Update on LLNL cross section evaluation efforts

USNDP annual meeting 2025

Prepared by LLNL under Contract DE-AC52-07NA27344.

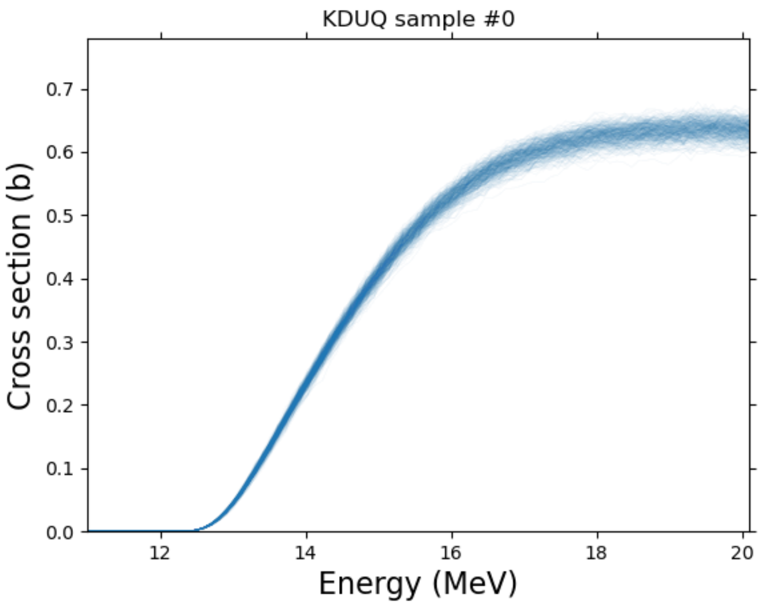
Nuclear Data and Theory Group

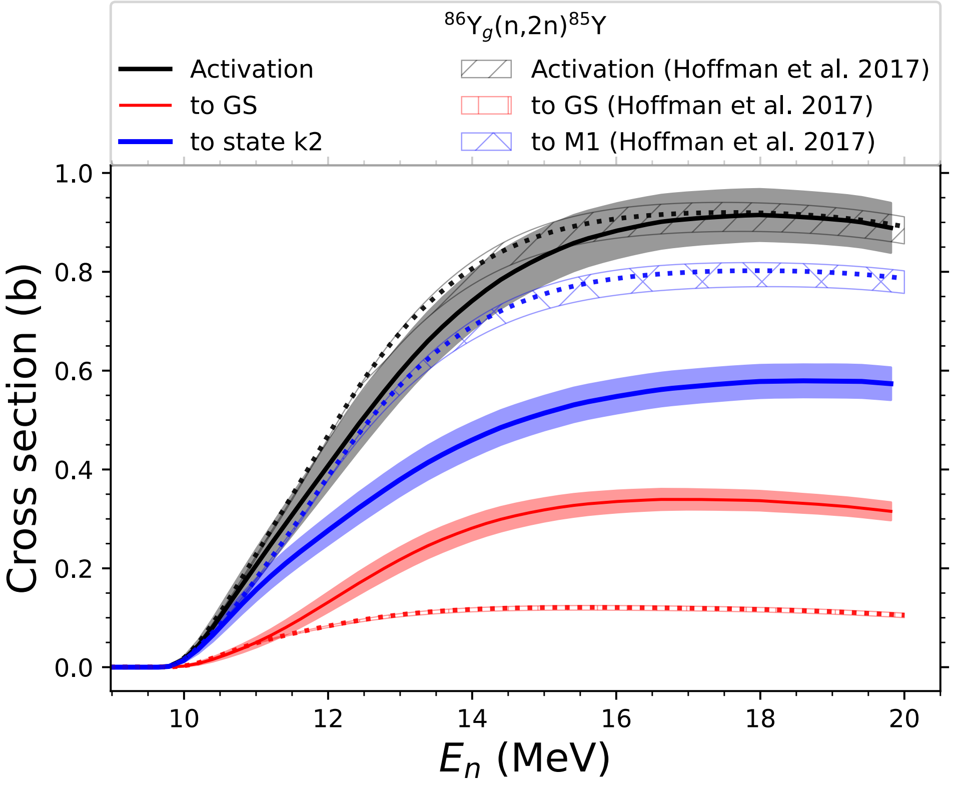
Outline

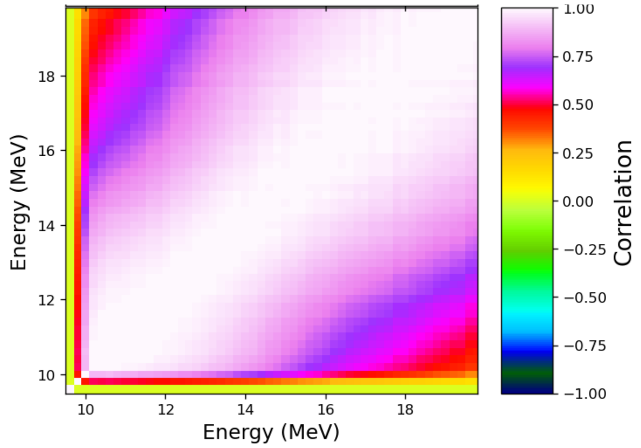
1. Activation cross sections with uncertainties and covariance
2. AI/ML efforts
3. Finalizing Pu239 evaluation

