Los Alamos NATIONAL LABORATORY

FPY Covariances

A.E. Lovell, T. Kawano, and P. Talou

CSEWG, November 2, 2022

LA-UR-22-31454

Funding provided by NA-22 and supported by NCSP.
Thanks also to M. Chadwick, S. Okumura, I. Stetcu, M. Herman, and M. Mumpower, W. Haeck, N. Gibson, A. Mattera, and A. Sonzogni.

Overview of cumulative fission product yield covariance development

- Combination of data and BeoH (LANL-developed deterministic fission fragment decay code) through a Kalman filter optimization
  - Optimization using cumulative fission product yields, average prompt/delayed neutron multiplicities
  - Data currently taken from EXFOR (A. Mattera, BNL, is correcting EXFOR data for updated nuclear structure information and providing data that is not in EXFOR)
  - Model stiffness is being addressed to ensure FPYs can be reproduced to the needed accuracy
- Covariances are calculated at discrete incident neutron energies
  - Kalman covariances scaled by the χ^2/N (to EXFOR experimental data)
  - Initial impact of diagonal uncertainties vs full correlations is being investigated (A. Sonzogni, et al., BNL)
- Discussions on the covariance format are still ongoing (more tomorrow)

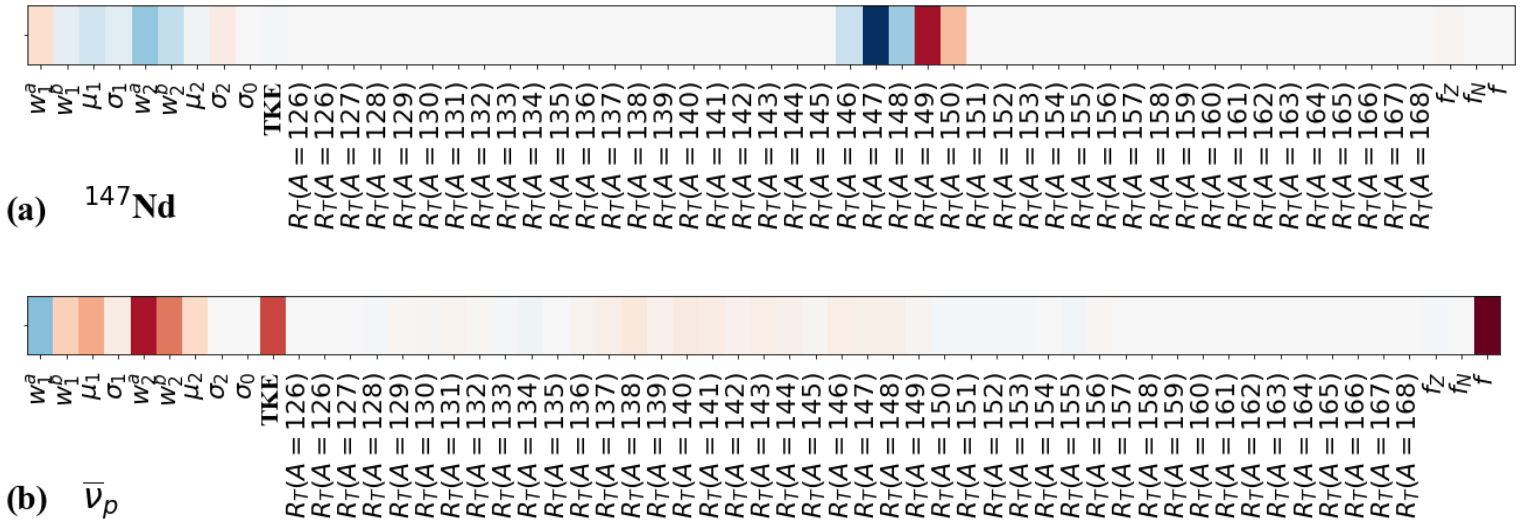
Fission product yield covariances status

- ^{252}Cf spontaneous fission
  - Bulk fitting has been performed
  - Covariances are calculated
- ^{235}U neutron induced fission - thermal to 20 MeV
  - Bulk fitting has been performed up to 20 MeV
  - Covariances calculated up to 20 MeV
- ^{238}U neutron induced fission – thermal to 20 MeV
  - Bulk fitting has been performed up to ~12 MeV (third-chance fission opening)
  - Covariances calculated up to ~12 MeV
- ^{239}Pu neutron induced fission – thermal to 20 MeV
  - Bulk fitting has been performed up to 20 MeV
  - Covariances calculated up to 20 MeV

All calculations shown here are preliminary! Improvements are still being made.

An overview using ^{252}Cf(sf)

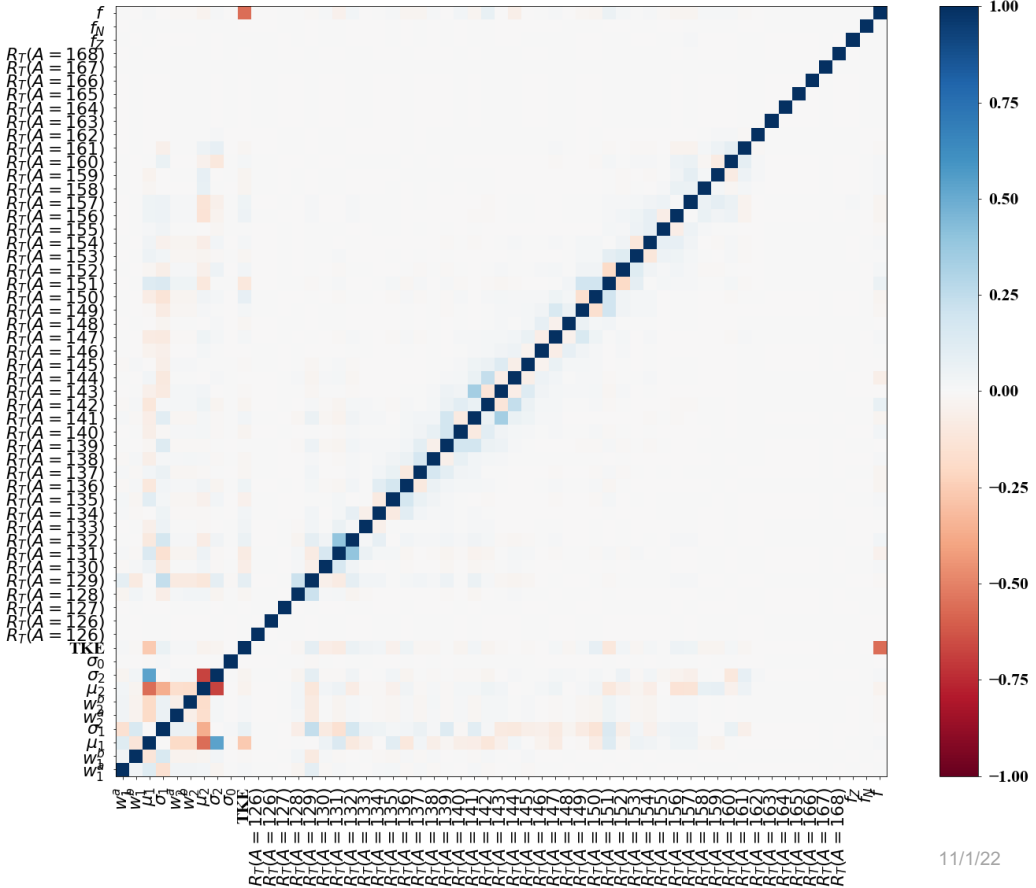
Parameter sensitivities for ^{147}Nd cumulative FPY and prompt average neutron multiplicity



