Fission Yields Modeling and Evaluation

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LANL-led, multi-institute re-evaluation of fission product yields

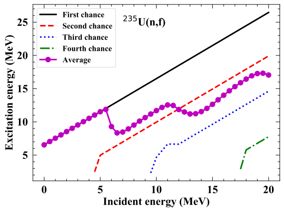
- New measurements, including recent effort to measure short-lived FPY and energy-dependent values
- New/updated models, including BeoH our LANL-developed, Hauser-Feshbach fission fragment decay code (e.g. PRC 103, 014615 (2021))
- Updated experimental FPY data with most recent structure information and updated decay data (consistency between independent and cumulative FPY with decay data)

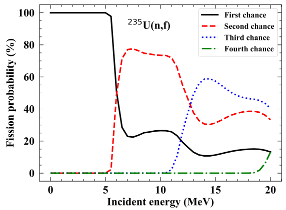
- ENDF/B-VIII.0 still largely based on the evaluation of England and Rider
- Only contains 3 energy points (thermal, fast, and 14 MeV), save an update for 239Pu to include a point at 2 MeV (Chadwick, Kawano, et al., 2010)
- No covariance information

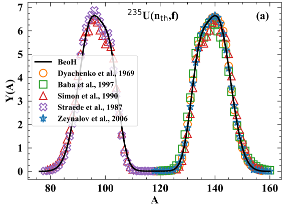
BeoH calculates prompt/delayed fission observables using the statistical Hauser-Feshbach theory

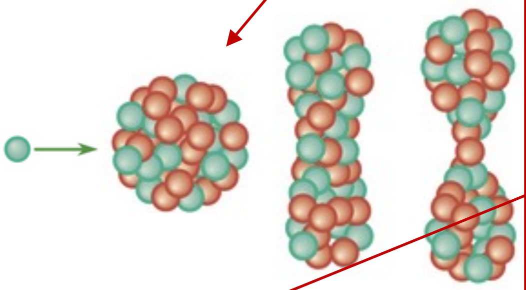
Decay data required for IFY → CFY

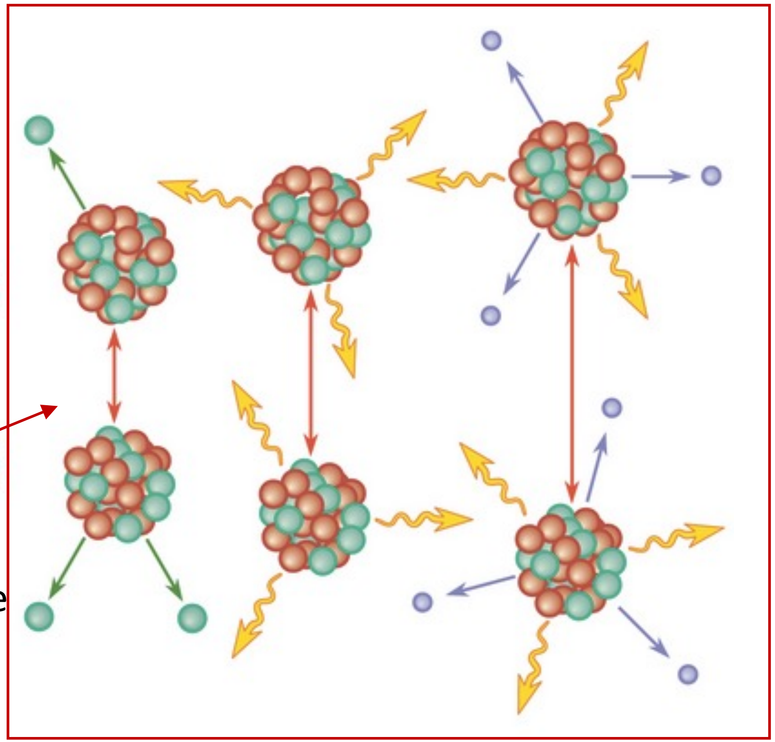
Input from CoH is needed (fission probabilities, excitation energy, etc.)