Activation cross sections with uncertainties and covariances

Forward-propagating parameter uncertainties





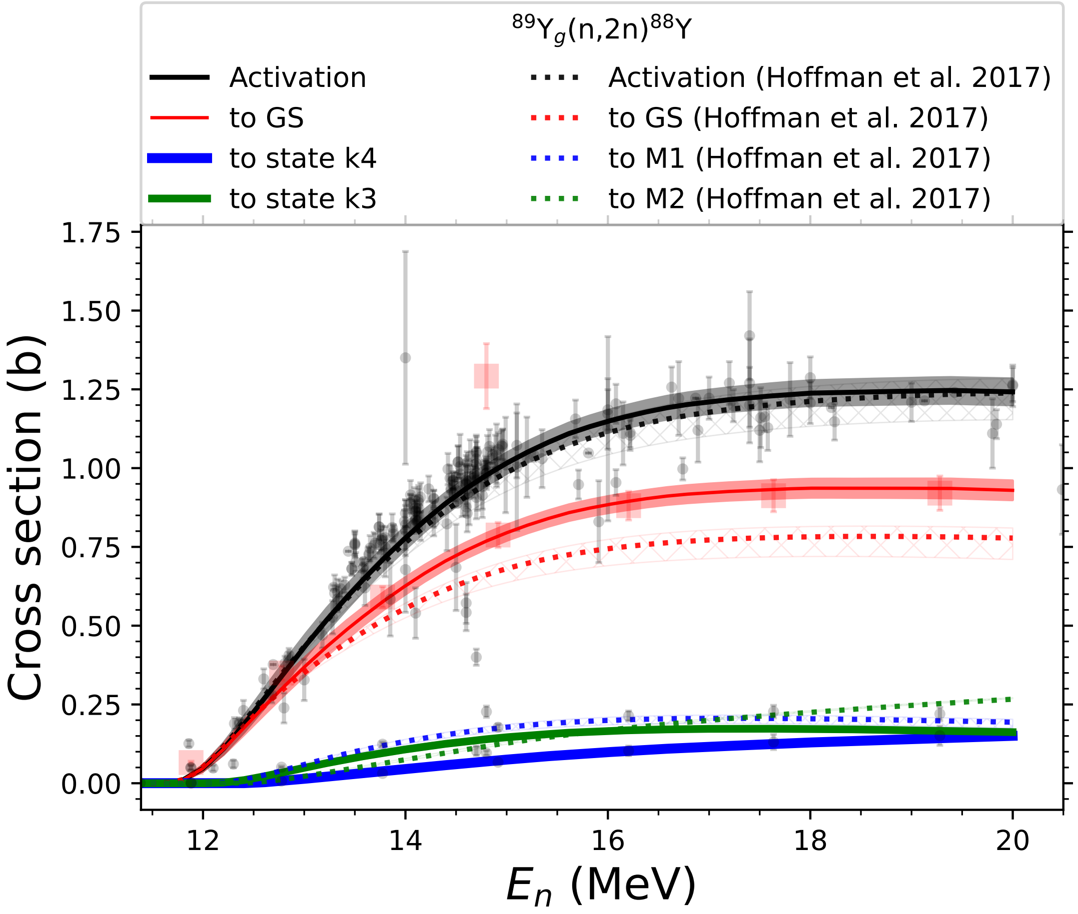


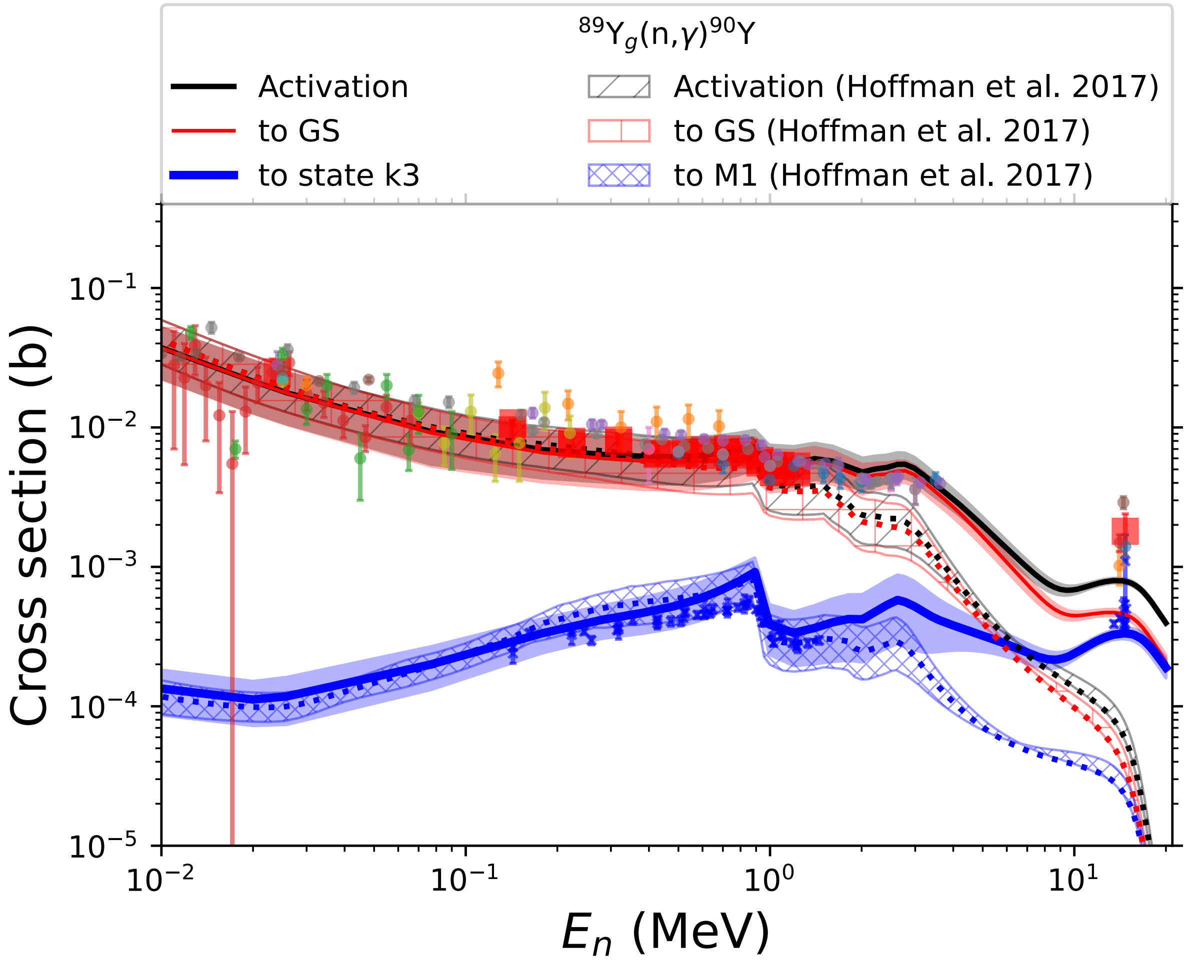
- Using uncertainty-quantified Koning-Delaroche OMP [Pruitt et al. 2023]
- Reaction model parameter systematics fit to data near stability
  - Uncertainties on $\langle\Gamma_\gamma\rangle_0$ and D_0,i.e. gamma strength function and level density
- GNDS files with neutron-induced cross sections for $^{85\text{-}91}$Y, $^{86\text{-}90}$Zr

Technical report is available: https://doi.org/10.2172/2997578

Validation by comparing to experimental data

No direct fit to the cross section data





- Validation for YAHFC reaction code
- Overall good performance with improvements over 2017 evaluation

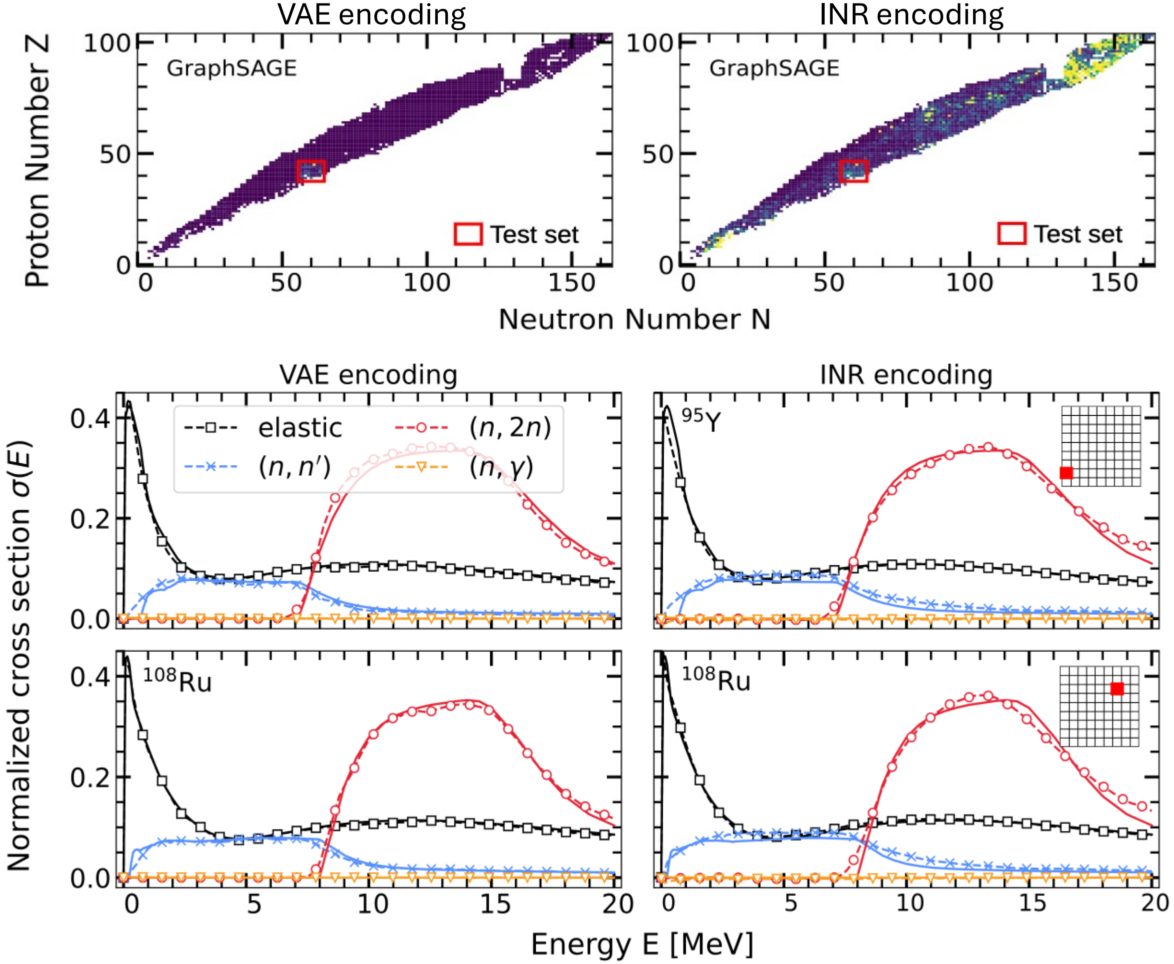
AI/ML

Graph neural networks can predict unknown cross sections with remarkable accuracy