Cumulative FPYs, prompt and delayed <v> including in the optimization.
The data (for fits discussed in this talk) are taken from EXFOR.

Parameter covariance matrix for ^{252}Cf(sf)

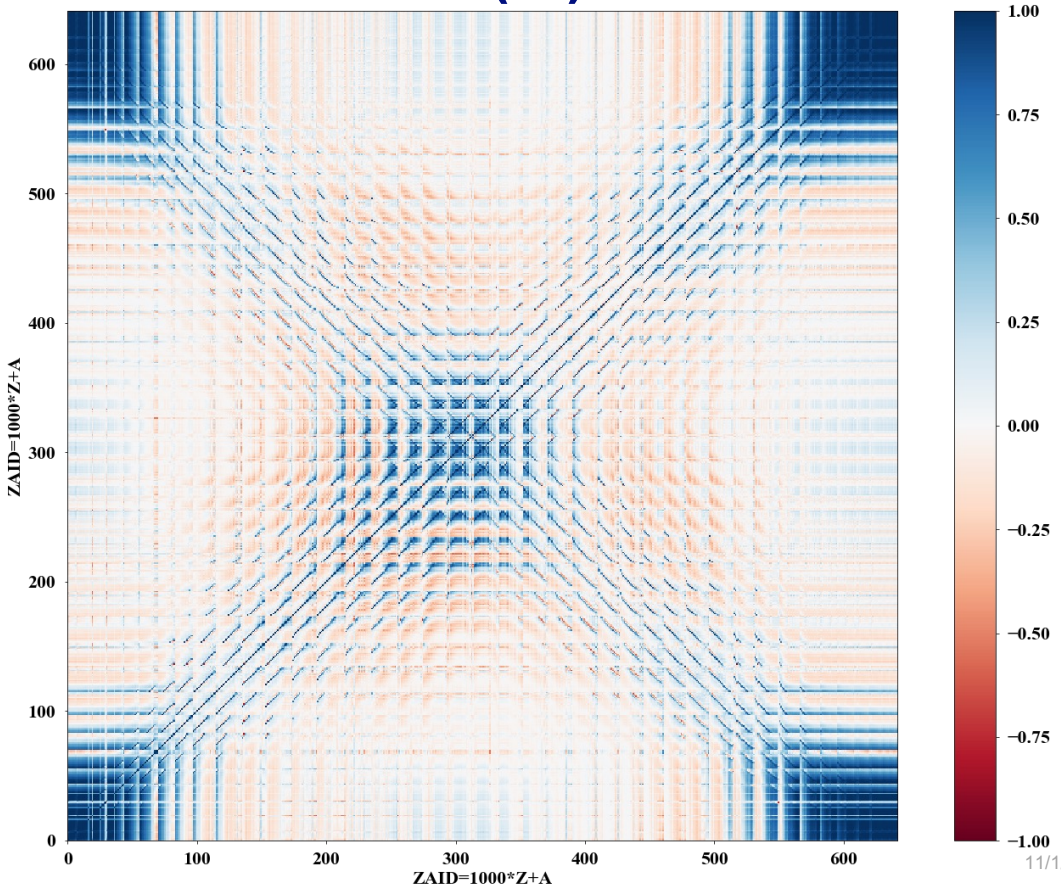
- Most parameters are uncorrelated ($R_T(A)$ values only impact a few FPYs each, most correlations are along the diagonal)
- Y(A) parameters are more highly correlated (first 9 parameters)
- TKE and f are highly anti-correlated (mainly through prompt <v>)



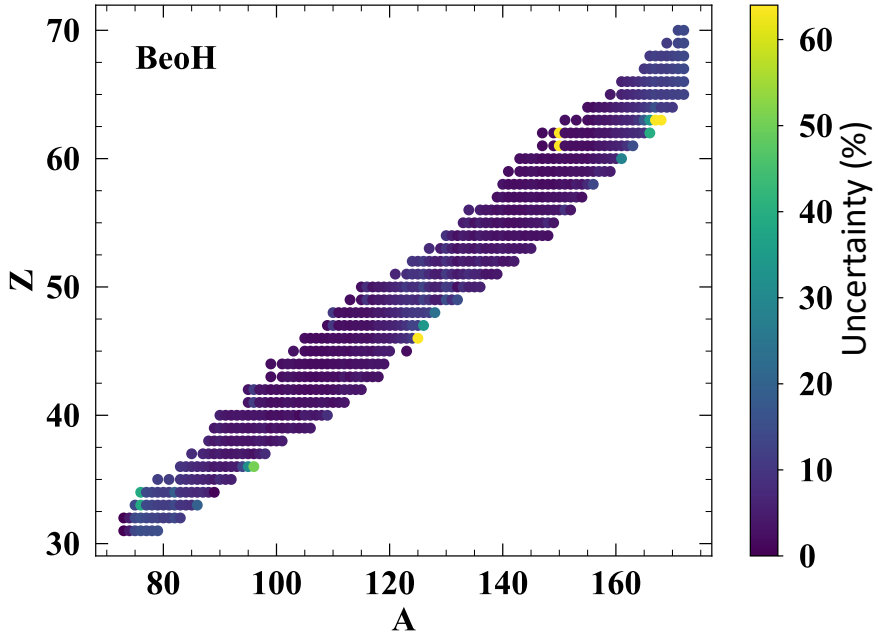
Cumulative FPY correlations for ^{252}Cf(sf)