The initial conditions of the fission fragments are parametrized and fit to data (mass, charge, kinetic energy, spin, parity)

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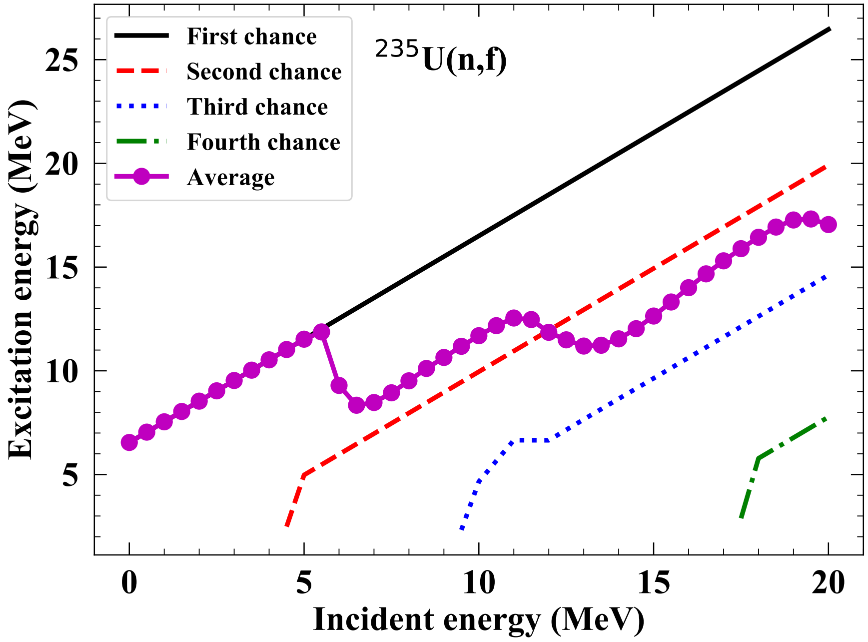
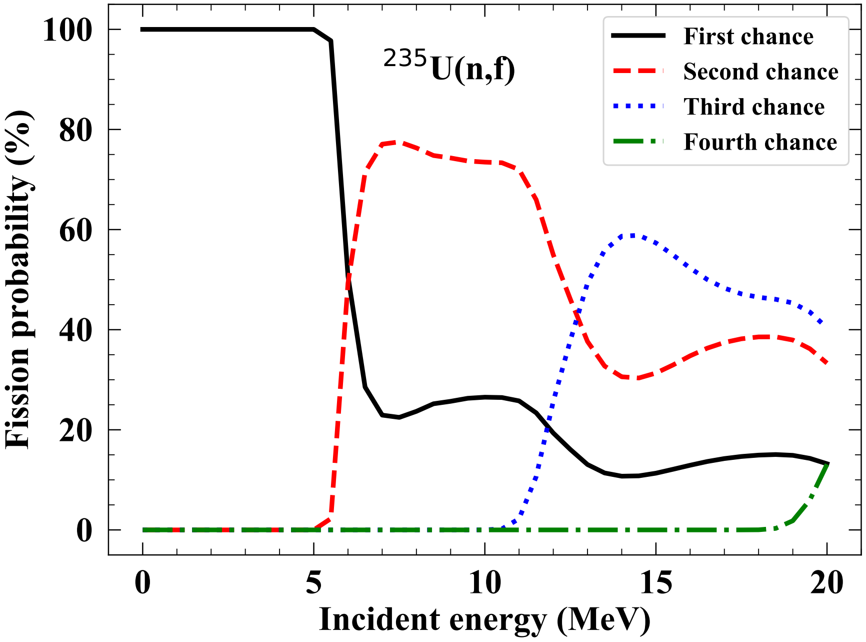
Pre-decay quantities are calculated with CoH

Most probable excitation energy causing fission

$$\langle E_f \rangle(m) = \frac{\int \sigma_f(m, E_x) E_x dE_x}{\int \sigma_f(m, E_x) dE_x}$$

