Update on LLNL evaluation efforts

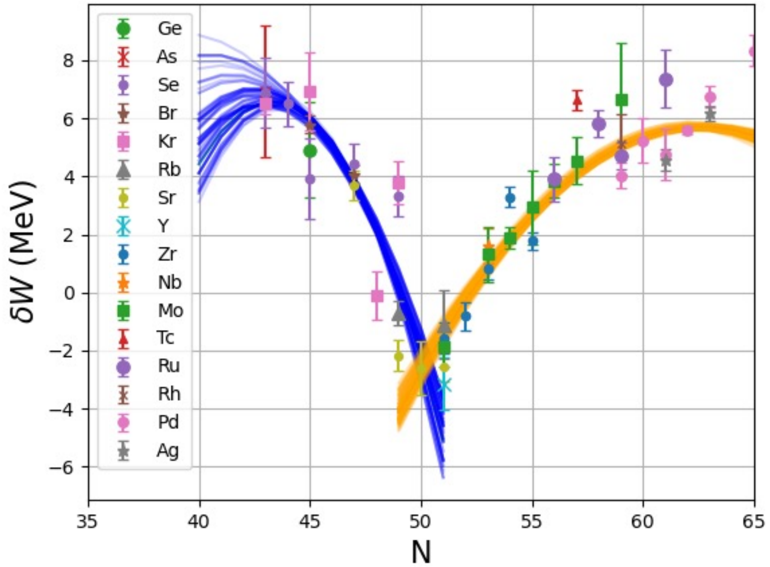
Nuclear Data Week 2025

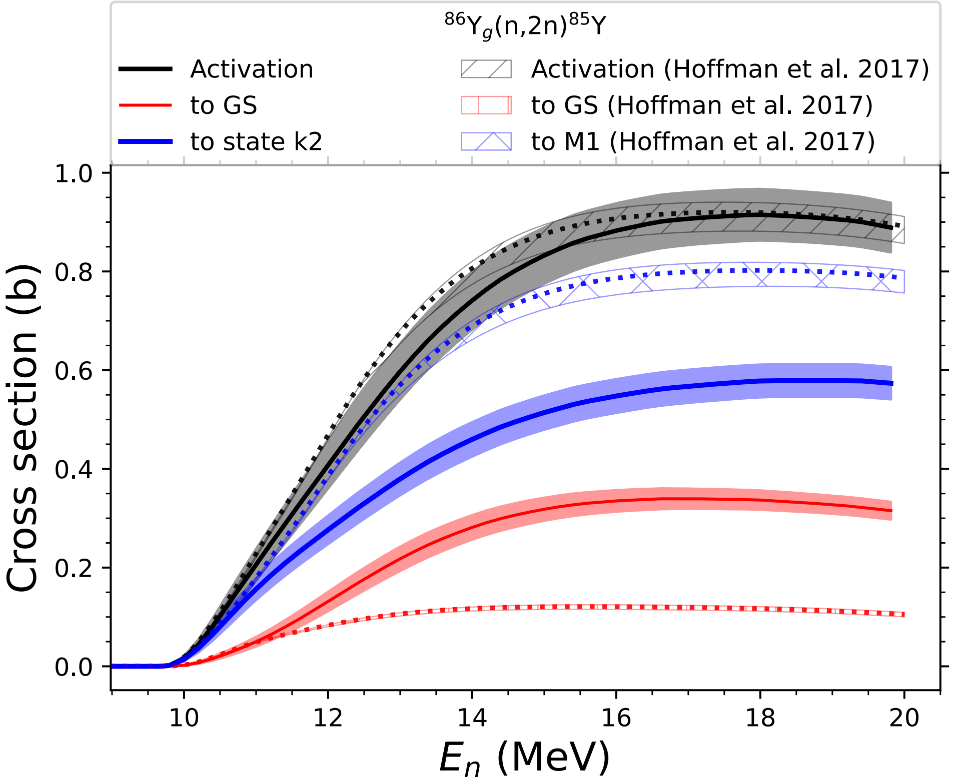
Andre Sieverding
Nuclear Data and Theory Group

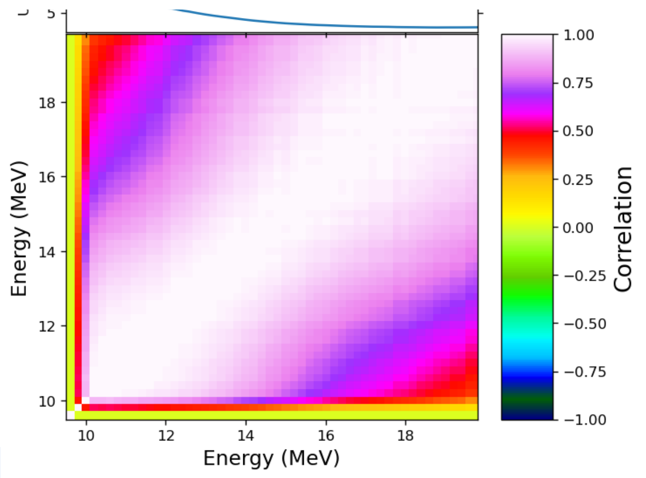
Prepared by LLNL under Contract DE-AC52-07NA27344.

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
- GNDS files with neutron-induced cross sections for $^{85-91}Y$, $^{86-90}Zr$

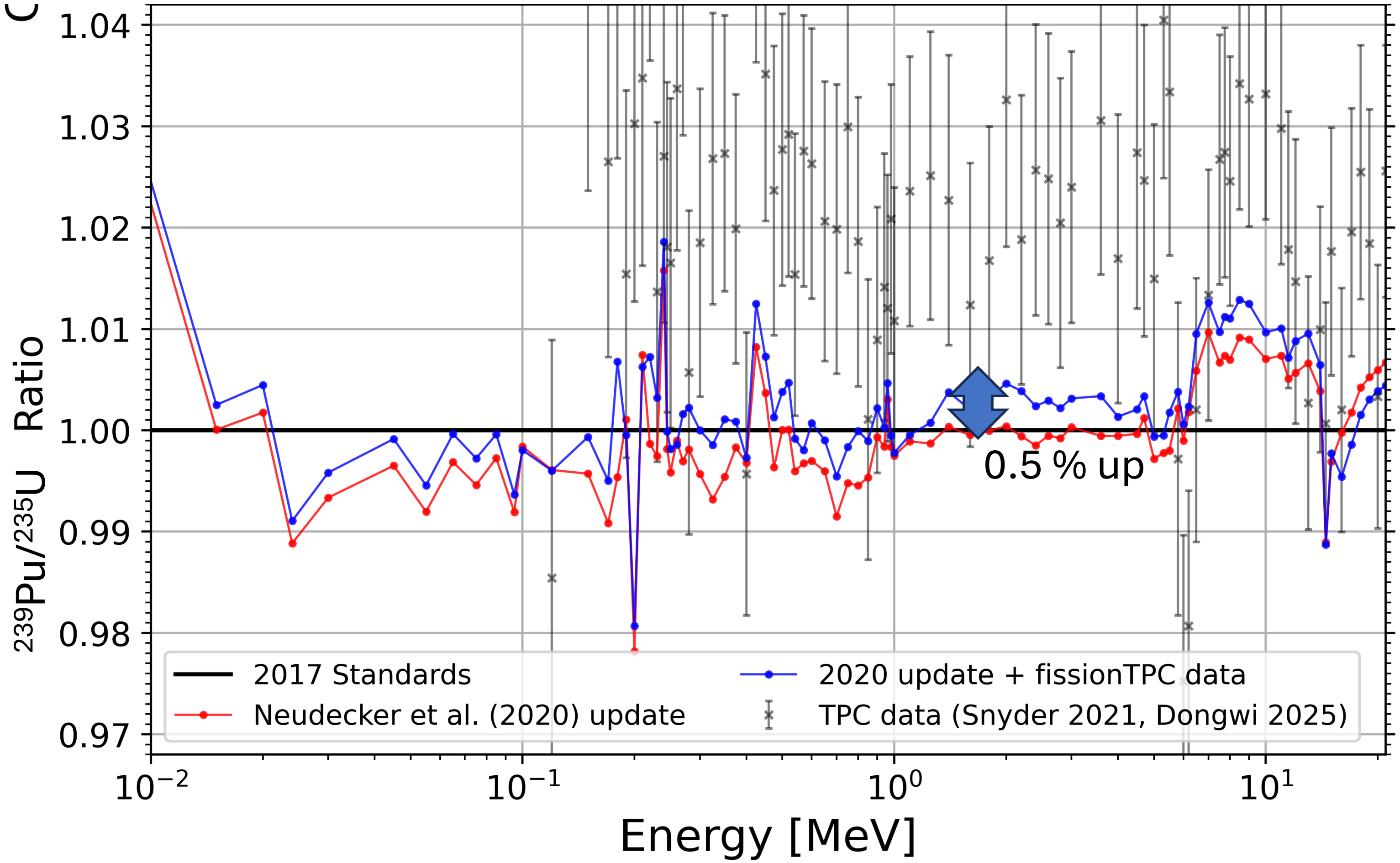
Technical report is available:
https://doi.org/10.2172/2997578