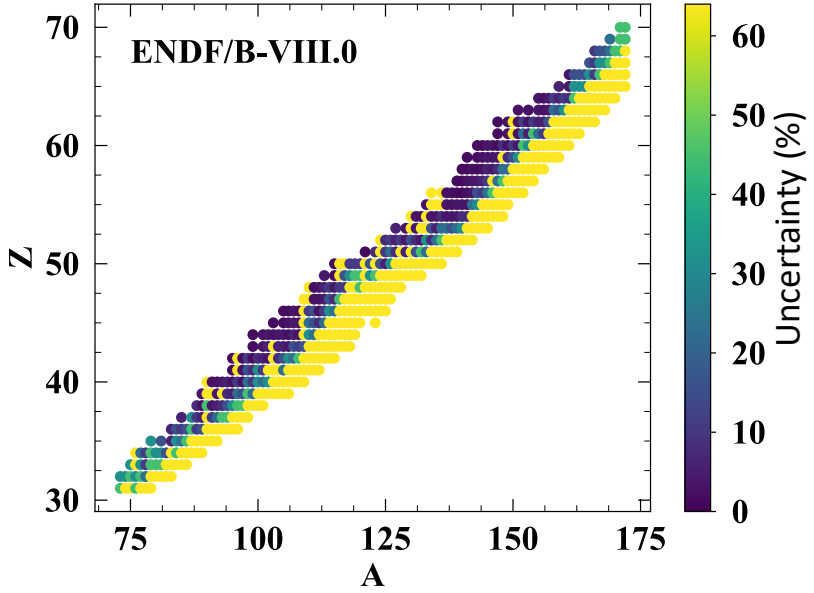
Cumulative FPYs are largely uncorrelated (from the inclusion of $R_T(A)$) but we see blocks of higher correlations.

$$\mathbb{F} = \mathbb{C}\mathbb{P}\mathbb{C}^T$$



Comparison between preliminary BeoH and ENDF/B-VIII.0 relative uncertainties for ^{252}Cf(sf)

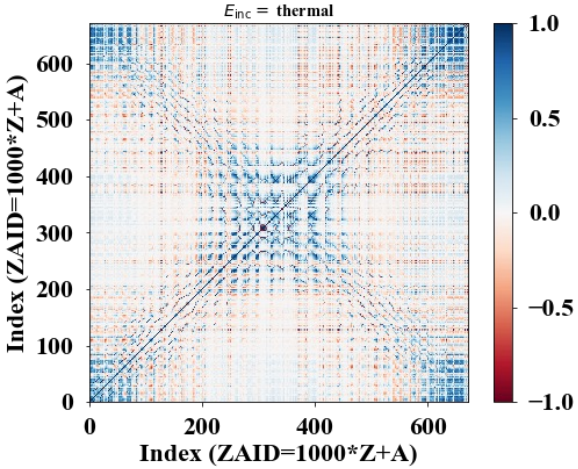


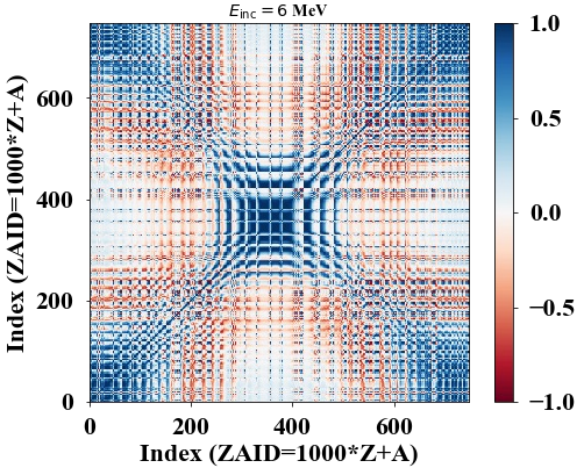


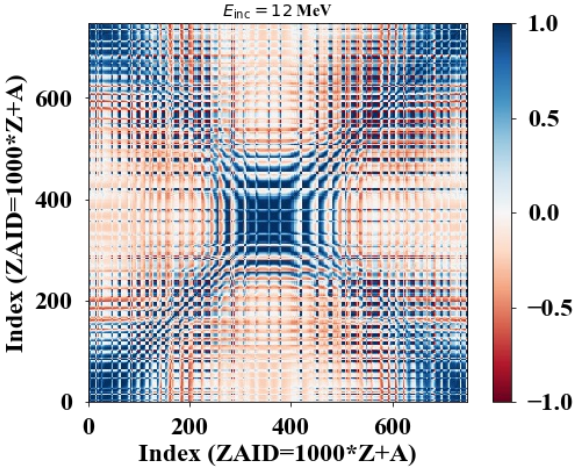
A piecewise approach is used to fit neutron-induced fission reactions

- First-chance parameters fit then fixed, second-chance parameters fit then fixed, third-chance parameters fit then fixed.
- Excitation energy sharing parameters only fit in the first-chance energy region – then kept the same for the other compounds (initial optimizations are to $\boldsymbol{\nu}$(A), most of the data is below 6 MeV incident neutron energy).
- Fourth-chance fission generally only contributes on the order of a few percent up to 20 MeV and little data to no data are available in this region; parameters are taken from CGMF and held constant.
- This approach possibly raises some questions about how to calculate uncertainties and covariances consistently.