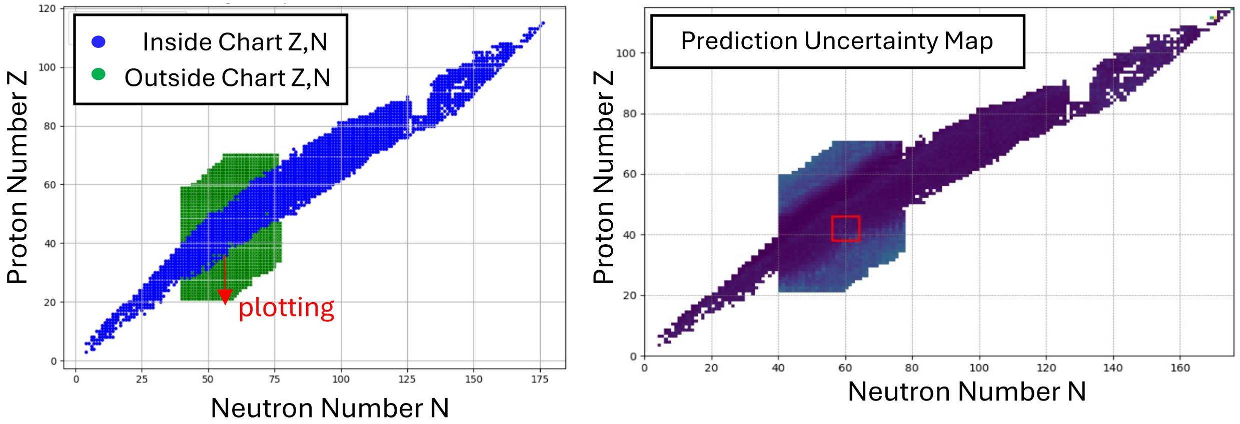
Hongjun Choi

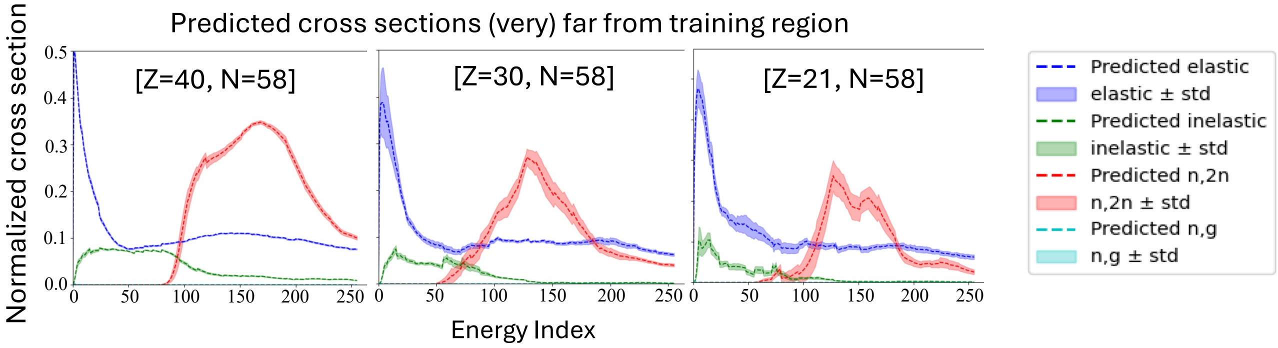
Sinjini Mitra

Shusen Liu



- Predicts extrapolated cross sections and estimates prediction uncertainty via Monte Carlo dropout.





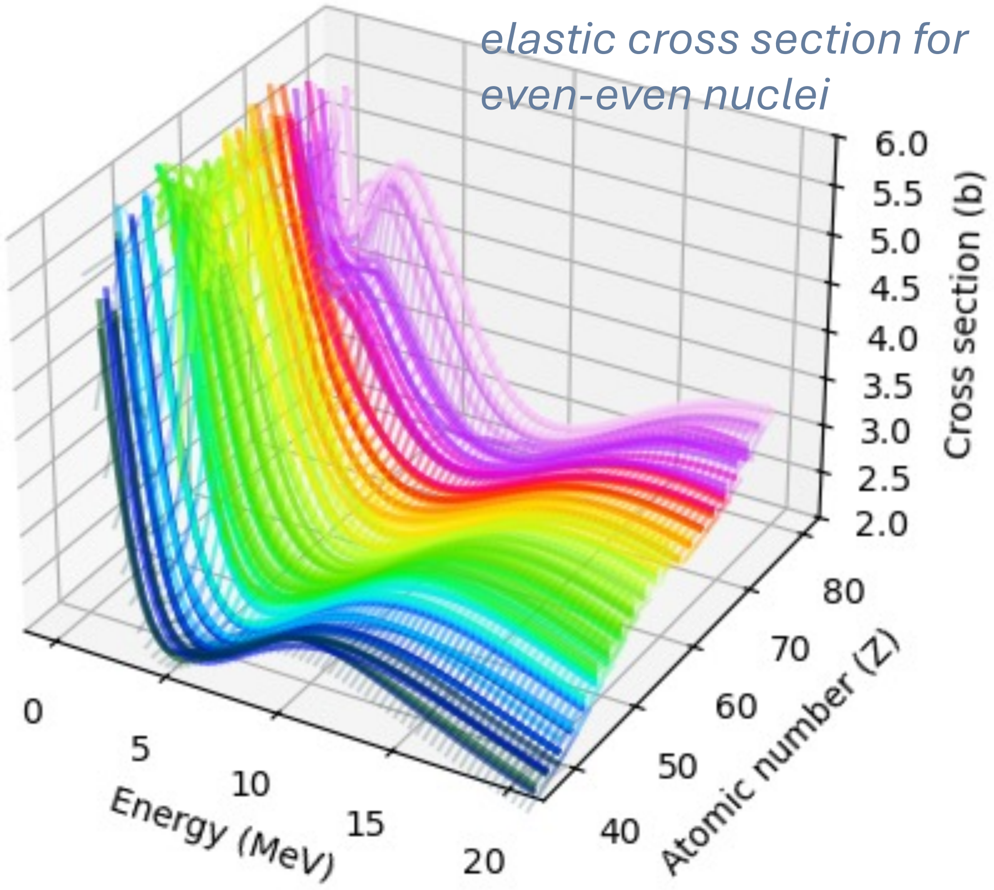
[Paper accepted in Phys. Rev. C 112, Issue 4, id.044601]

How to estimate uncertainties? How to propagate data or evaluated uncertainties?

Gaussian process model for cross sections

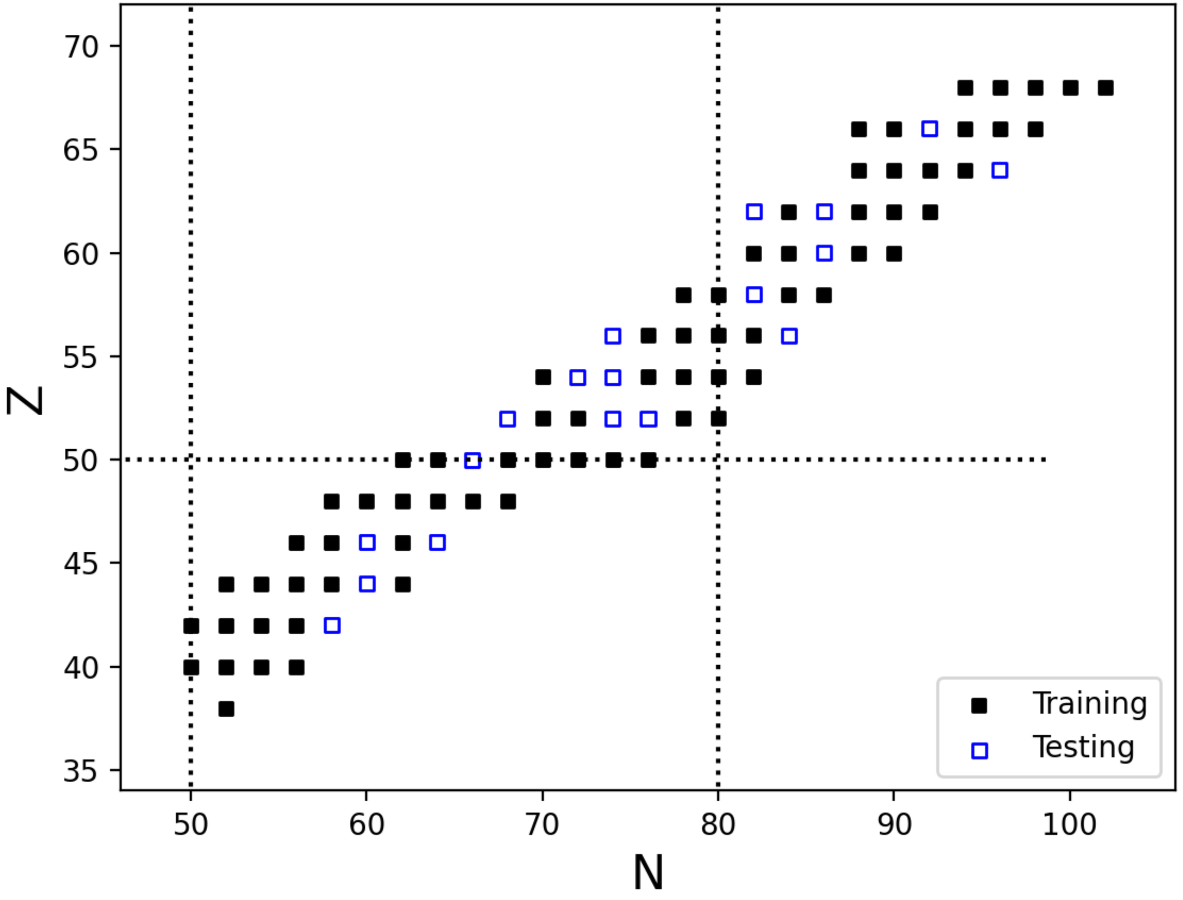
- The elastic scattering cross section is generally smooth and a "bulk property" of nuclei
- Most naïve approach:
  - Describe $\sigma(N, Z, E)$ as 3->1 Gaussian process regression
  - Focus on even-even nuclei to increase smoothness (for now)
  - For simplicity we use TENDL as baseline dataset

