Gaussian Process Regression for the Evaluation of Energy-Dependent Fission Product Yields

Konstantinos Stergiou [1] Vaia Prassa [2] Charalampos Moustakidis [1]

[1]Department of Physics, AUTh, Greece [2]Department of Physics, UTh, Lamia, Greece

1. Introduction

Accurate knowledge of Fission Product Yields (FPY) is fundamental for nuclear reactor physics and waste management. However, experimental data for neutron-induced fission are often sparse. This work explores the application of **Gaussian Process Regression (GPR)** to evaluate independent fission charge yields and investigate their energy dependence across actinide targets.

2. Data Acquisition & Methodology

The GPR framework was trained using a dual-model approach:

- **Model A (Baseline):** Trained on evaluated data extracted from the **JENDL-5** library via automated scraping.
- **Model C (Extended):** Augmented with synthetic datasets generated by the **GEF** code (from Thermal to 20 MeV) to fill gaps in incident energy distributions.

Kernel optimization via Akaike Information Criterion (AIC) selected a composite **Matérn + Rational Quadratic + White Noise** ARD kernel. This architecture effectively captures smooth physical trends, multi-scale variations, and aleatoric uncertainties:

$$k(x, x') = \sigma_f^2\Big(k_{\text{Matérn}}(x, x') + k_{\text{RQ}}(x, x')\Big) + \sigma_n^2 \delta_{x,x'}$$

3. Physical Feature Sensitivity (ARD)

Automatic Relevance Determination (ARD) extracts the inverse length-scale ($1/\ell$) of each feature, revealing its physical significance. The analysis confirms that Fragment Charge (Z) dominates the process, while Incident Energy (E_n) heavily influences the extended model.