Finalizing ^{239}Pu evaluation

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

- Based on calculations with LLNL's **YAHFC** reaction code + Fresco coupled channels
- Fission: **GMAP evaluation including fissionTPC ^{239}Pu/^{235}U**
- Cross sections below **30 keV** and fission product data are taken from ENDF/B VIII.1

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

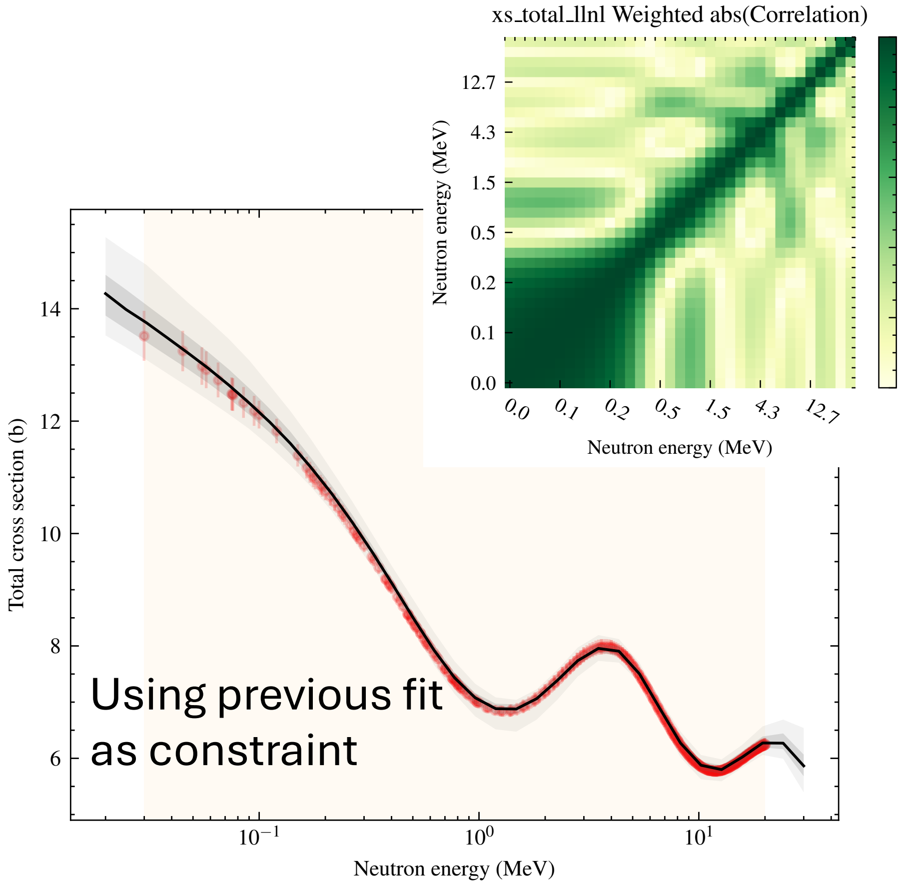


Up next: Add covariance data

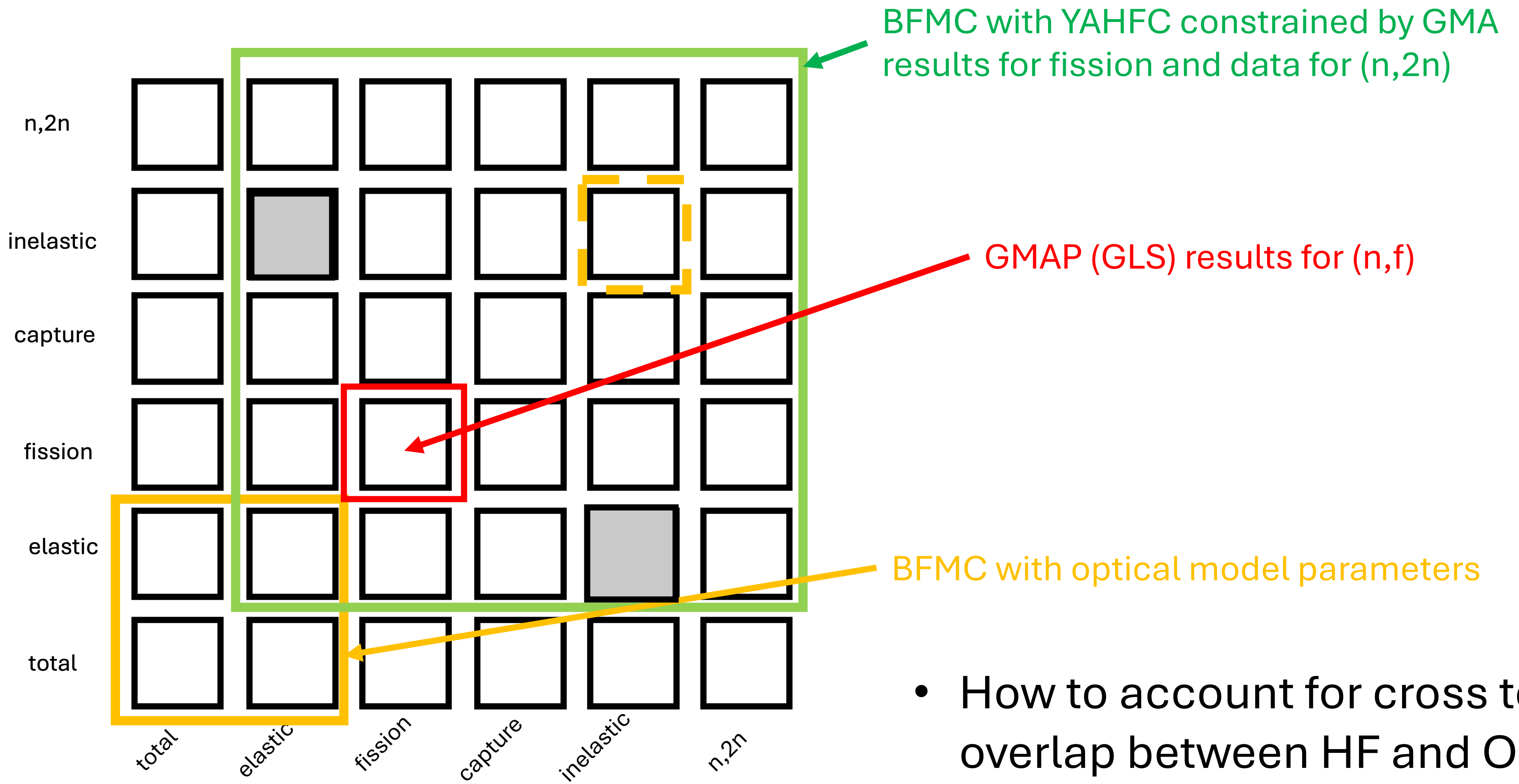
Covariance data from Backward-forward Monte-Carlo (BFMC)