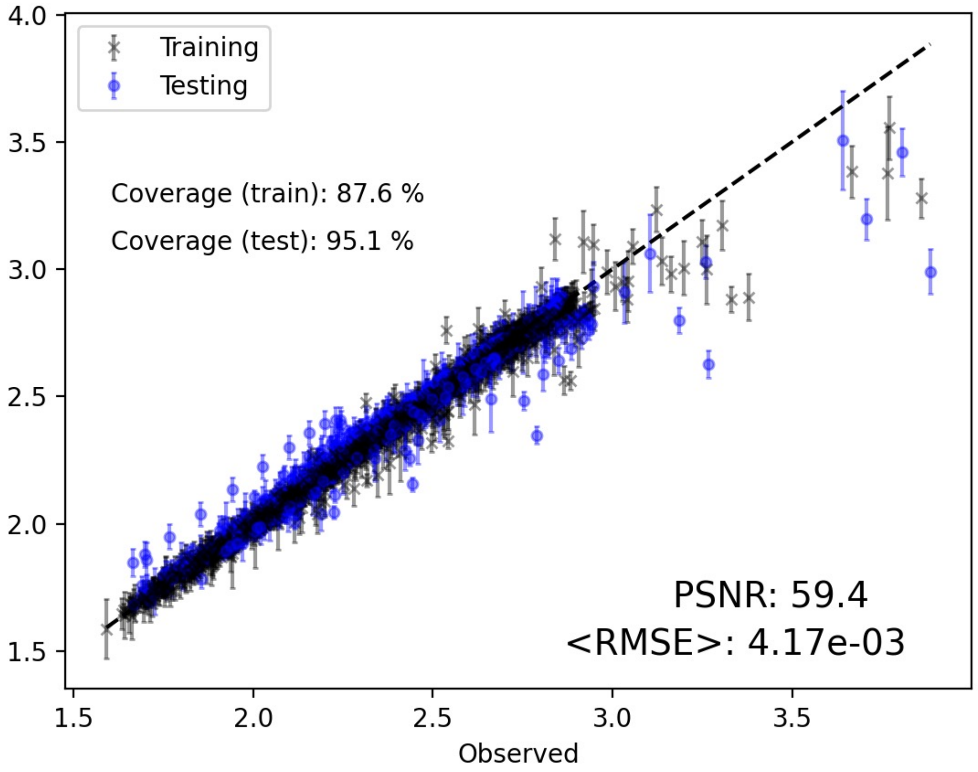
elastic cross section for even-even nuclei