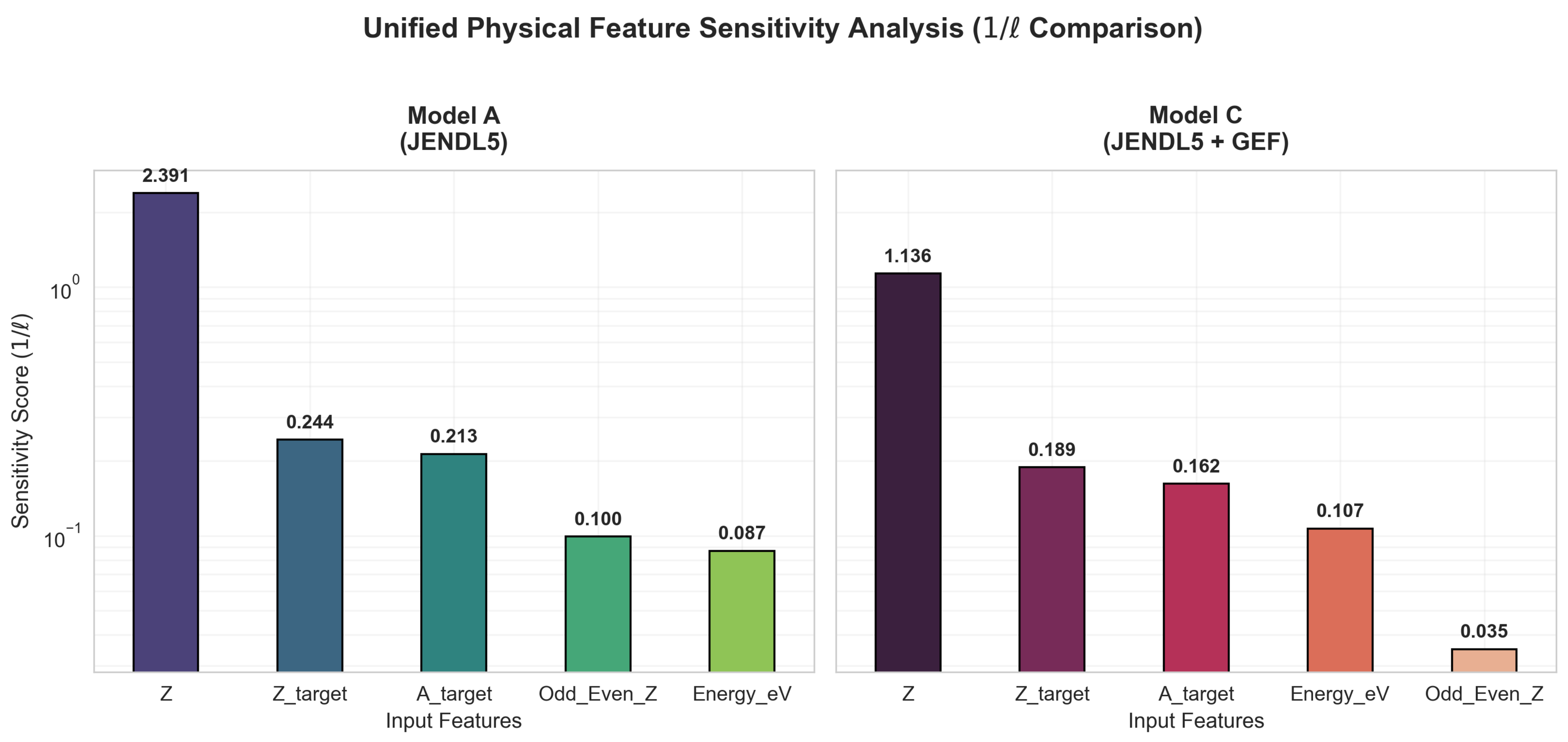

Figure 1. Feature sensitivity comparison between JENDL-5 and the Extended Hybrid Model.

4. Global Cognitive Interpretation (SHAP)

Shapley Additive Explanations (SHAP) decode the GPR's internal logic. The global interpretation illustrates how the model incorporates asymmetric structural distributions alongside energy-dependent phenomenological variations.

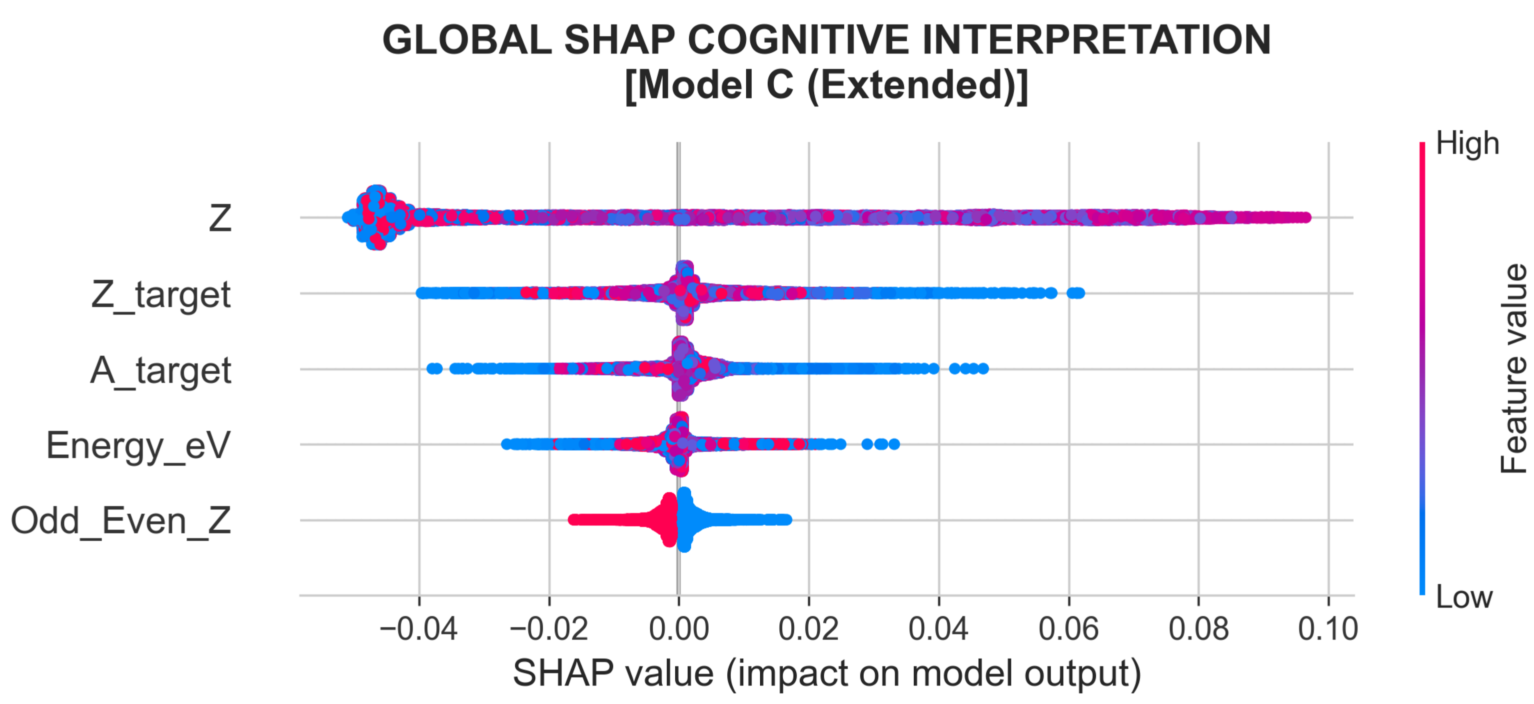

Figure 2. Global SHAP values for Model C (Extended Framework).