Development by O.C. Gorton

- BFMC | $p(X_i)$ can be computed:
  - $E[x] = \int xp(x)dx \approx \frac{1}{N}\sum_i X_i w_i$
  - With uninformative prior
  - And $w_i \propto \exp\left[\left(-\frac{\chi_i^2}{\chi_{min}^2}\right)^2\right]$ Bauge et al. (2007)
- Applied to HF and OMP parameters **separately**

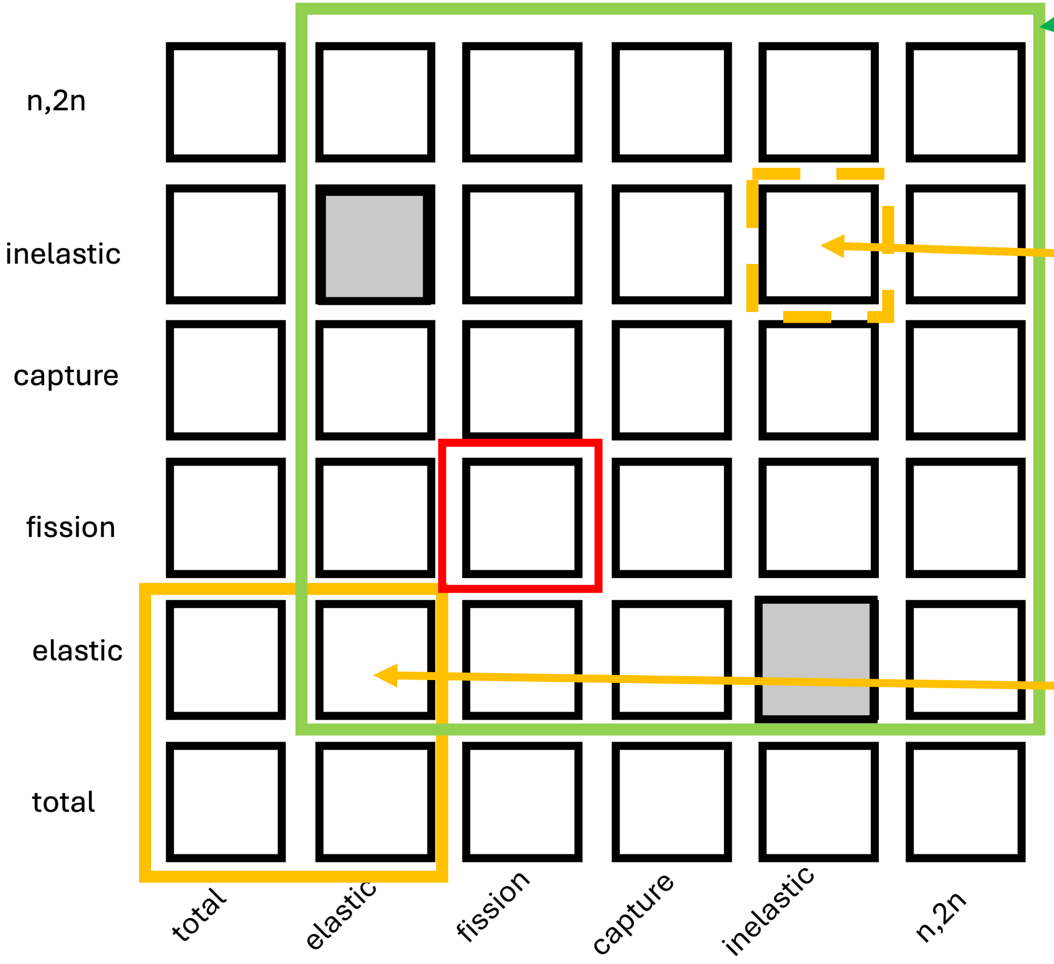


Merging covariance data for all components



- How to account for cross terms and overlap between HF and OMP parameters?

Merging covariance data for all components



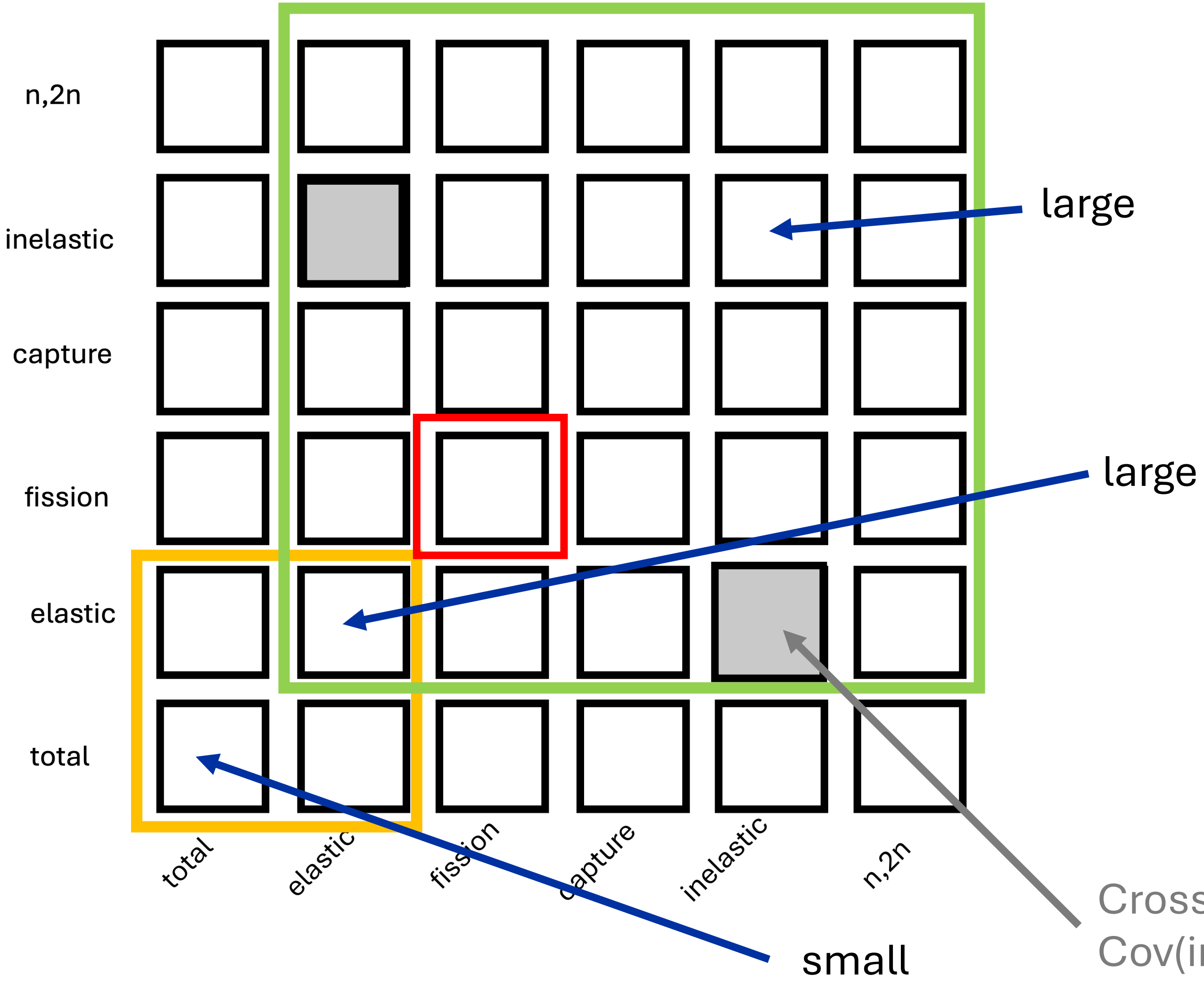
BFMC with YAHFC constrained by GMA results for fission and data for (n,2n)