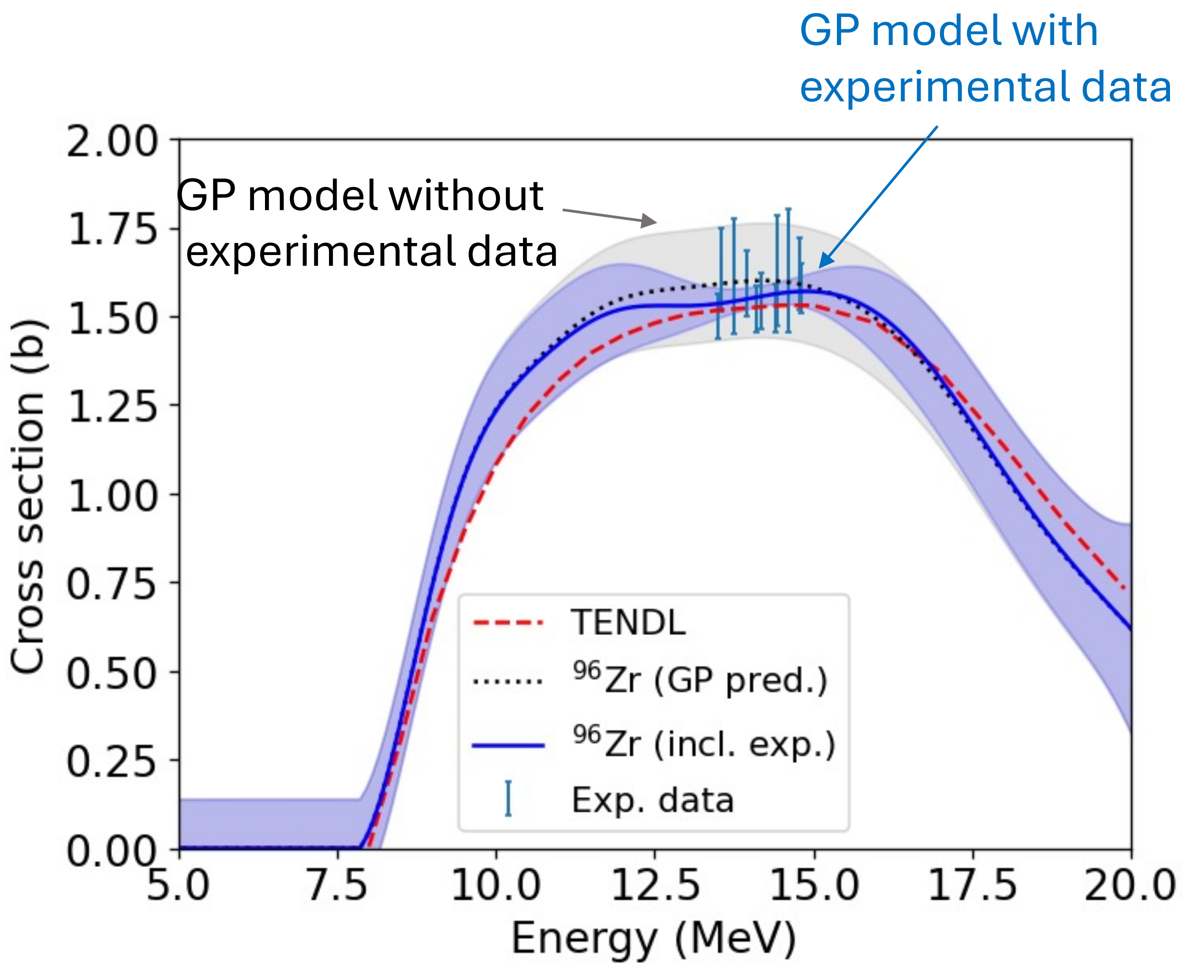
Elastic scattering cross section

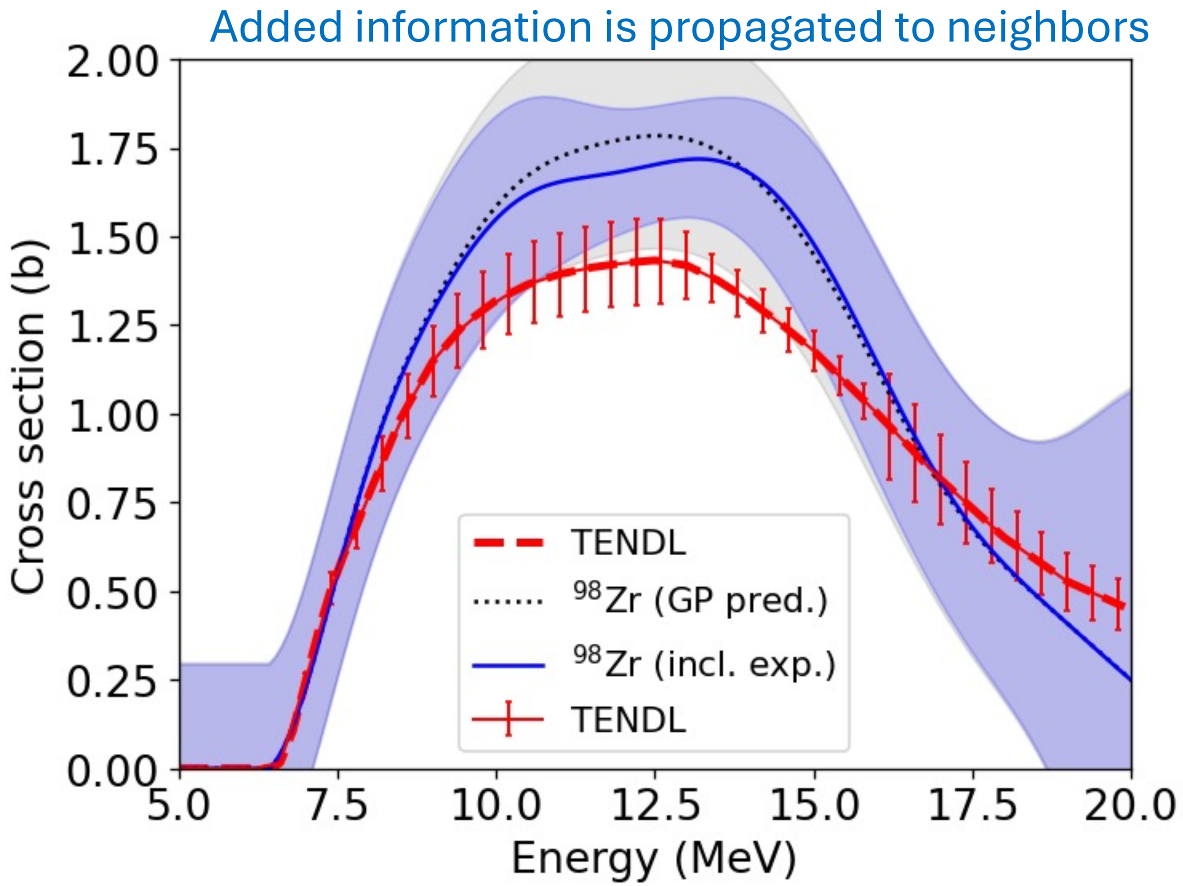
- Even-even nuclei only
- Random split between training and test cases
- Good performance on testing set
- Mostly interpolation





Combine with data



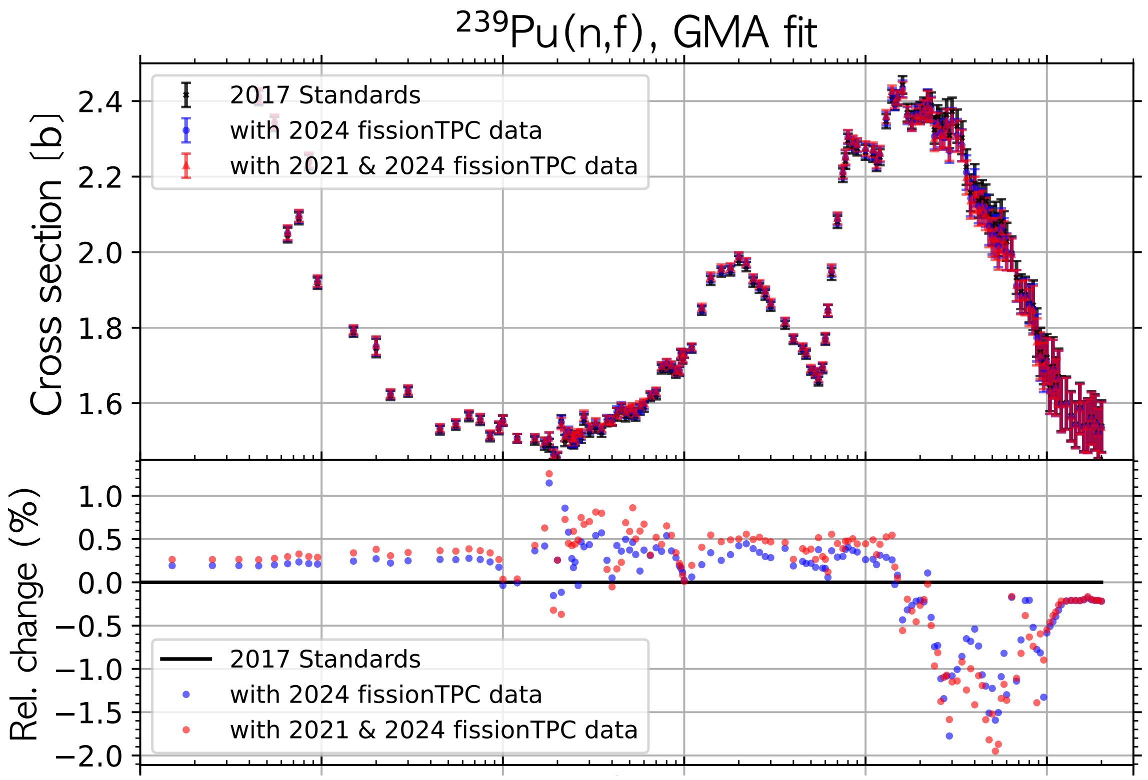


Adding new experimental data reduces the uncertainty of the prediction but still uses the knowledge of the model where no data is available

Finalizing ^{239}Pu evaluation

Summary of the LLNL n+^{239}Pu evaluation (so far)

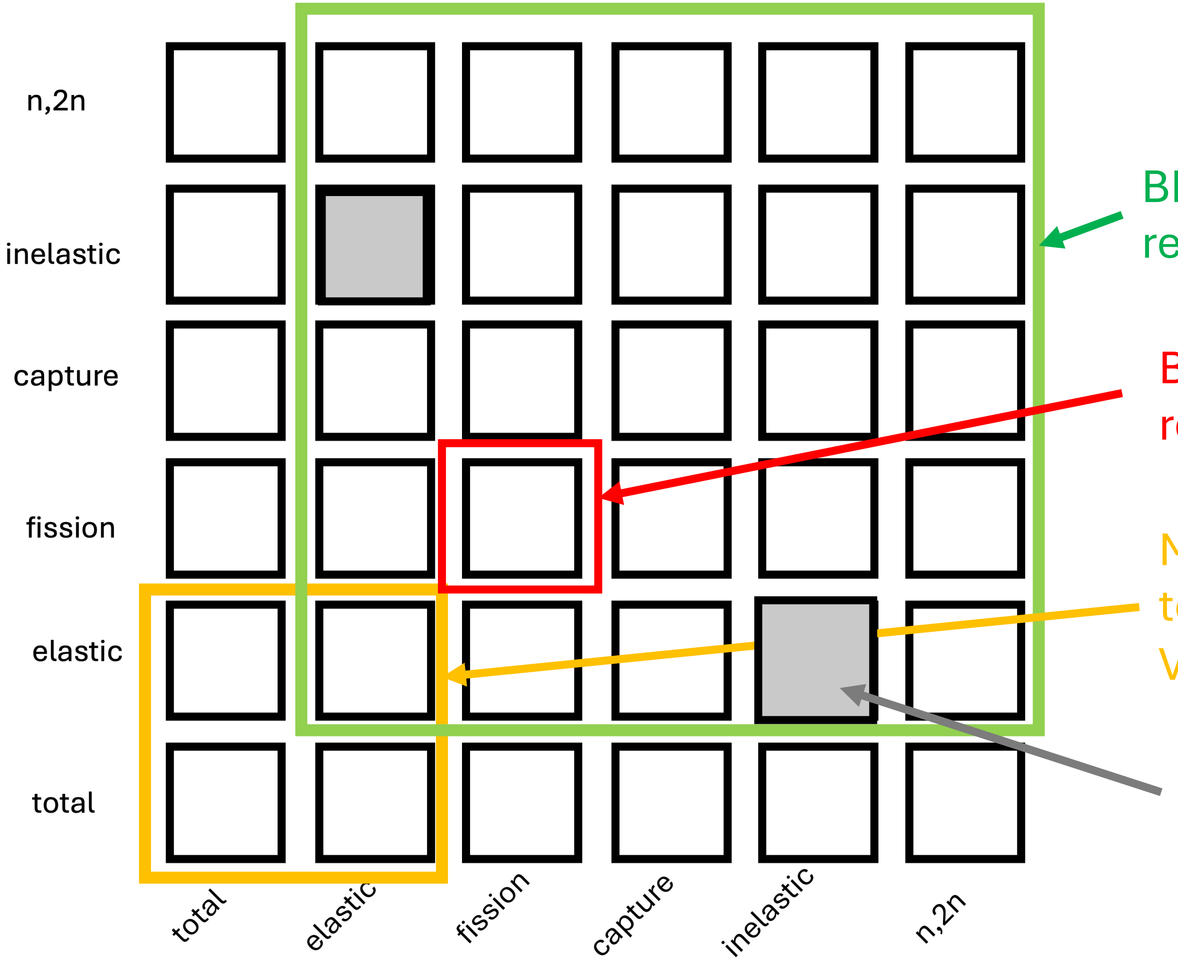
- Total cross section: Re-fit of OMP parameters to data using Soukhovitskiĩ (2016,2020) with FRESCO
- Fission: GMAP evaluation including fissionTPC datasets (generalized least squares fit across neutron standard cross sections)
- Other channels computed with LLNL's YAHFC reaction code with parameters optimized to (n,f) and (n,2n) data
- Cross sections below **30 keV** and fission product data are taken from ENDF/B VIII.1



