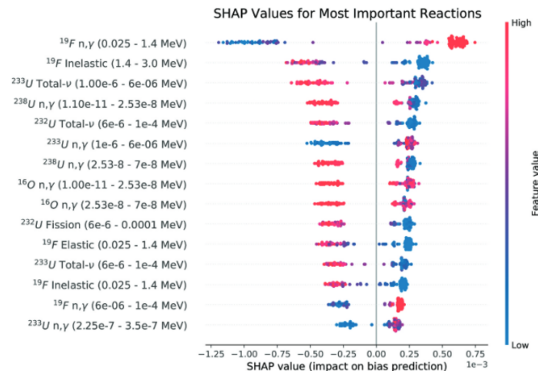
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Previous Work on ML Predictions of k -eigenvalue Benchmarks

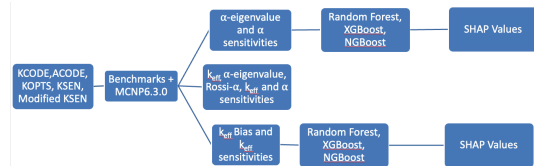
- Used the 1100+ criticality safety benchmarks from Whisper
- Random Forest trained on sensitivities/biases to predict k_{eff} bias
- Investigated the k_{eff} bias in ^{233}U aqueous solution benchmarks
- Inconsistencies in the ^{19}F inelastic scattering cross section data [1]



SHAP Beeswarm Plot for the Random Forest predictions of k_{eff}

Previous Work on ML Predictions of α -eigenvalue Benchmarks

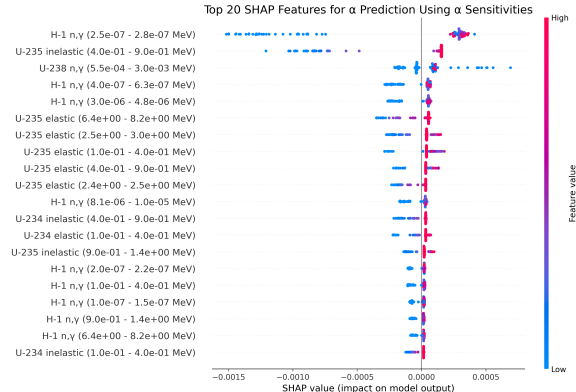
- Predict α -eigenvalues and k_{eff} bias using α -eigenvalue sensitivities
- Use SHAP values to explain top features
- Evaluate the significance of using α sensitivities to identify nuclear data impactful to α predictions, compared with k_{eff} sensitivities [2]



Method Map

SHAP α Sensitivity Results

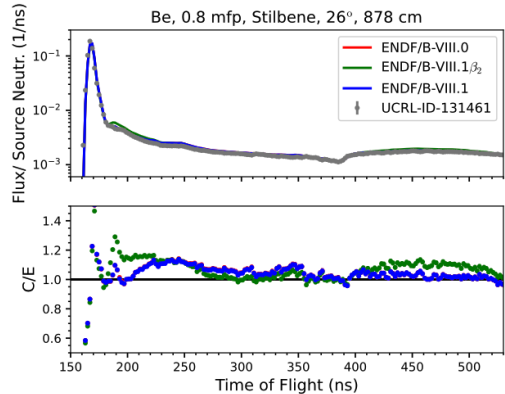
- Contribution of energy-resolved α -eigenvalue sensitivities to the Random Forest predictions across all benchmarks
- The reason why other features are not dominating is because they likely do not exhibit patterns within the sensitivity coefficients that drive the α predictions. [3]



SHAP Beeswarm Plot for the Random Forest predictions of α -eigenvalues

Lawrence Livermore National Laboratory Pulsed Sphere (LPS) program

- Spheres of many different, but distinct materials were irradiated one at a time by a D+T neutron source right in the center of the spheres
- Different neutron detectors (e.g., Pilot-B, NE-213, Stilbene) as a function of time of flight (TOF) at three different angles.
- Limitations in documentation leading to sub-optimal models [6, 4]

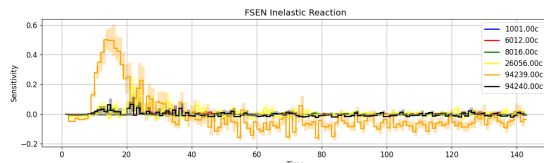
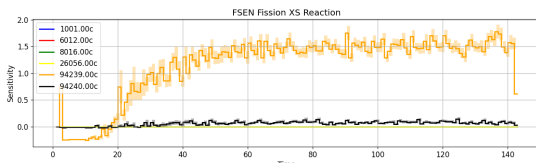


Simulated ^9Be LPS spectra are compared to experimental data

FSEN Sensitivity

- Time-dependent sensitivities are computed using a new fixed-source sensitivity tally in the MCNP[®] code
- New fixed-source sensitivity capability (FSEN option) is similar to the existing k-eigenvalue (KSEN option) method
- Adjoint weighted technique which differs from brute force calculations (FRENDY/SANDY codes) and is similar to the differential operator method (PERT card) [5]