HF-covariance + scaled non-elastic covariance

- $\Sigma_{inel} = M_f\, C_{nonel}^{OMP} M_f^T + \Sigma_{\text{inel}}^{HF}$
- $M_f = \frac{\sigma_{inel}^{HF}}{\sigma_{nonel}^{OMP}} diag\left(\Sigma_{nonel}^{OMP}\right)^{1/2}$

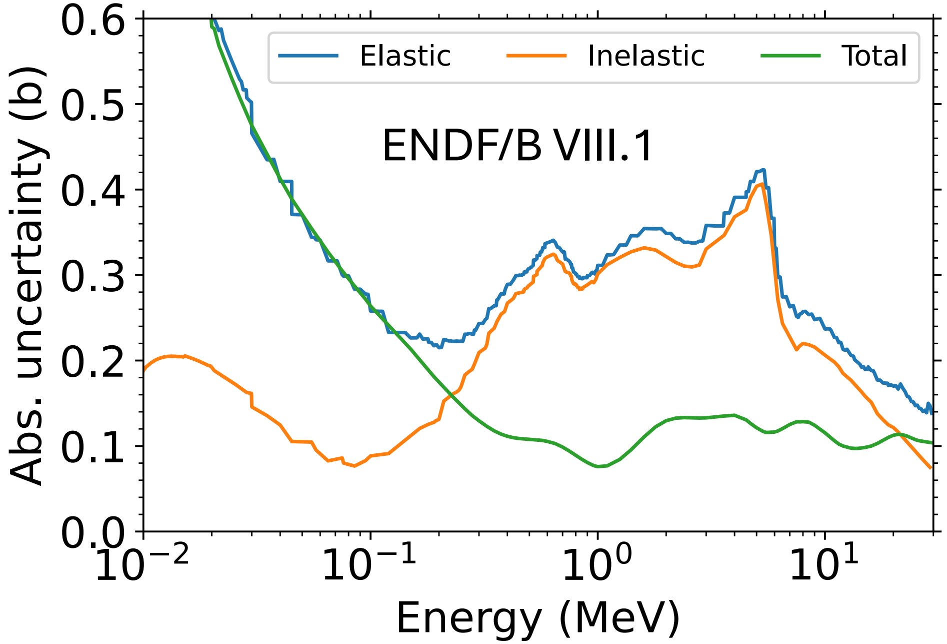
Total covariance + inelastic + …

Merging covariance data for all components



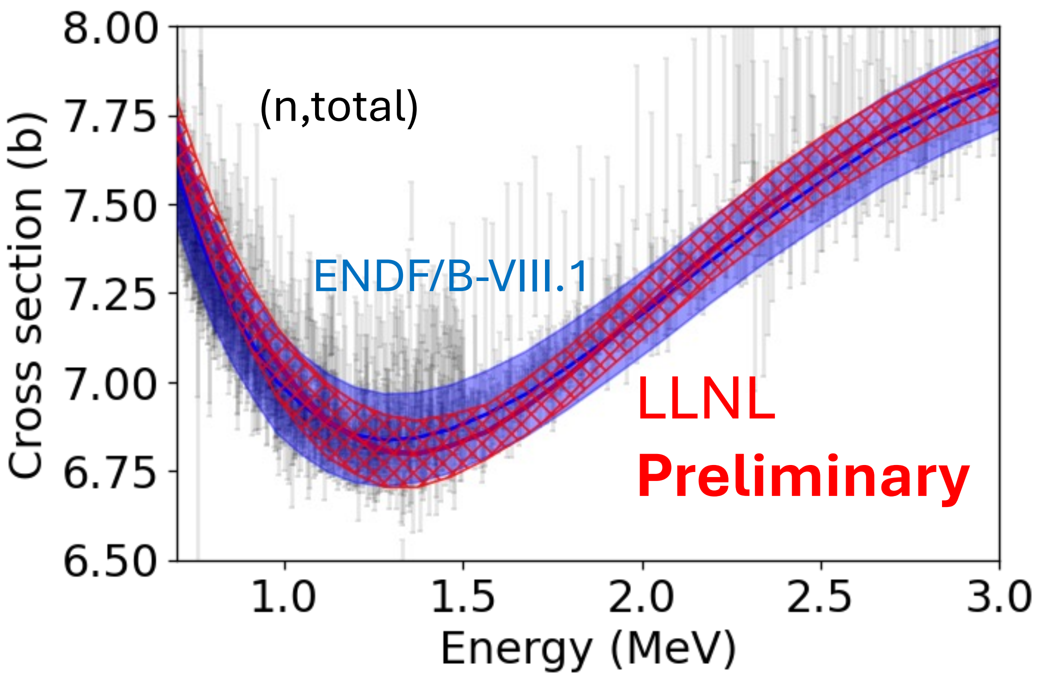
Cross-channel covariance
Cov(inel,el):=Cov(tot,tot) - [rest]

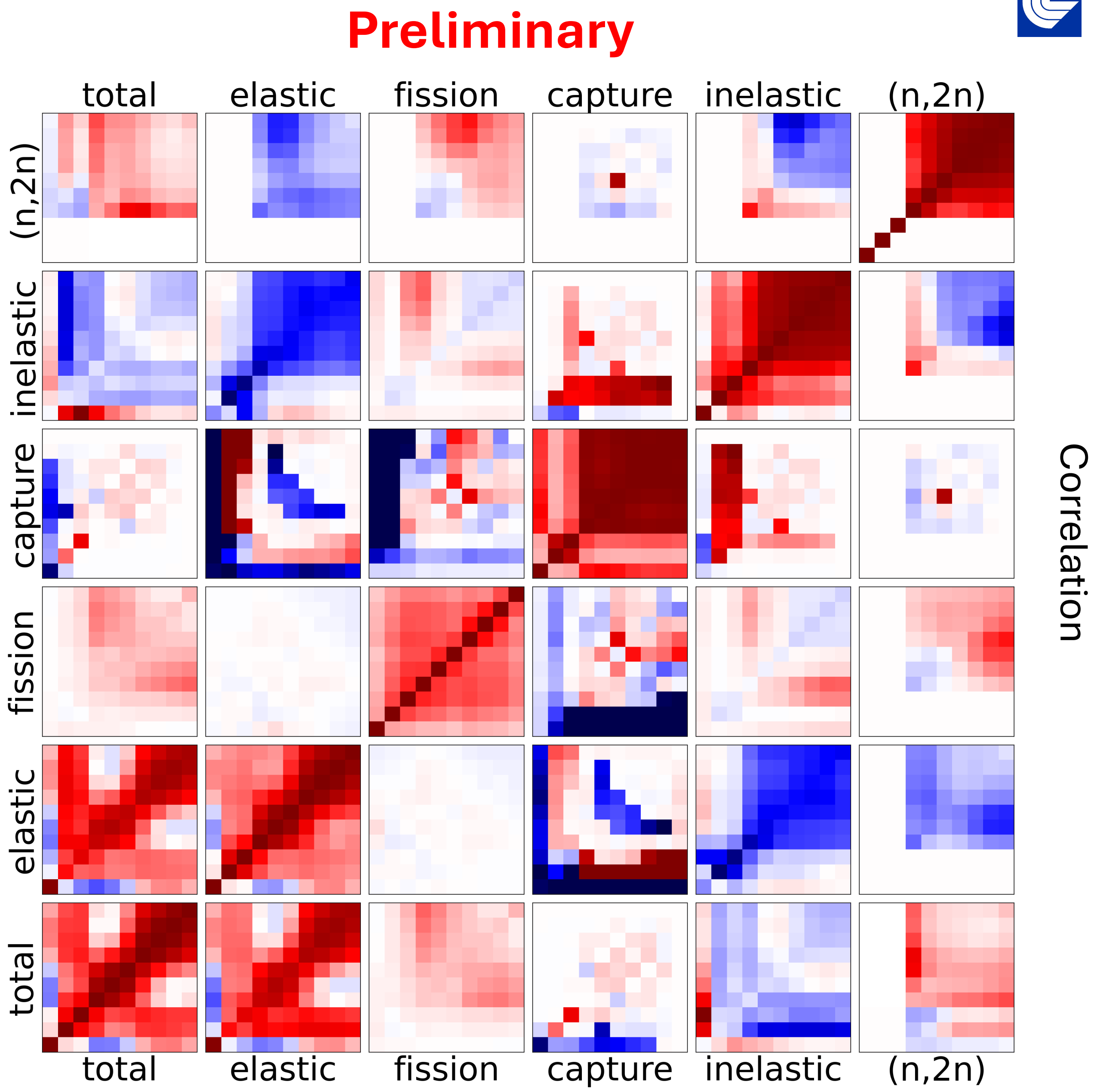
$$Cov(tot, tot) = Cov(el, el) + Cov(inel, inel) + Cov(inel, el) + \cdots$$