^{239}Pu(n,f) correlations matrices are being developed at discrete energies from thermal to 20 MeV

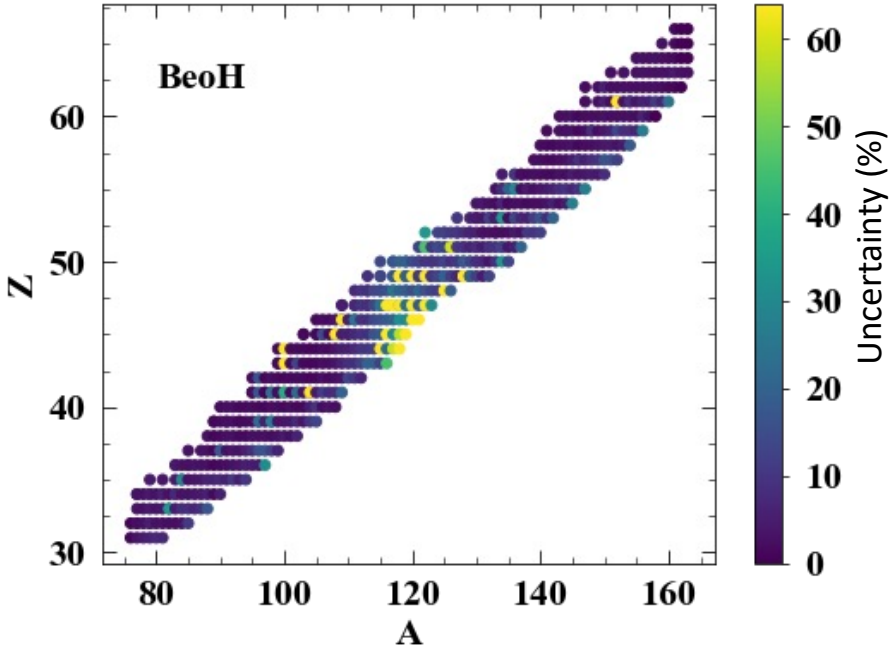


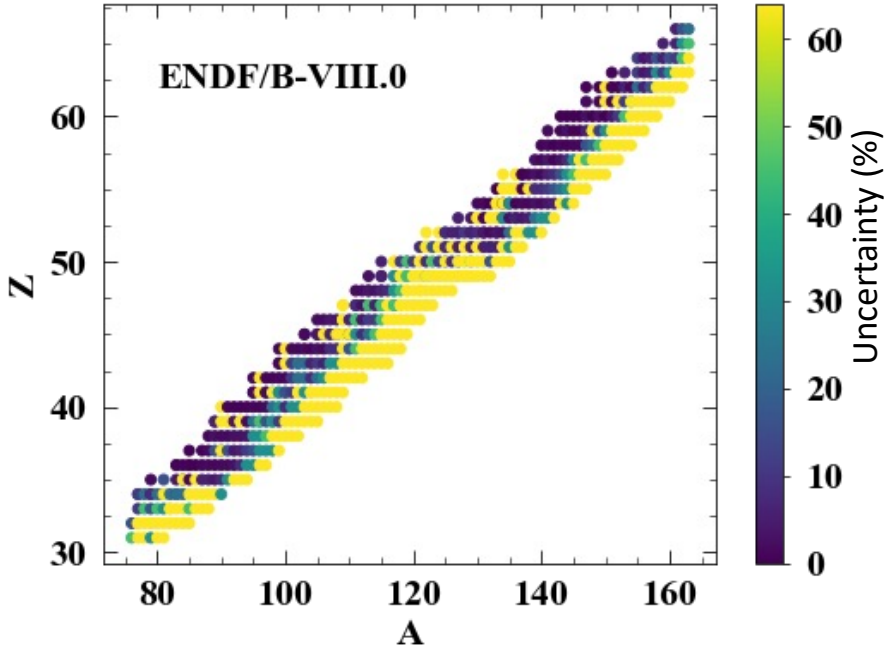




Because parameters in the fourth-chance energy region are currently not fit, we currently use the covariance matrix from the highest energy point in the third-chance region for the covariances up to 20 MeV.

Comparison of relative percent uncertainties for ^{239}Pu(n,f) at thermal



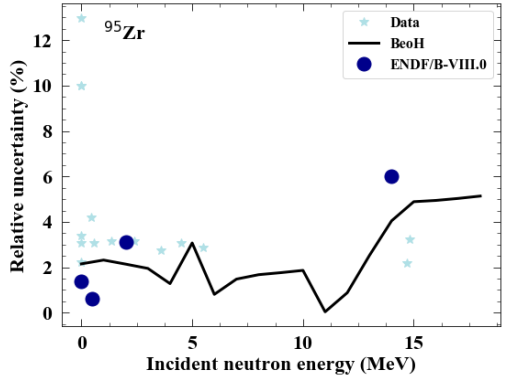


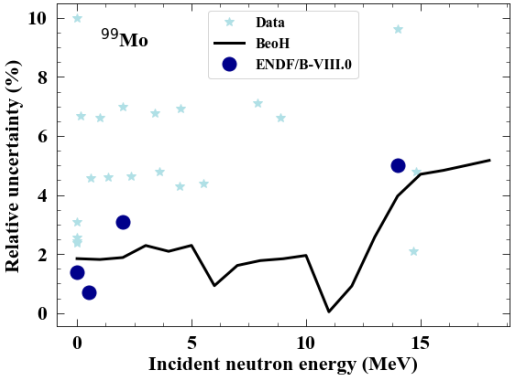
^{239}Pu(n,f) thermal cumulative FPY percent uncertainty comparison

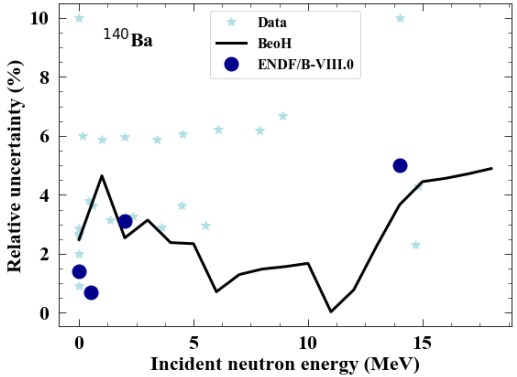
^{239}Pu(n_{th},f) Y_C(A,Z)	ENDF/B-VIII.0	IRDFF-II	Present (prelim)
^{95}Zr	1.4%	1.1%	2.2%
^{99}Mo	1.4%	0.7%	1.8%
^{103}Ru	2.0%	2.1%	1.7%
^{106}Ru	2.0%	2.3%	2.2%
^{137}Cs	64.0%	1.22%	10.2%
^{140}Ba	1.4%	1.1%	2.5%
^{144}Ce	0.7%	0.9%	2.6%