[c.f. presentation at Nuclear Data Week 2024]

Up next: Add covariance data

Adding covariance data



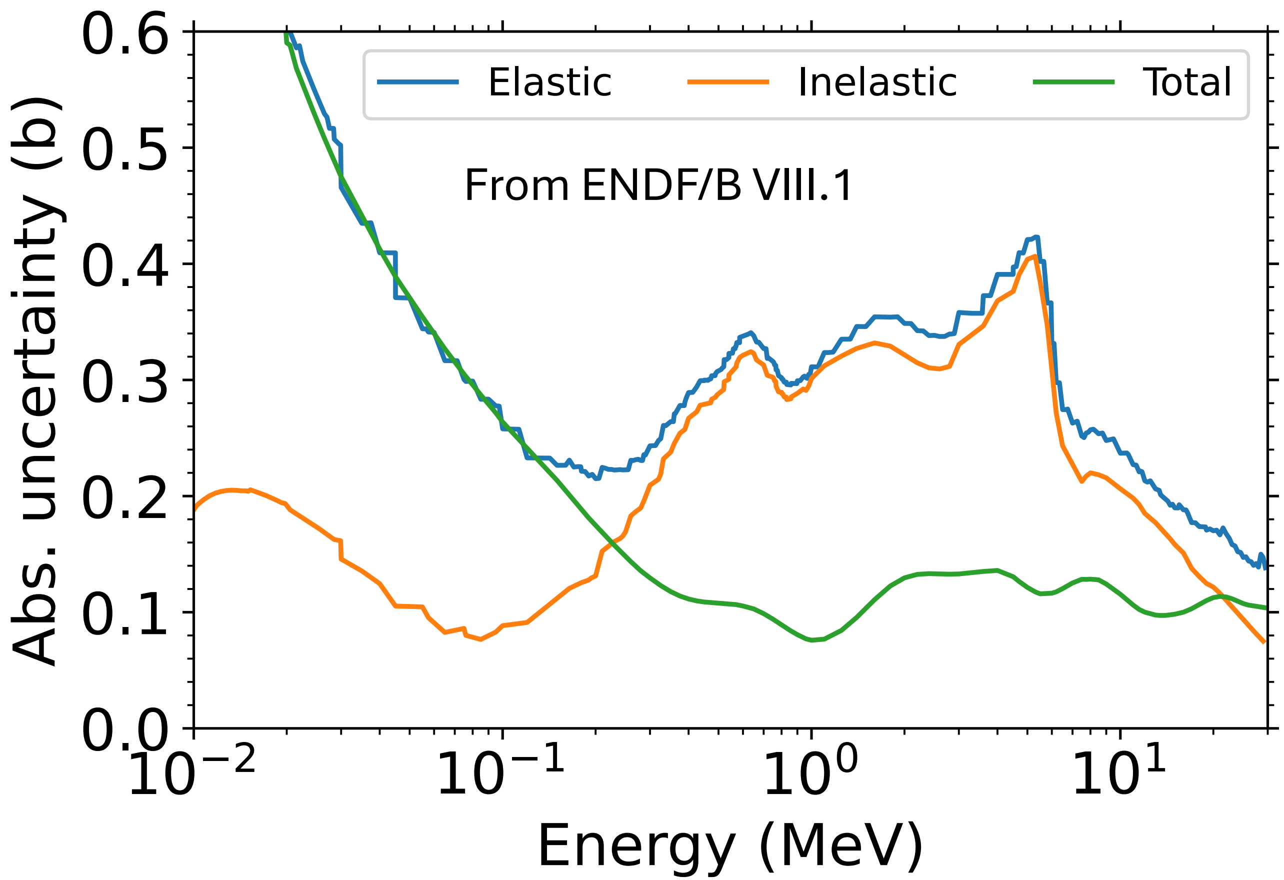
BFMC with YAHFC constrained by GMA results for fission and data for (n,2n)

BFMC with YAHFC constrained by GMA results for fission and data for (n,2n)

MCMC fit with FRESCO ; rescaled to match total and elastic uncertainty from ENDF/B VIII.1

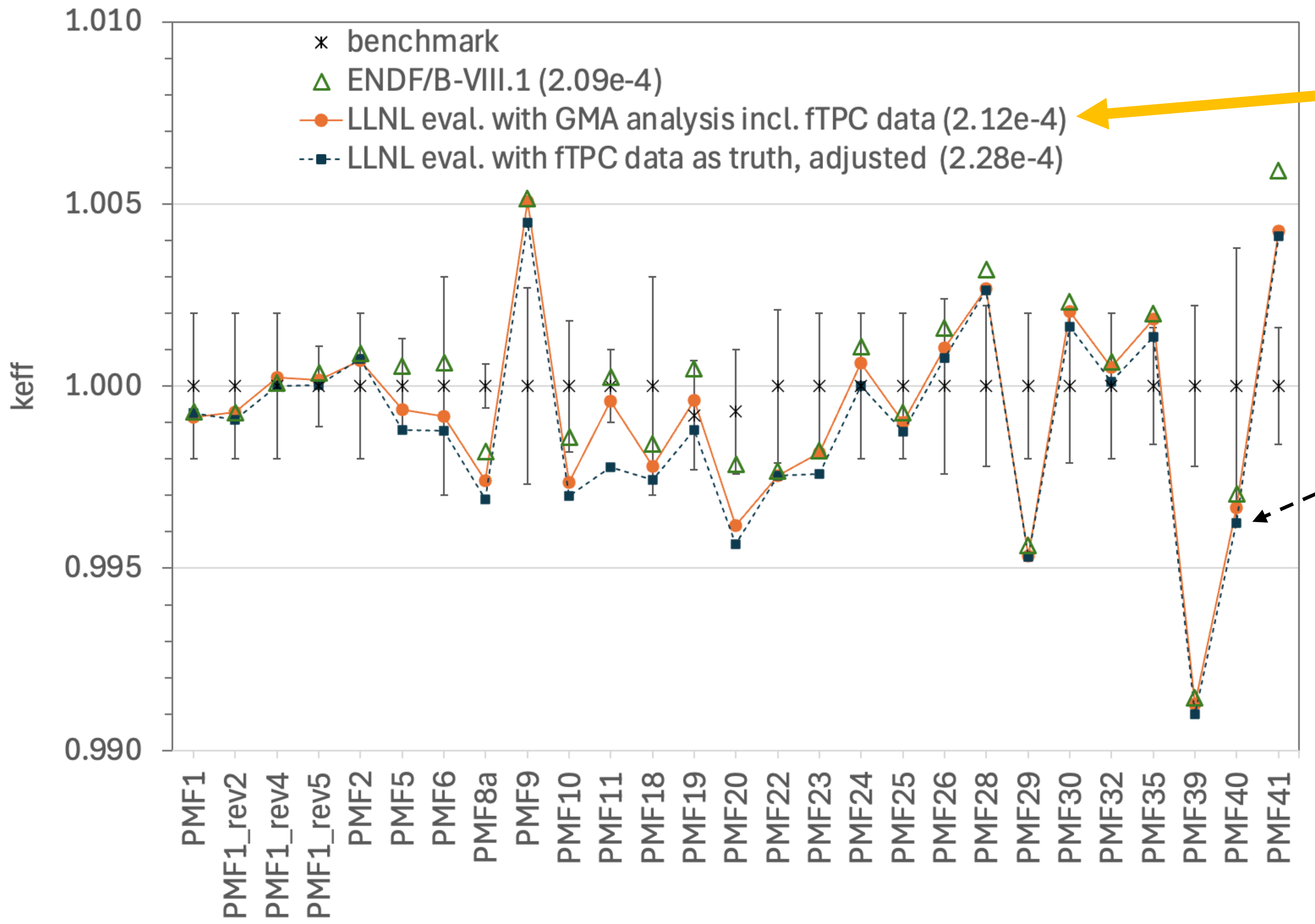
Cross-channel covariance Cov(inelastic,elastic) adjusted to ensure consistency