Combined covariance matrix

- Combined matrix is positive semi-definite
- Total uncertainty is close to ENDF/B VIII.1



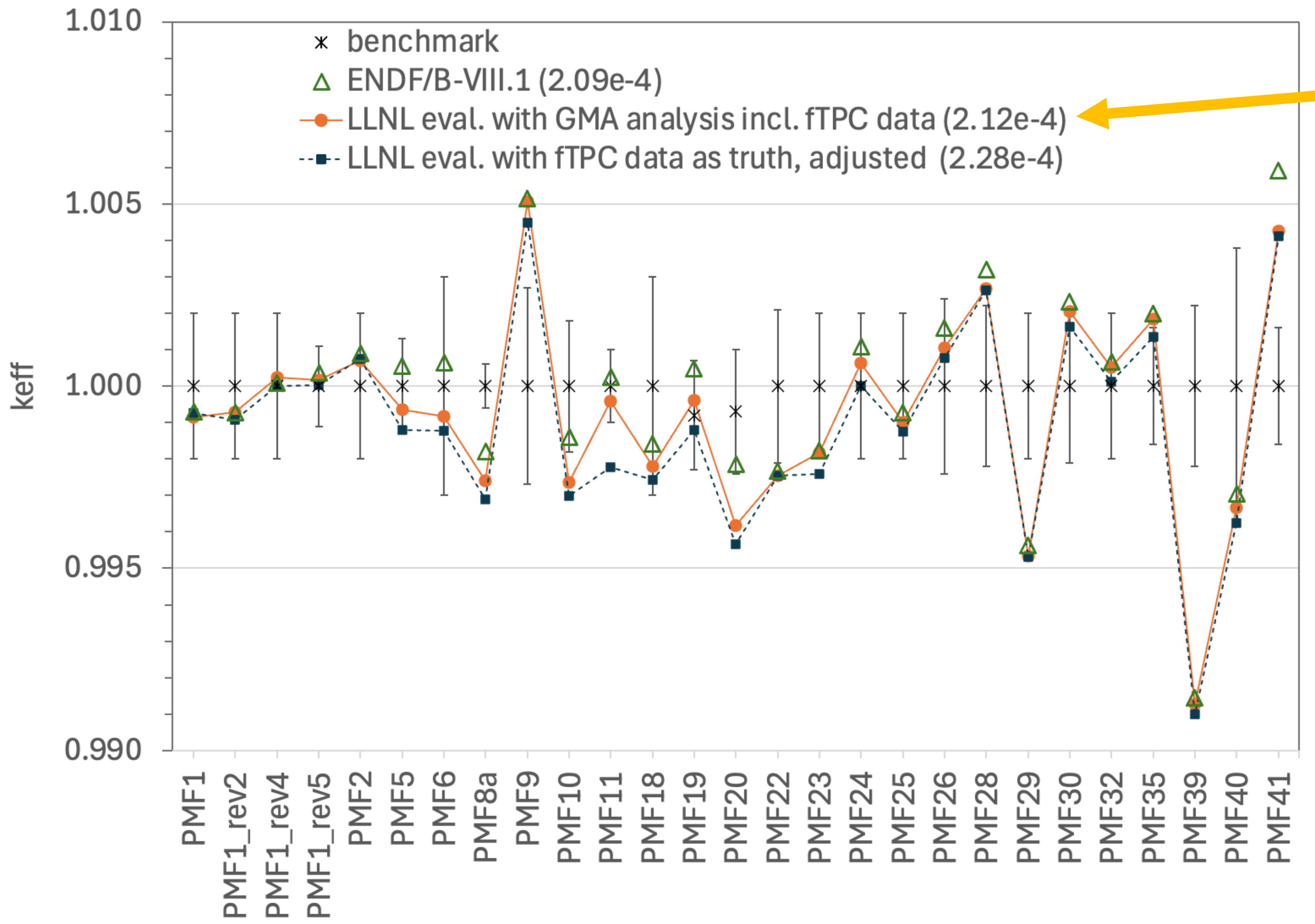


To Do

- To obtain a better elastic-inelastic cross channel covariance, we need to include the OMP parameters in the BFMC evaluation

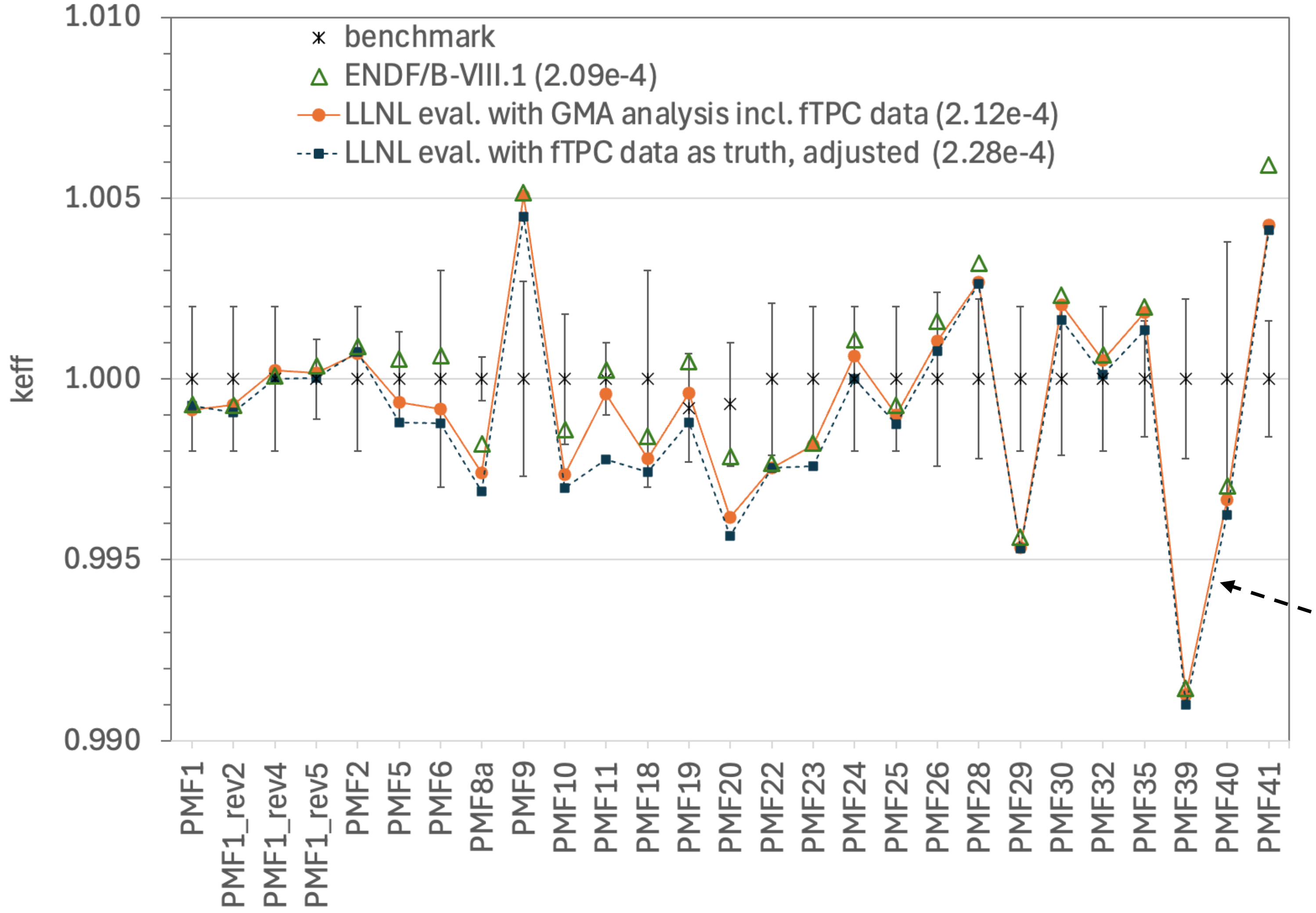
Adjusting the library to the fission TPC 239Pu/235U data