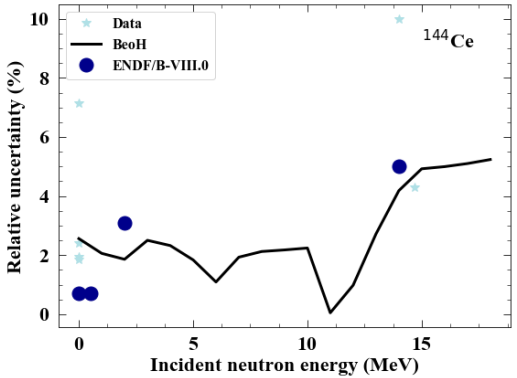
IRDFF-II: A. Trkov, et al., NDS 163 1 (2020)

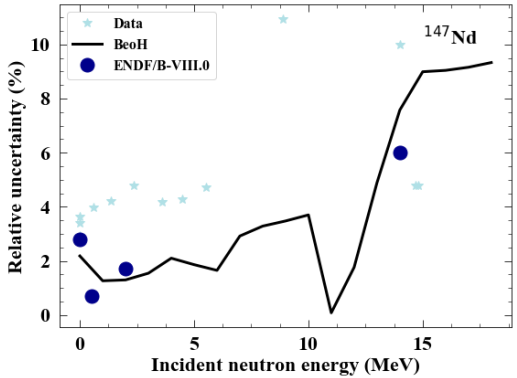
^{239}Pu(n,f) relative uncertainties for select cumulative FPY