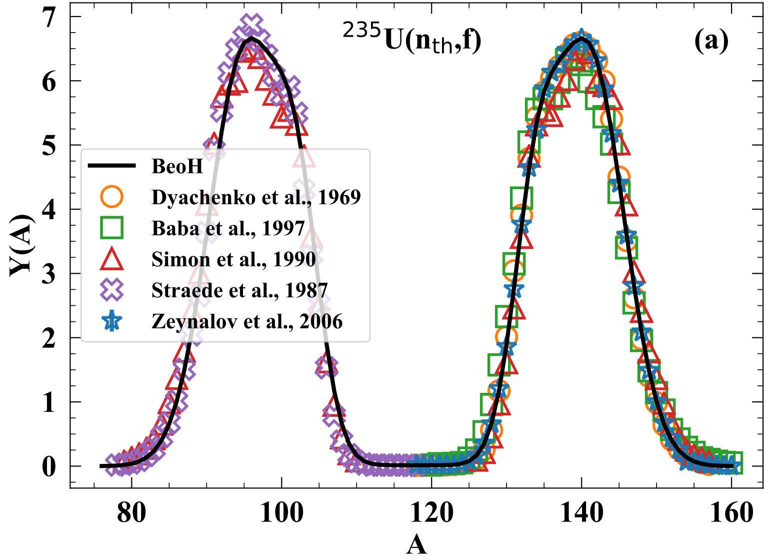


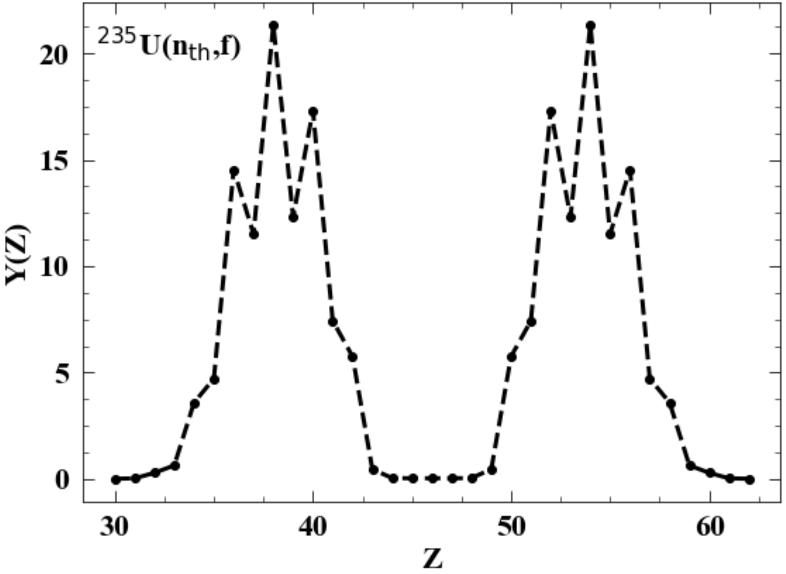
Fission probabilities (fission barriers and level densities can be fit to cross sections)



Fission fragment initial conditions are constrained by experimental data where available

Mass yields, Y(A), are taken to be a sum of Gaussians; each weight, mean, and standard deviation is a function of incident energy (similar to CGMF/FREYA/etc.).



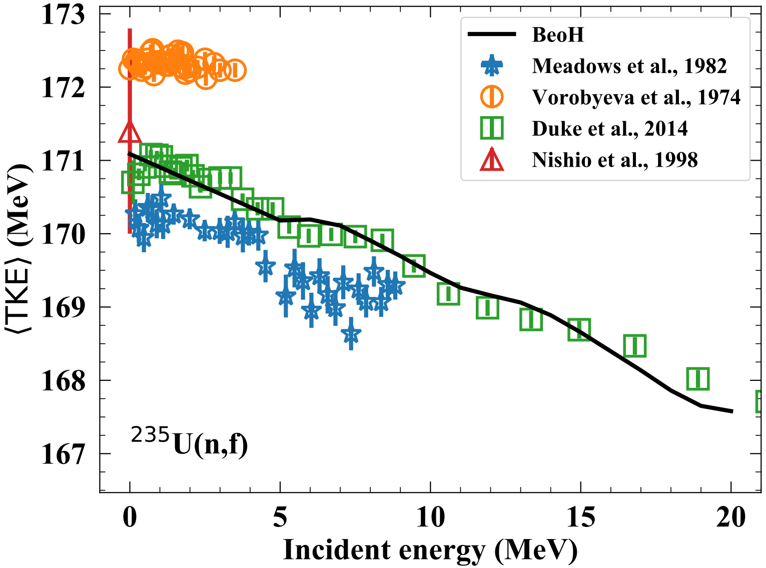


The Wahl systematics are used to calculate the charge distribution, Y(Z|A).