Validation and Verification



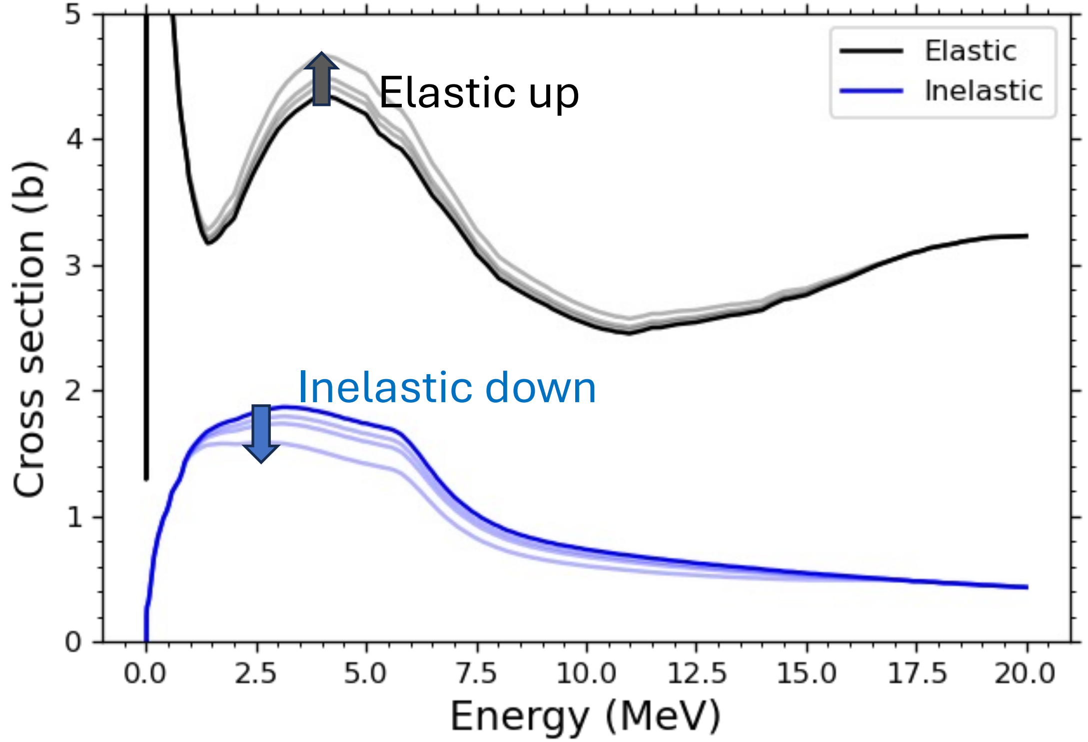
- GMAP analysis of fissionTPC data: **No adjustment needed**
- Almost as good as ENDF/B VIII.1 across PMF benchmarks
- Uncertainty propagation is work in progress

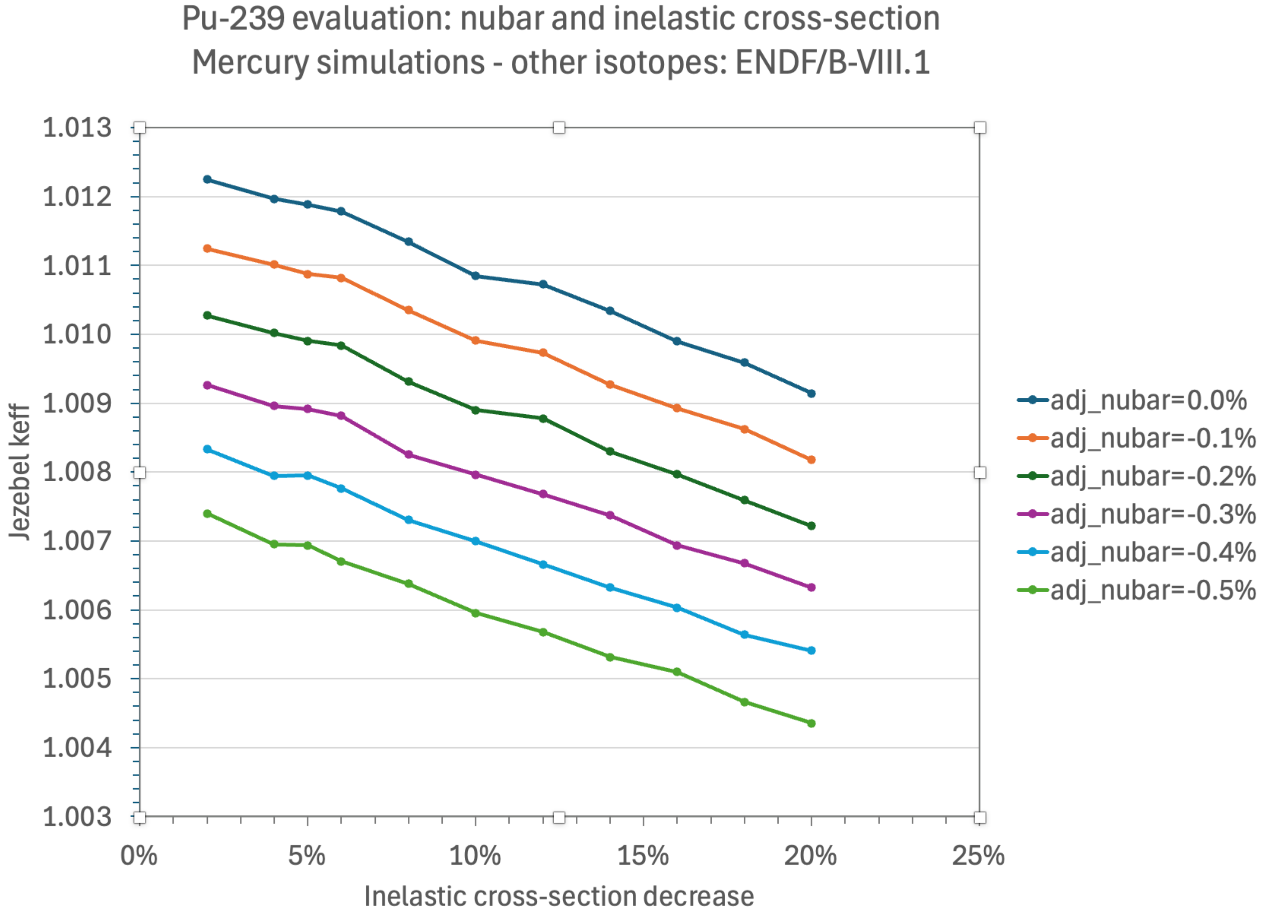
Validation and Verification



- Thought experiment:
  - What if the $^{239}Pu/^{235}U$ fission TPC data was the only available data?
- **Requires -1.4 % adjustment of $\overline{\nu}$**