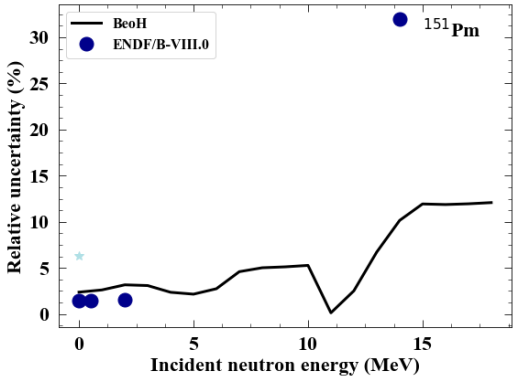




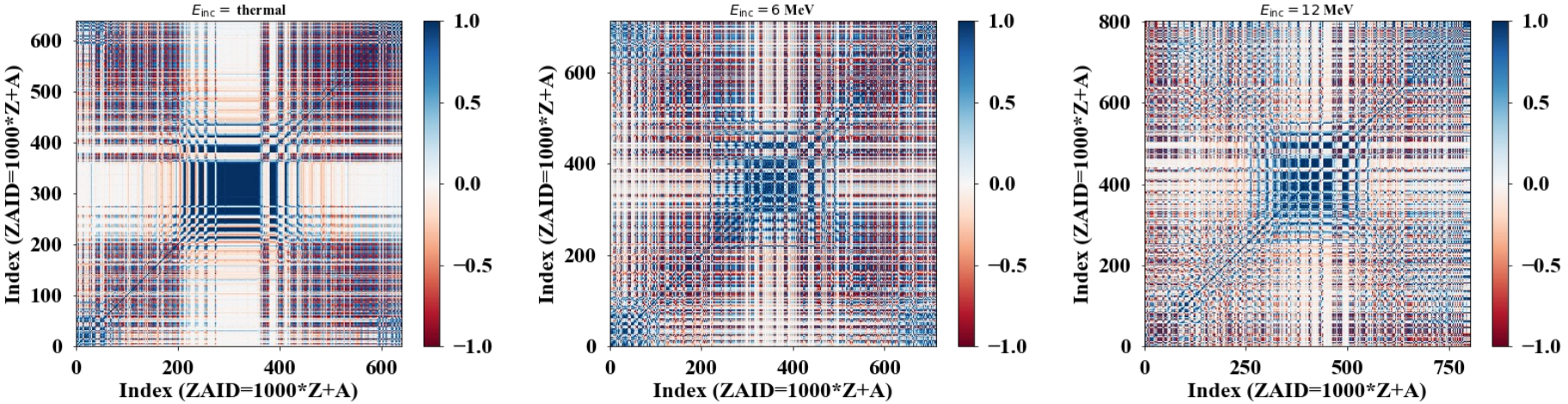






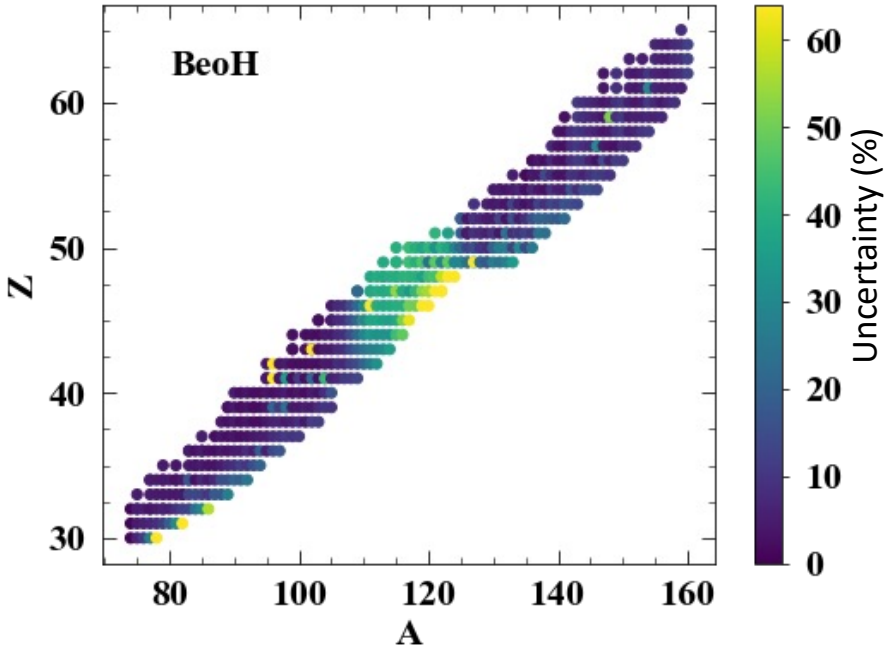


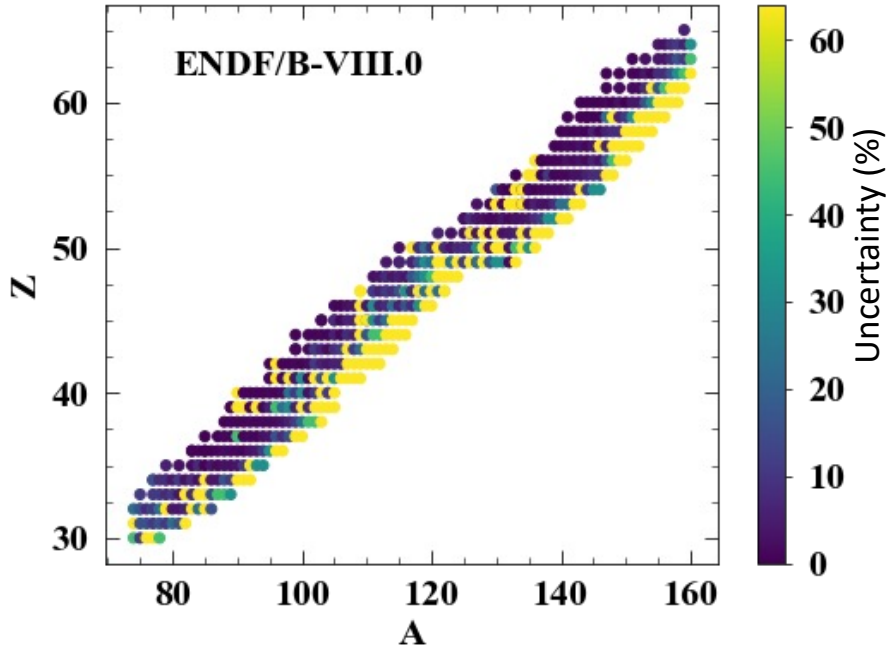
^{235}U(n,f) correlations matrices are being developed at discrete energies from thermal to 20 MeV



Because parameters in the fourth-chance energy region are currently not fit, we currently use the covariance matrix from the highest energy point in the third-chance region for the covariances up to 20 MeV.

Comparison of relative percent uncertainties for $^{235}U(n,f)$ at thermal



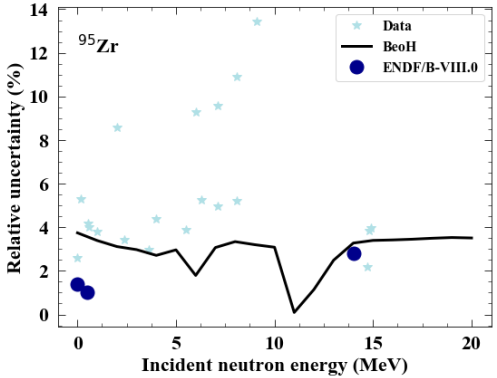


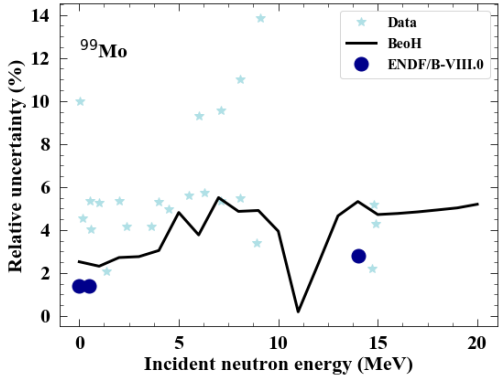
^{235}U(n,f) thermal cumulative FPY percent uncertainty comparison

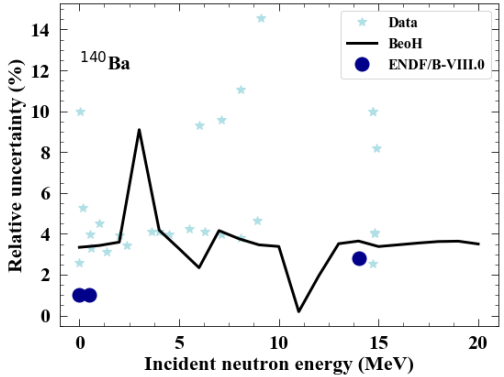
^{235}U(n_{th},f) Y_C(A,Z)	ENDF/B-VIII.0	IRDFF-II	Present (prelim)
^{95}Zr	1.4%	1.0%	3.7%
^{99}Mo	1.4%	1.3%	2.5%
^{103}Ru	1.4%	2.1%	2.2%
^{106}Ru	1.4%	2.3%	7.7%
^{137}Cs	0.5%	1.04%	4.0%
^{140}Ba	1.0%	1.0%	3.3%
^{144}Ce	0.7%	0.9%	8.9%

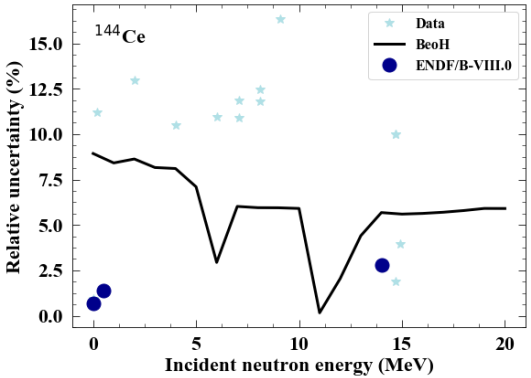
IRDFF-II: A. Trkov, et al., NDS 163 1 (2020)

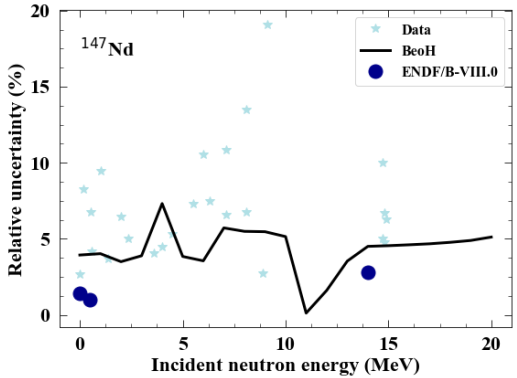
^{235}U(n,f) relative uncertainties for select cumulative FPY