Fission fragment initial conditions are constrained by experimental data where available

<TKE>(E_{inc}) was parametrized to reproduce the shape of the data of Duke, et al., up to E_{inc}=20 MeV.

<TKE>(A) is Gaussian, with the means and widths fit to mass-dependent data.



The spin distribution is proportional to the available states in the level density formula, with an adjustable scaling factor on the spin cut-off parameter, f.

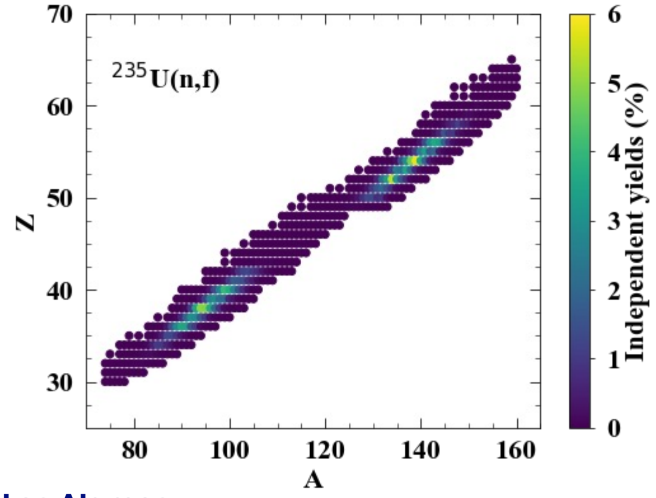
$$R_{l,h}(J) = \frac{J+1/2}{f^2\sigma_{l,h}(U)} \exp\left\{-\frac{(J+1/2)^2}{2f^2\sigma_{l,h}^2(U)}\right\}$$

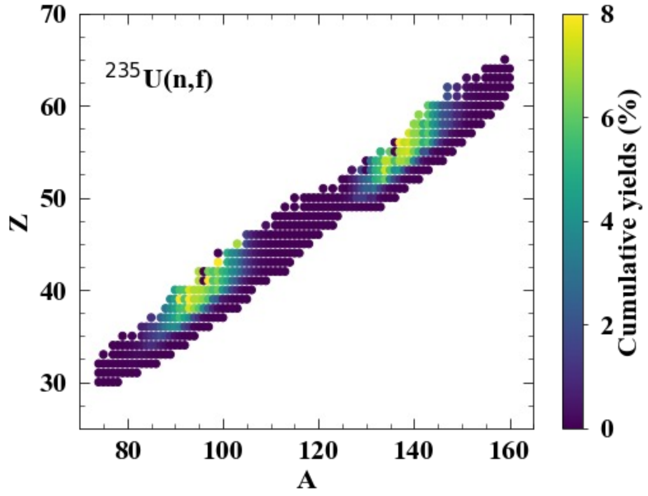
Positive and negative parities are taken to be equally probable.

Independent yields to cumulative yields

Once the initial conditions of all fragments are determined, the Hauser-Feshbach statistical decay is performed for each fission fragment.

Then, a time-independent calculation is performed, using decay data library information (from ENDF/B-VIII.0) to calculate the cumulative yields from the independent yields. Isomeric states are kept track of for the independent and cumulative yields.