Beyond $\bar{\nu}$: adjusting "by hand"





Benchmarks are still out of reach

Turn more knobs: Capture, PFNS, Angular distributions … too many to do by hand

Conclusions

- LLNL n+Pu239 evaluation (using the 2021 and 2025 fissionTPC data with GMAP, YAHFC) from 30 keV – 20 MeV is close to finalized
- Performance in criticality benchmarks is very close to ENDF/B VIII.1
- Taking fissionTPC ratio with 2017 ^{235}U fission standard makes adjustment hard to achieve by hand

Backup/additional slides

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

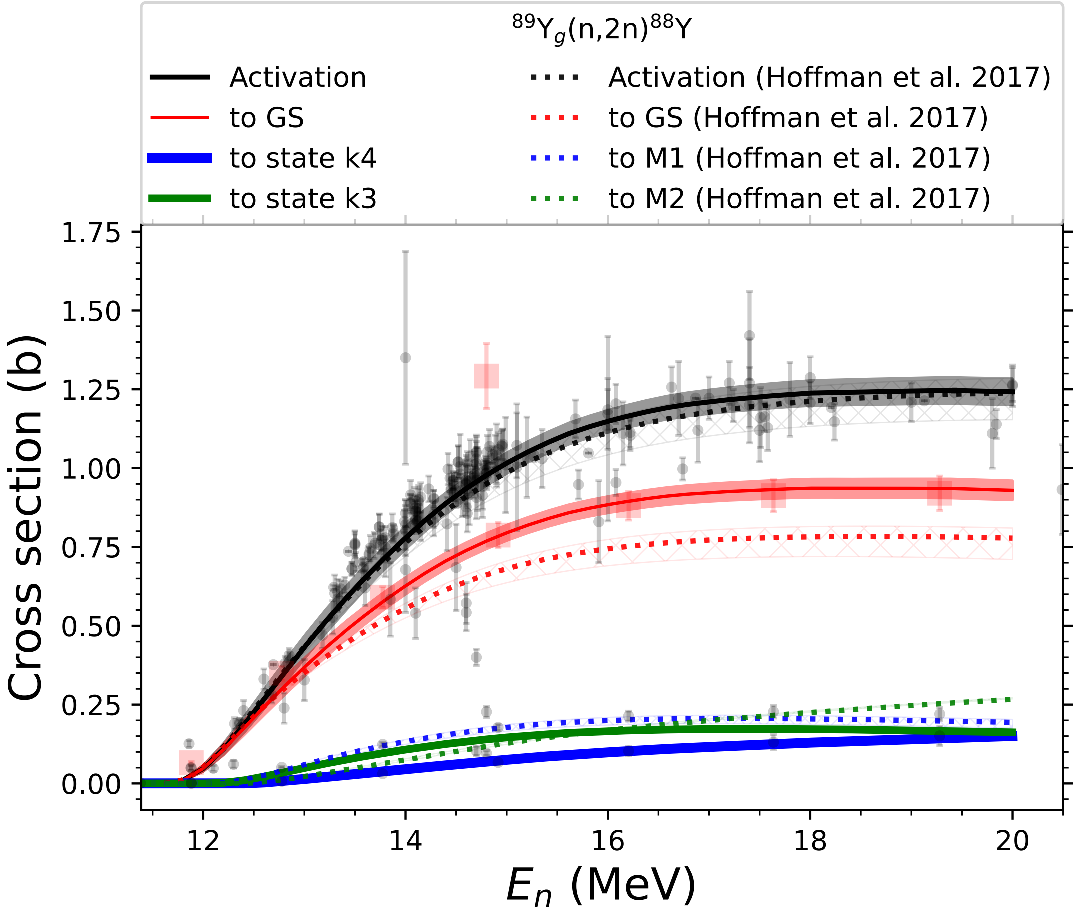
Development by O.C. Gorton

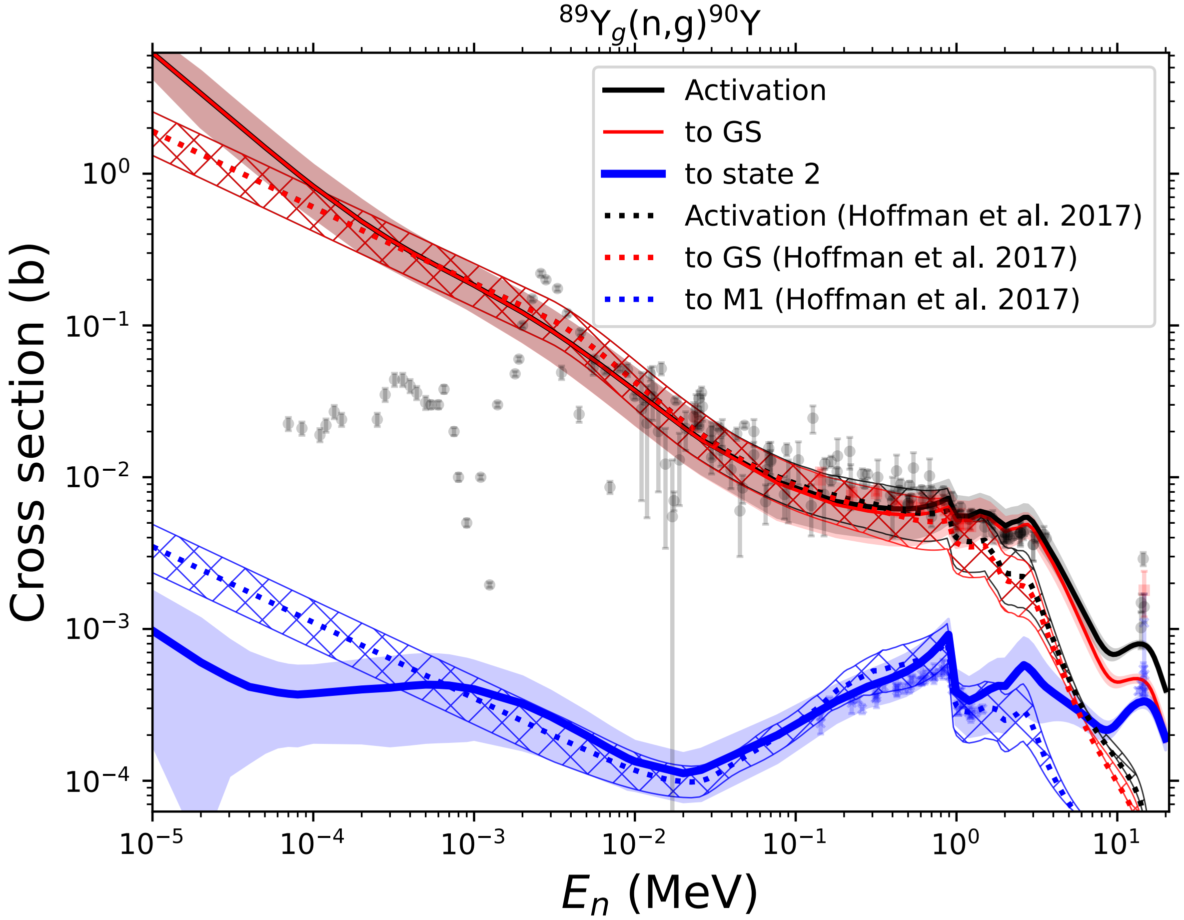
Goal: approximate statistics of random variable x, such as the expected value: $E[x] = \int xp(x)dx$

- 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 $X_i \sim U(x_{min}, x_{max})$, $w_i = p(X_i) \to \bar{p}(X_i)$
- 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