Covariances for ^{239}Pu



- Tight constraints on the total cross section enforce a strong correlation between the elastic scattering and inelastic cross sections between 300 keV and 20 MeV

Validation and Verification



- GMAP analysis of fissionTPC data: No adjustment needed
- Almost as good as ENDF/B VIII.1 across PMF benchmarks

- Taking the Pu239/U235 fission TPC data directly (no averaging with other measurements through GMA) **requires -1.4 % adjustment of $\bar{\nu}$** (which is outside of the uncertainties)

Conclusions

- Workflow and code development for large-scale HF reaction calculation, including uncertainty propagation
- AI/ML approaches for cross sections:
  - Neural networks
  - Gaussian processes
- Actinide evaluations:
  - n+Pu239 covariances with backward-forward Monte-Carlo

    To do: Include OMP parameters in MC sampling to capture correlations between reaction channels and elastic scattering
  - Adjustment of n+^{239}Pu to agree with fissionTPC Pu9/U5 data with more than $\bar{\nu}$?

Backup

Importance-sampling Backward-forward Monte-Carlo (iBFMC)

Development by O.C. Gorton

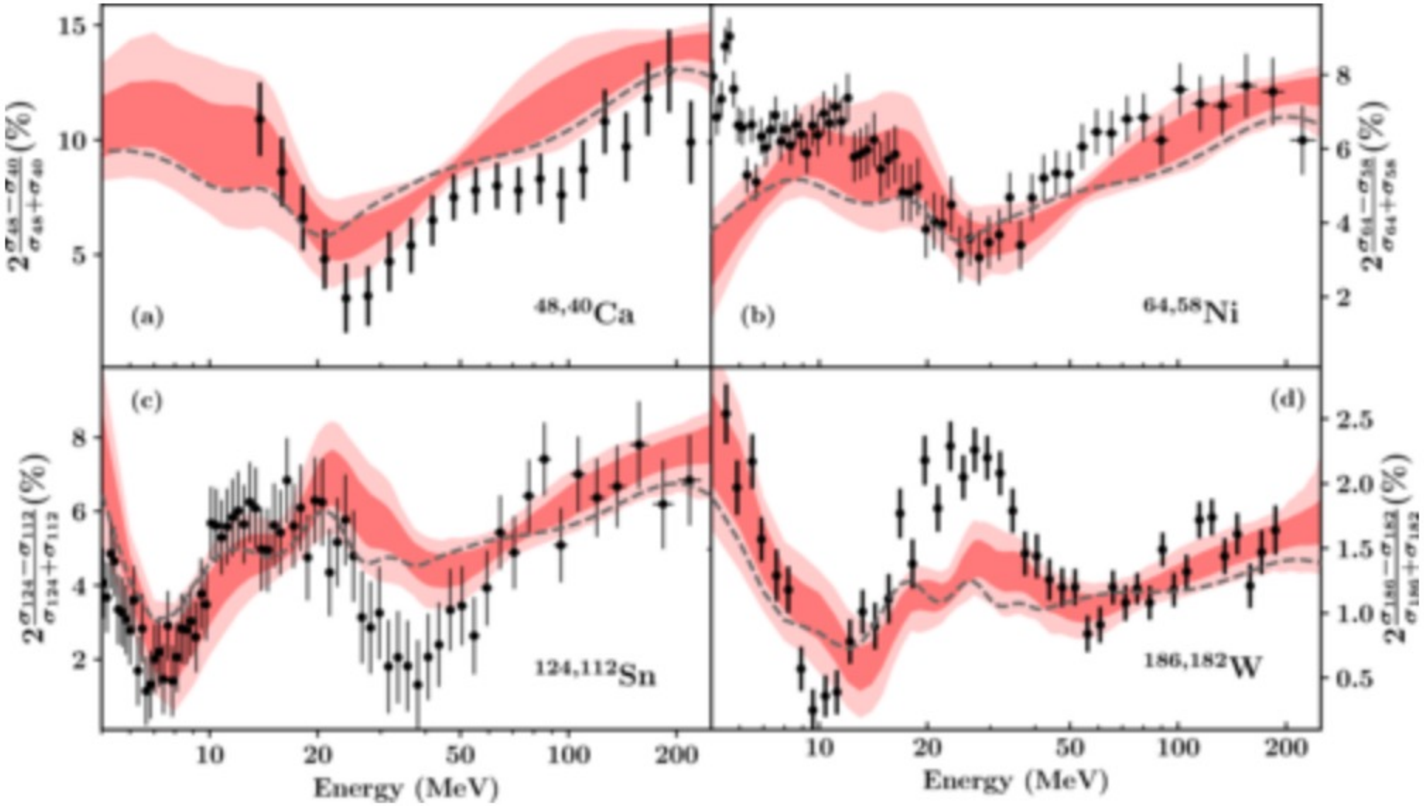
Goal: approximate statistics of random variable x, such as the expected value: $E[x] = \int xp(x)dx$

- Direct Monte Carlo | $p(x)$ can be sampled:
  - $E[x] = \int xp(x)dx \approx \frac{1}{N}\sum_i X_i$ where $X_i \sim p(x)$
- BFMC | $p(X_i)$ can be computed:
  - $E[x] \approx \frac{1}{N}\sum_i X_i w_i$ where $X_i \sim U(x_{min}, x_{max})$, $w_i = p(X_i) \rightarrow \bar{p}(X_i)$
- Importance sampling BFMC | $p(x)$ can be sampled approximately:
  - $E[x] \approx \frac{1}{N}\sum_i X_i \frac{w_i}{g_i}$ where $X_i \sim g(x)$, $w_i = p(X_i)$, $g_i = g(X_i)$

Sampling from a uniform distribution often yields very few samples with non-zero weight