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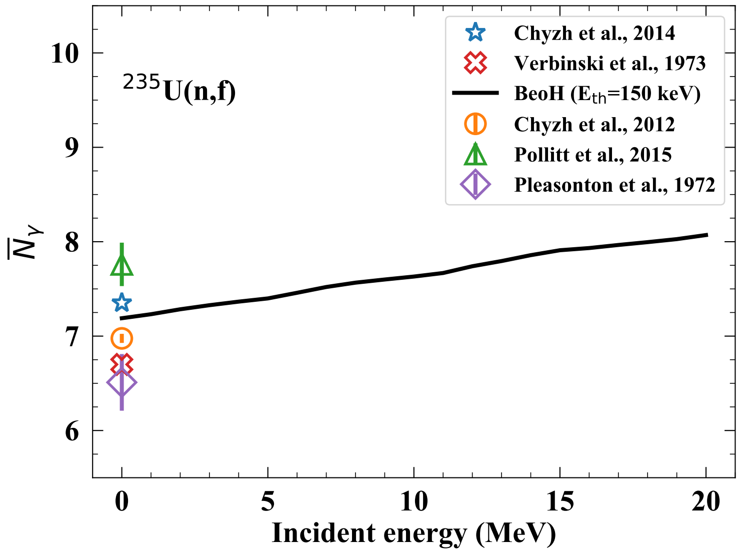
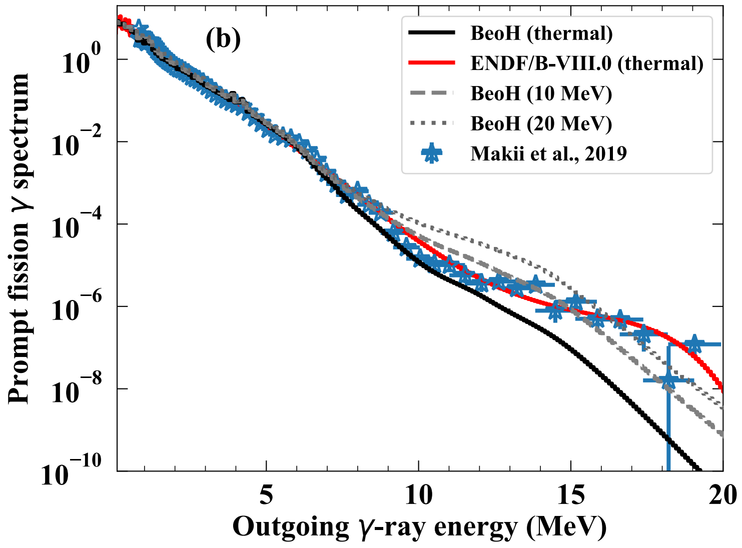
Prompt gamma-ray observables can be calculated

Average prompt γ-ray multiplicity



Experimental energy cut-offs can be included, for better comparison to data

Prompt γ-ray energy spectrum



Using BeoH, we can see trends in the tail of the spectrum as the incident energy increases (not currently included in ENDF/B-VIII.0)

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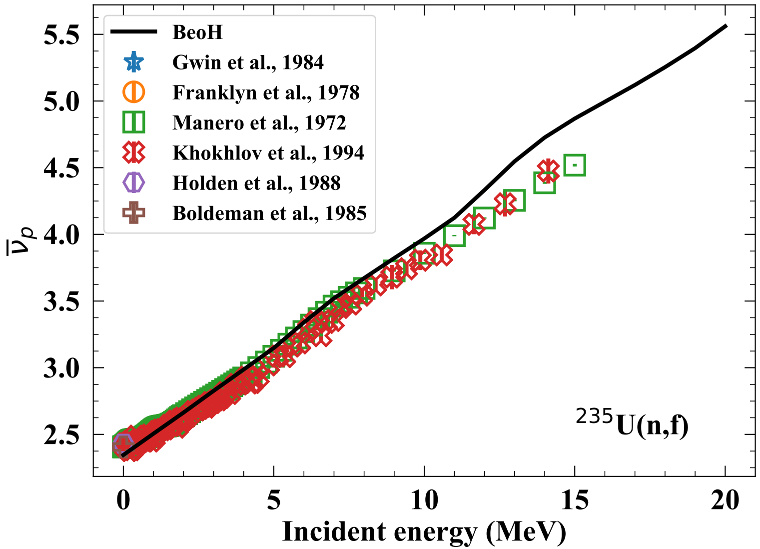
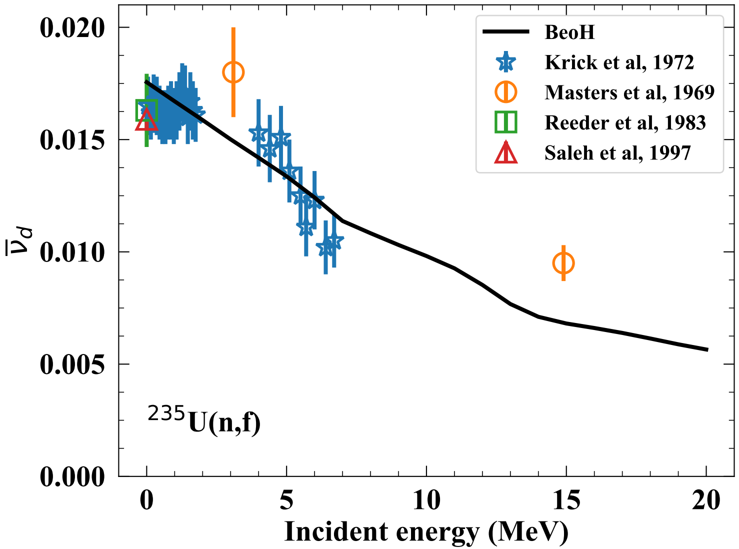
Prompt and delayed neutron observables can be calculated