Validation by comparing to experimental data

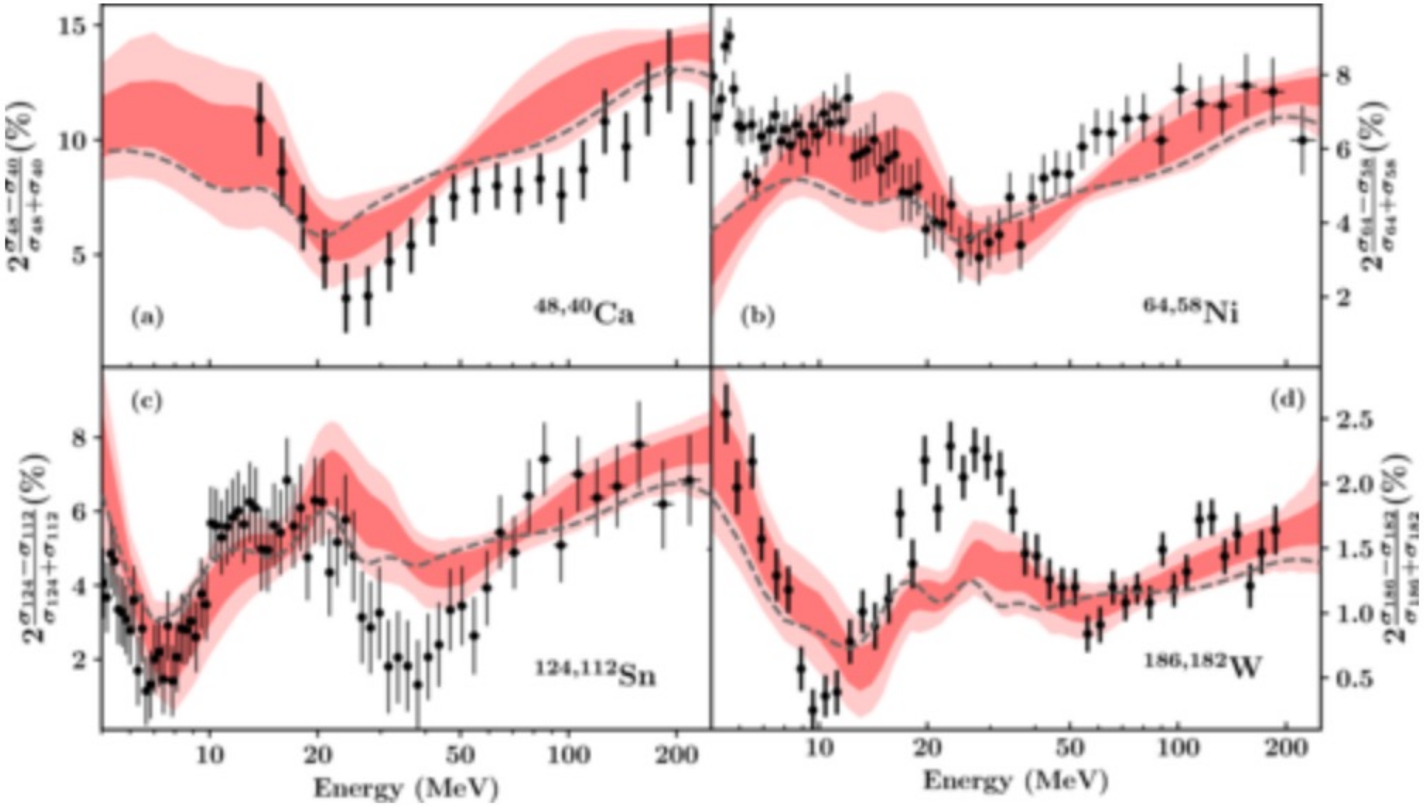




- Overall good performance for (n,2n). Capture cross sections need to be improved
- Validation for YAHFC reaction code

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



Level Densities – shell corrections

- The fitted systematic is similar to hoffman:

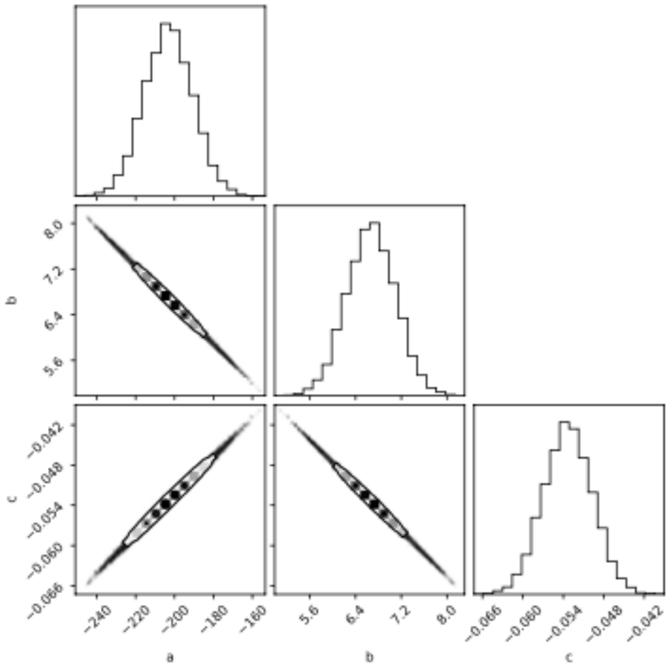
N <= 50

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

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.



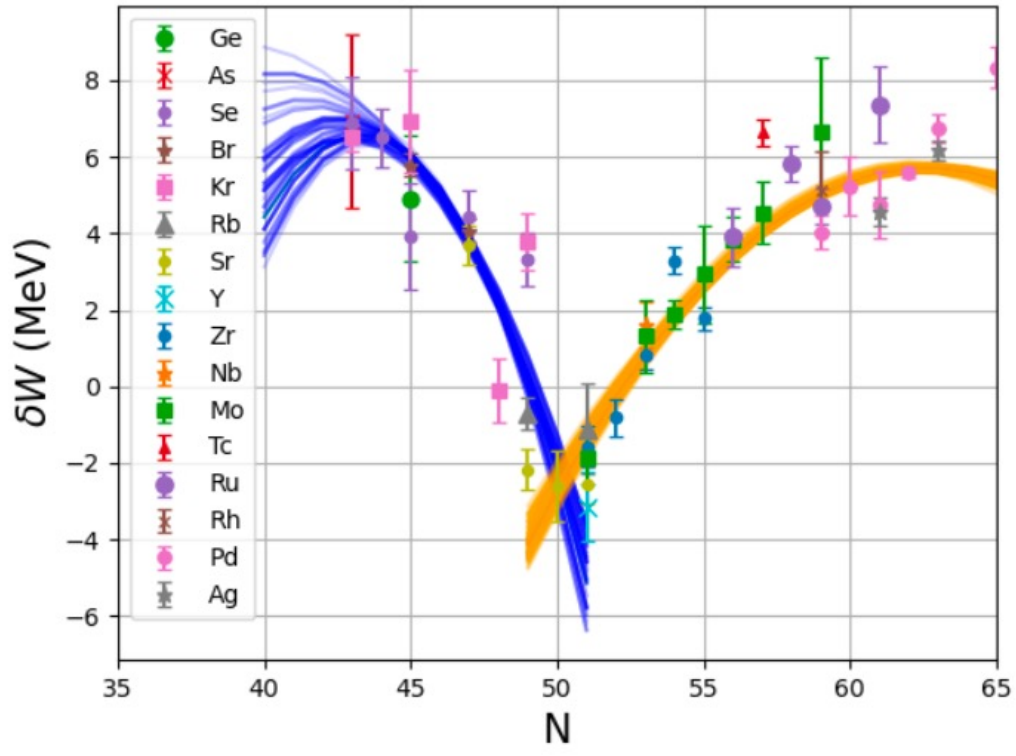


Figure 2: Results of the Monte-Carlo fitting procedure for the shell correction parameter δW.

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:

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