5. Physics Extraction: Fission Valley Filling

A key indicator of a successful fission model is its ability to replicate the *Peak-to-Valley (P/V) ratio* transition. As incident neutron energy increases, shell effects wash out, and symmetric fission modes activate. Model C perfectly maps this transition up to 20 MeV.

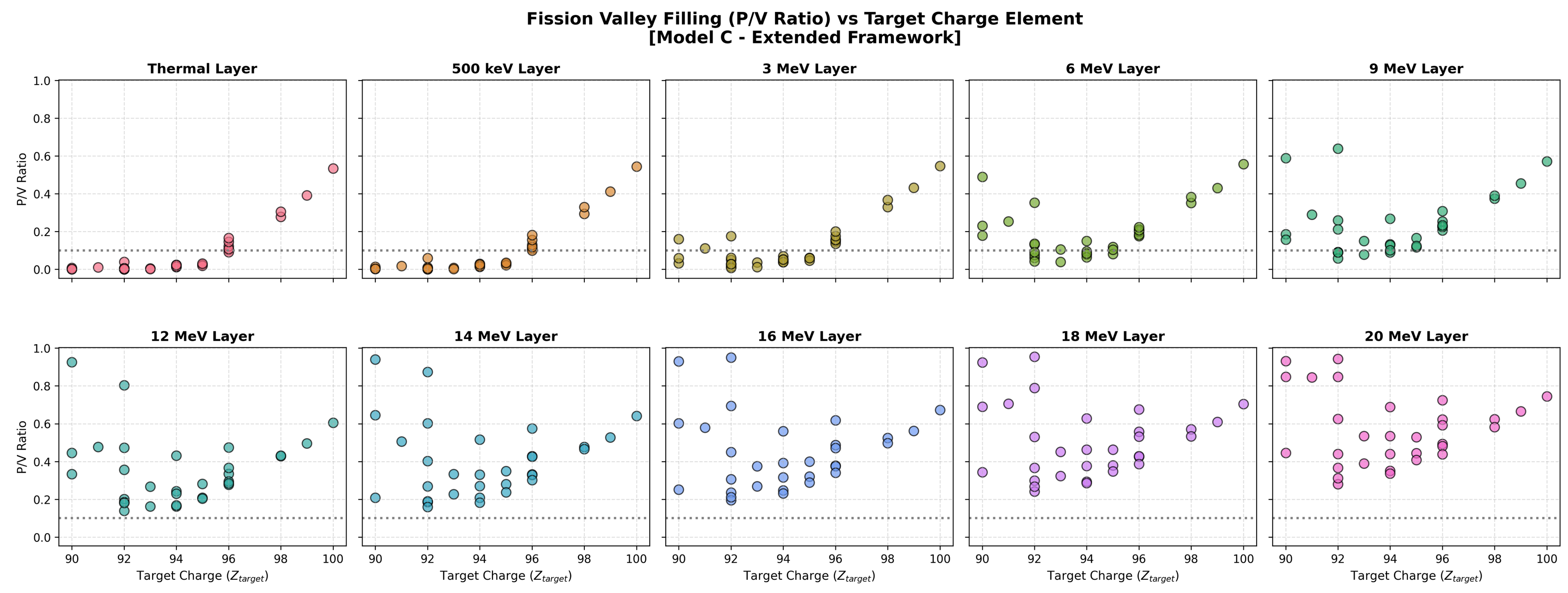

Figure 3. Evolution of the P/V ratio across energies, demonstrating the filling of the symmetry valley.

6. Blind Validation vs. EXFOR Experimental Data

To assess true predictive power, the GPR models were benchmarked against unseen experimental data from the **EXFOR** database. The Extended Model (Model C) demonstrates superior performance, yielding lower reduced chi-squared (χ^2_ν) values and accurately reconstructing the distributions even when experimental measurements are incomplete (e.g., partial peaks in ^{245}Cm).