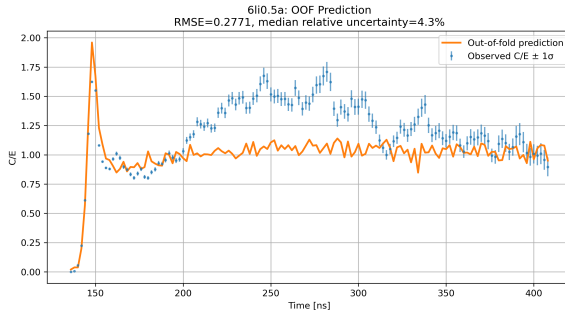
Example ^{239}Pu 0.7 MFP LPS Sensitivity Profiles



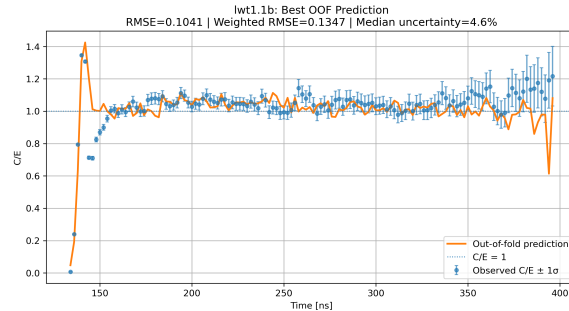
Machine Learning Models

- Different MLs will be used (Random Forest, HistGradientBoostingRegressor, XGBoost, CatBoost and more)
- Different Inputs
 - Experiment name + Physical features
 - Sensitivity data
 - Experiment name + Sensitivity data
- Target C/E

Current Predictive Power

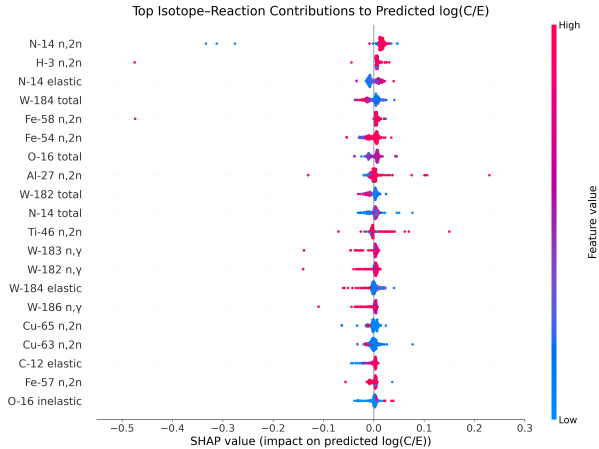


Out of Fold Time of Flight Prediction Plot
for 6Li0.5a experiment



Out of Fold Time of Flight Prediction Plot
for lwt1.1b experiment

SHAP Plot



SHAP Beeswarm Plot for the CatBoost predictions of C/E

Future and Ongoing Work

- Explore ML models for better metrics
- Use SHAP analysis to explain the features (i.e., sensitivities) of our models that drive the predictions
- Lack of data leads to poor results – new and modern pulsed-sphere-like experiments would be beneficial for this kind of analysis

References

- [1] Pavel A Grechanuk, Michael E Rising, and Todd S Palmer. “Application of Machine Learning Algorithms to Identify Problematic Nuclear Data”. In: *Nuclear Science and Engineering* 195.12 (2021), pp. 1265–1278. DOI: 10.1080/00295639.2021.1935102.
- [2] Antonio Huerta. “Quantifying the Impact of Nuclear Data on Predictive Radiation Transport α -eigenvalue Calculations”. MA thesis. Department of Nuclear Science and Engineering: Oregon State University, 2025. URL: https://ir.library.oregonstate.edu/concern/graduate_thesis_or_dissertations/bv73c846c.
- [3] Antonio Huerta et al. “The Role of Nuclear Data Sensitivities in Prompt -eigenvalue Predictions of Delayed-Critical Benchmarks”. In: *Nuclear Science and Engineering* (2026). DOI: 10.1080/00295639.2026.2715893.
- [4] Denise Neudecker et al. “The Need for a New LLNL Pulsed Sphere Neutron Leakage Spectra Series”. In: *Fusion Science and Technology* 82 (2026), pp. 1143–1160. URL: <https://api.semanticscholar.org/CorpusID:286337215>.
- [5] Michael Evan Rising and Alexander Rich Clark. “Development of a New Fixed-source Sensitivity Tally Capability in the MCNP® Code [Slides]”. eng. In: Los Alamos National Lab. (LANL), Los Alamos, NM (United States). United States, 2022.
- [6] C Wong et al. *LIVERMORE PULSED SPHERE PROGRAM: PROGRAM SUMMARY THROUGH JULY 1971*. Tech. rep. California Univ., Livermore. Lawrence Livermore Lab., Jan. 1972. URL: <https://www.osti.gov/biblio/4658057>.