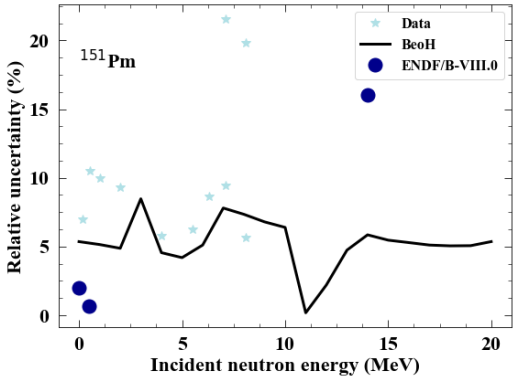




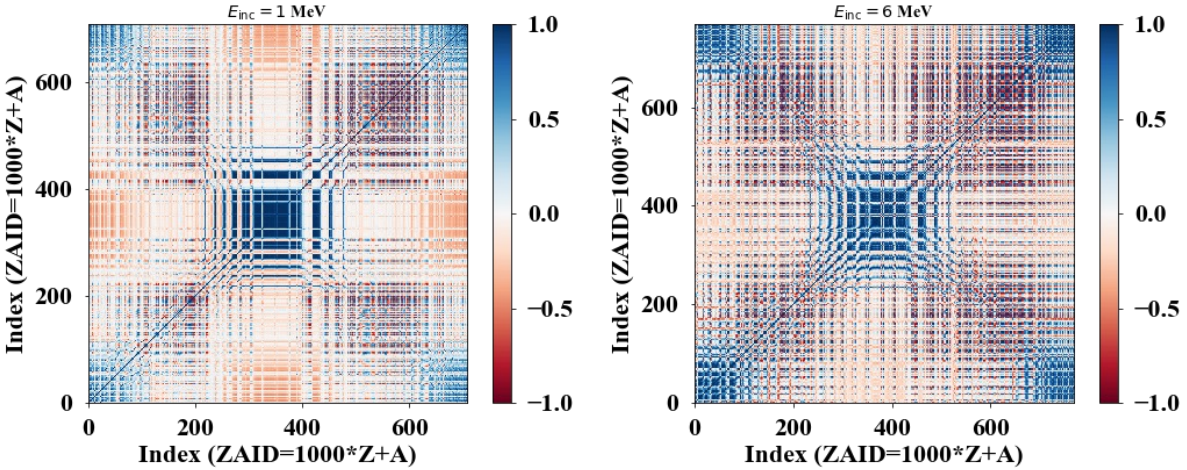






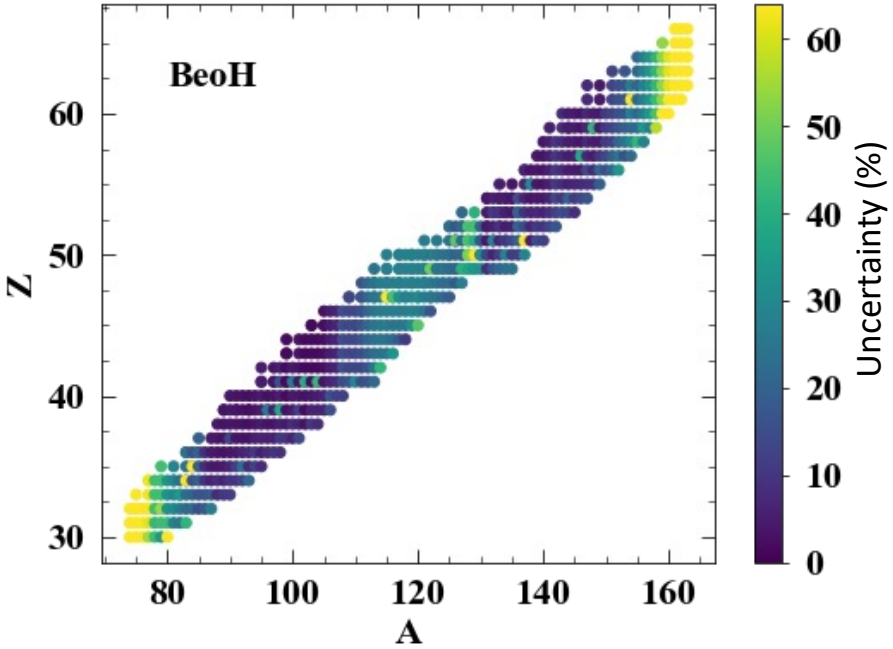


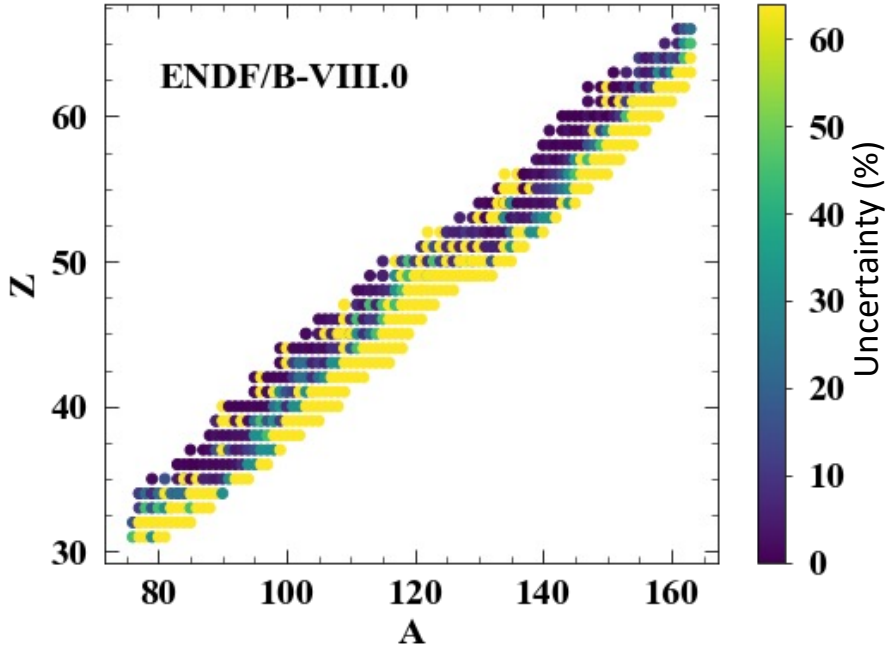
^{238}U(n,f) correlations matrices are being developed



The optimization of the third-chance parameters is still being performed.