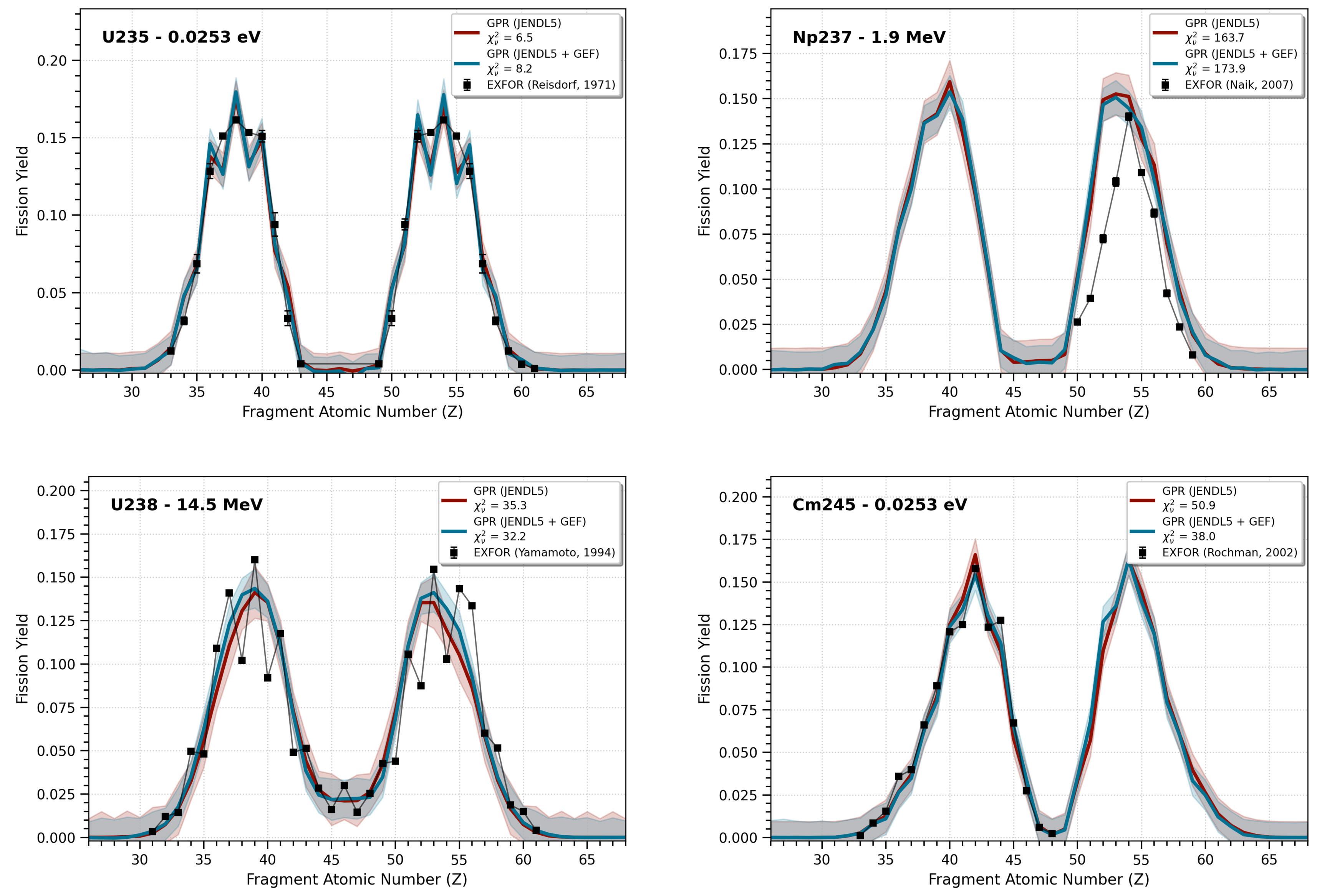

Figure 4: Comparative benchmarks showing GPR predictions vs. EXFOR data.

7. Conclusions

- **Physical Robustness:** The hybrid GPR approach successfully maps fundamental evaluated libraries (JENDL-5) and physical phenomenology simulated by GEF (Valley Filling, Odd-Even staggering).
- **Generalization:** The model acts as an automated, uncertainty-aware tool, successfully predicting distributions for systems with missing or partial data (e.g., ^{245}Cm).
- **Impact:** This framework offers a reliable alternative for generating nuclear data in regions where experimental setups are unfeasible, critical for fast-reactor designs.

8. Acknowledgements & References

The authors acknowledge the IAEA for the **EXFOR** experimental database and the Japan Atomic Energy Agency for the **JENDL-5** library. Special thanks to the developers of the **GEF** code for providing the underlying theoretical fission framework.

1 K.-H. Schmidt et al., *General Description of Fission Observables: GEF Model*, Nucl. Data Sheets 131, 107-221 (2016).

2 O. Iwamoto et al., *Japanese Evaluated Nuclear Data Library Version 5: JENDL-5*, J. Nucl. Sci. Technol. 60 (2023).

Email: stergiou.sci@gmail.com **GitHub:** github.com/StergiouKostas **LinkedIn:** linkedin.com/in/konstantinos-stergiou-sci