Neutron Transmission Coefficients

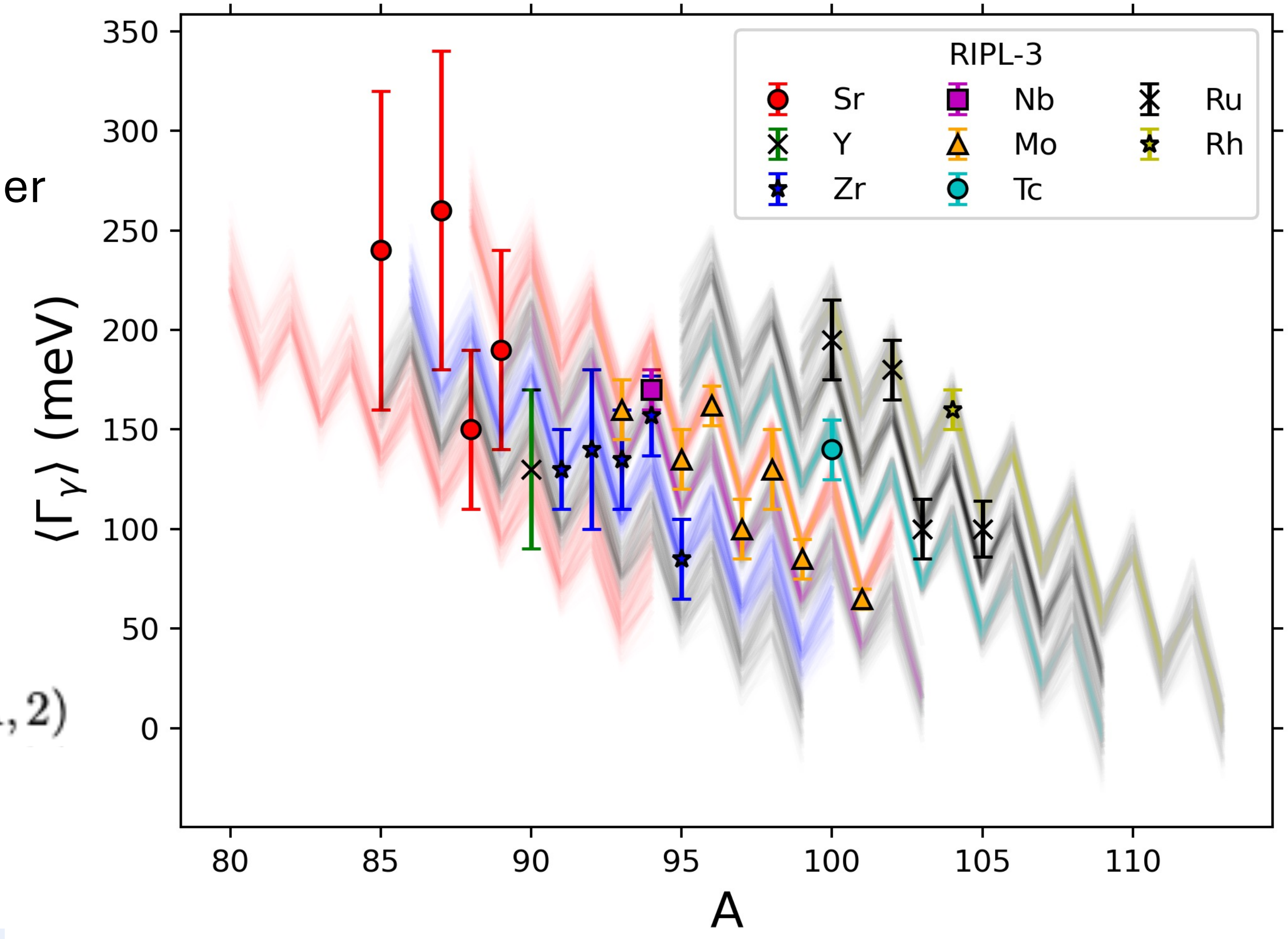
- Pruitt & Escher have re-evaluated the parameters of the Koning-Delaroche optical model
- Including MCMC UQ
- We consider a subset of 50 samples (out 400+) of pre-calculated neutron transmission coefficients



Gamma-ray Transmission Coefficients

- Average radiative width trends:
- $<\Gamma_\gamma>_0$ increases with charge number (Z)
- $<\Gamma_\gamma>_0$ generally decreases with mass number along an isotopic chain (N)
- $<\Gamma_\gamma>_0$ shows an odd-even staggering in A, only observable for even-Z nuclei
- We choose to fit with an empirical form:

$$\langle\Gamma_\gamma\rangle_0(Z, A) = c_0 + c_1 A^2 + c_2 Z^2 + c_3 Z \bmod(\mathrm{A}, 2)$$



Level Densities – shell corrections

- The fitted systematic is similar to hoffman:

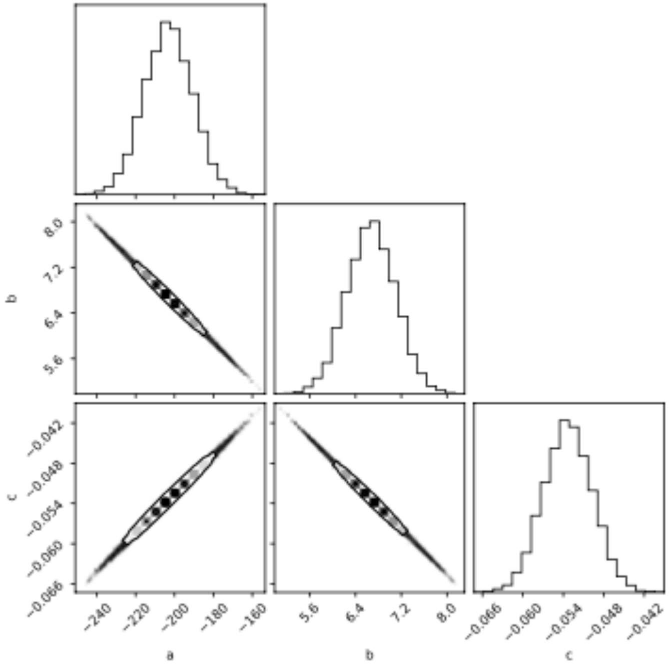
N <= 50

$$c_0 = -364 \pm 70$$
$$c_1 = 17.2 \pm 3.0$$
$$c_2 = -0.20 \pm 0.03$$

N > 50

$$c_0 = -202 \pm 12$$
$$c_1 = 6.67 \pm 0.43$$
$$c_2 = -0.053 \pm 0.004$$

- Uncertainties represent the 1σ quantile of the distributions that results from the MC fitting procedure. Close to normal distributions.



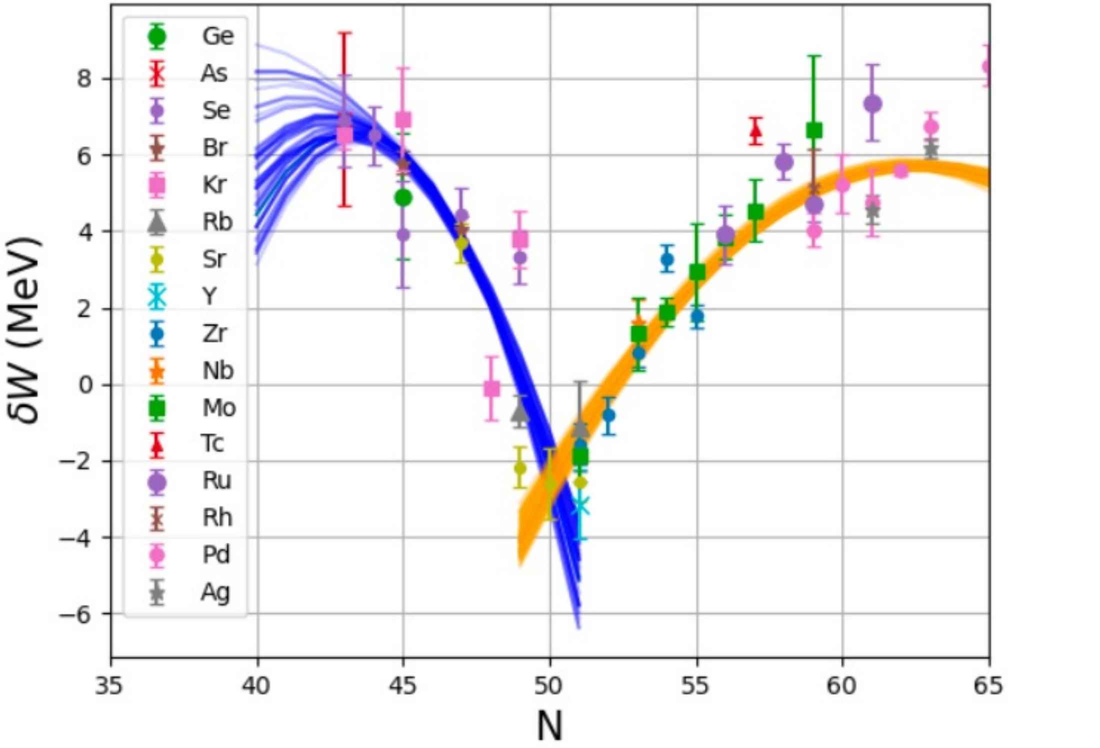


Figure 2: Results of the Monte-Carlo fitting procedure for the shell correction parameter δW.