Comparison of relative percent uncertainties for ^{238}U(n,f) at 0.5 MeV



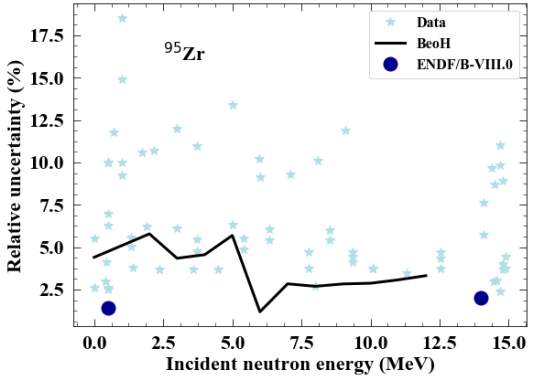


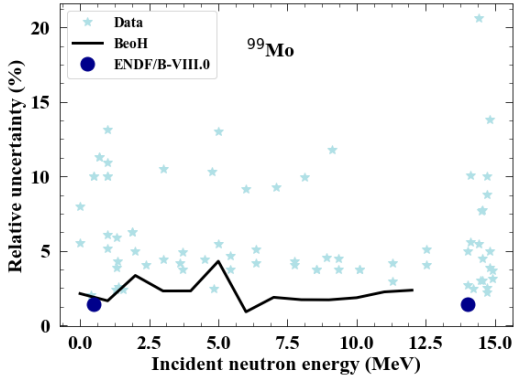
^{238}U(n,f) 0.5 MeV cumulative FPY percent uncertainty comparison

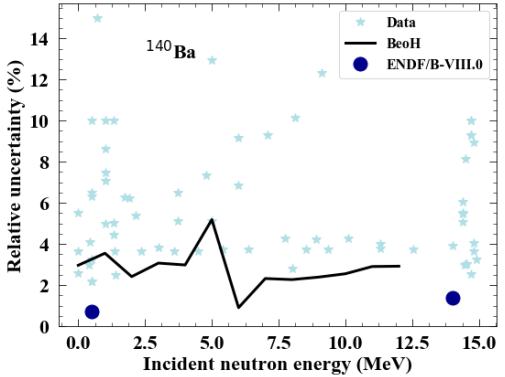
^{238}U($n_{0.5\ MeV}$,f) Y_C(A,Z)	ENDF/B-VIII.0	IRDFF-II	Present (prelim)
^{95}Zr	1.4%	1.6%	4.8%
^{99}Mo	1.4%	1.6%	1.9%
^{103}Ru	1.4%	1.8%	1.8%
^{106}Ru	1.4%	5.3%	5.1%
^{137}Cs	1.0%	2.33%	6.6%
^{140}Ba	0.7%	1.29%	3.3%
^{144}Ce	1.4%	2.25%	5.0%

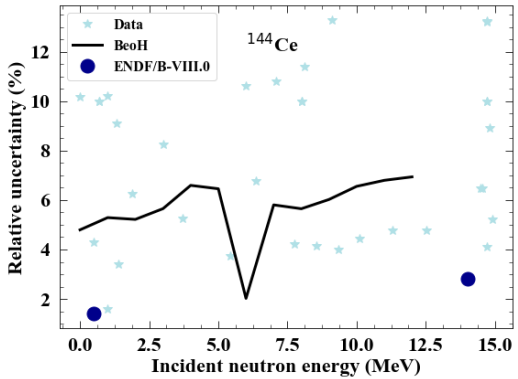
IRDFF-II: A. Trkov, et al., NDS 163 1 (2020)

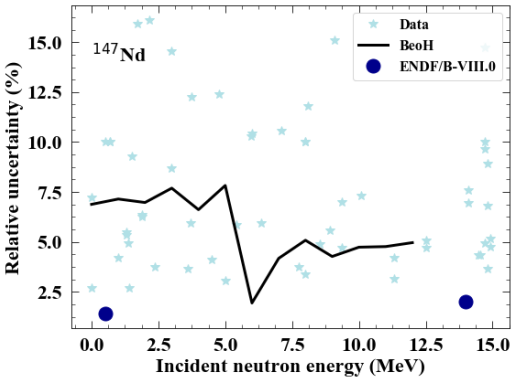
^{238}U(n,f) relative uncertainties for select cumulative FPY

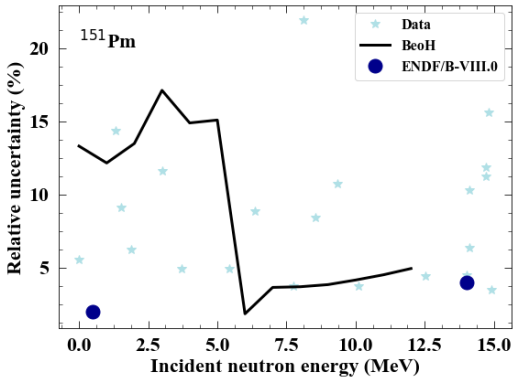












Conclusions and future work

- Covariances are being developed for the FPY re-evaluation, for ^{252}Cf(sf), ^{235,238}U(n,f), and ^{239}Pu(n,f)
- For neutron-induced fission, covariances are being developed from thermal to 20 MeV (optimization for ^{238}U(n,f) after ~12 MeV still in progress)
- Results shown here are preliminary
  - Further optimization will take place – accounting for model stiffness, new decay data from BNL (Sonzogni), updated FPY values from BNL (Mattera) – which could change correlations and uncertainties
- Here, results for the cumulative FPYs were shown, but we have consistent calculations with independent yields and covariances from BeoH
- Currently, only considering covariances at single incident energies (no cross-energy correlations included)
- Covariance format in ENDF is still under development