Average prompt neutron multiplicity



Average delayed neutron multiplicity



There is good agreement between the BeoH calculations as a function of incident energy and the experimental data but still room in the model space for improvement

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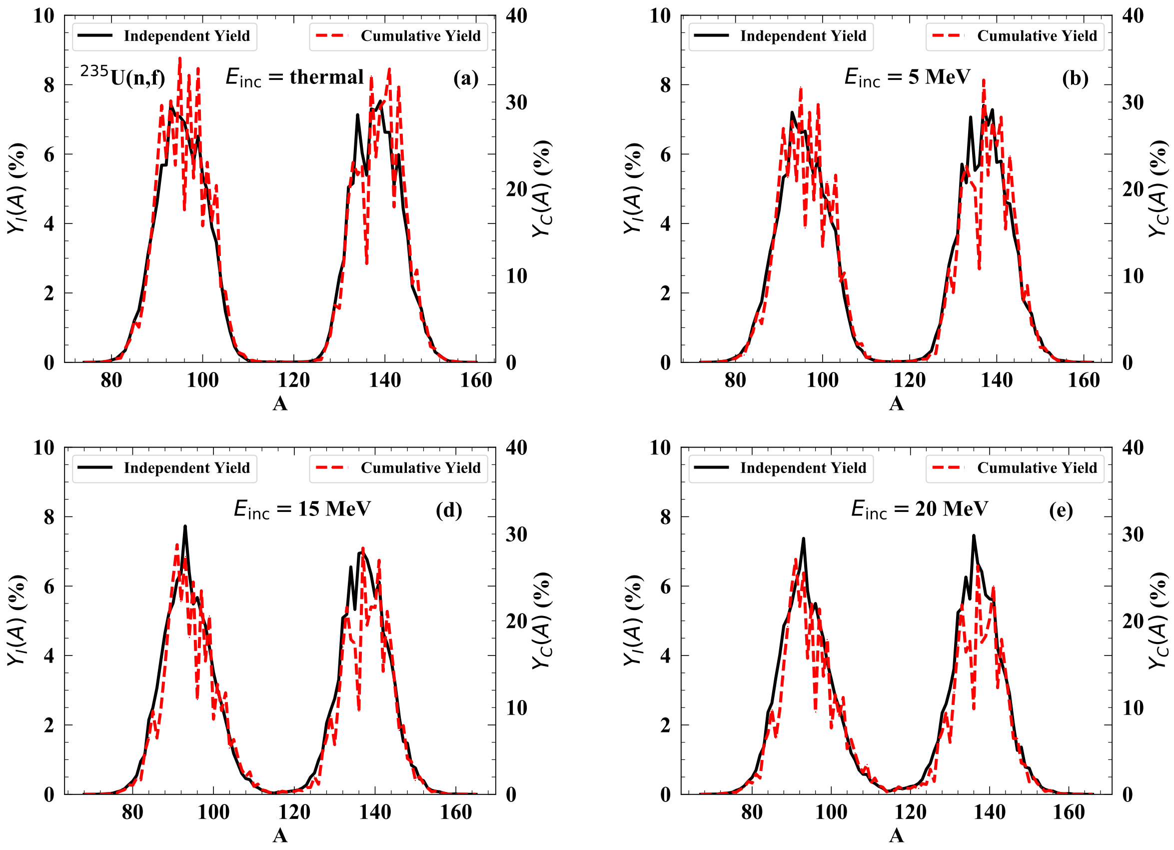
Independent and cumulative mass yields



Both independent and cumulative yields show changes as the incident neutron energy is increased

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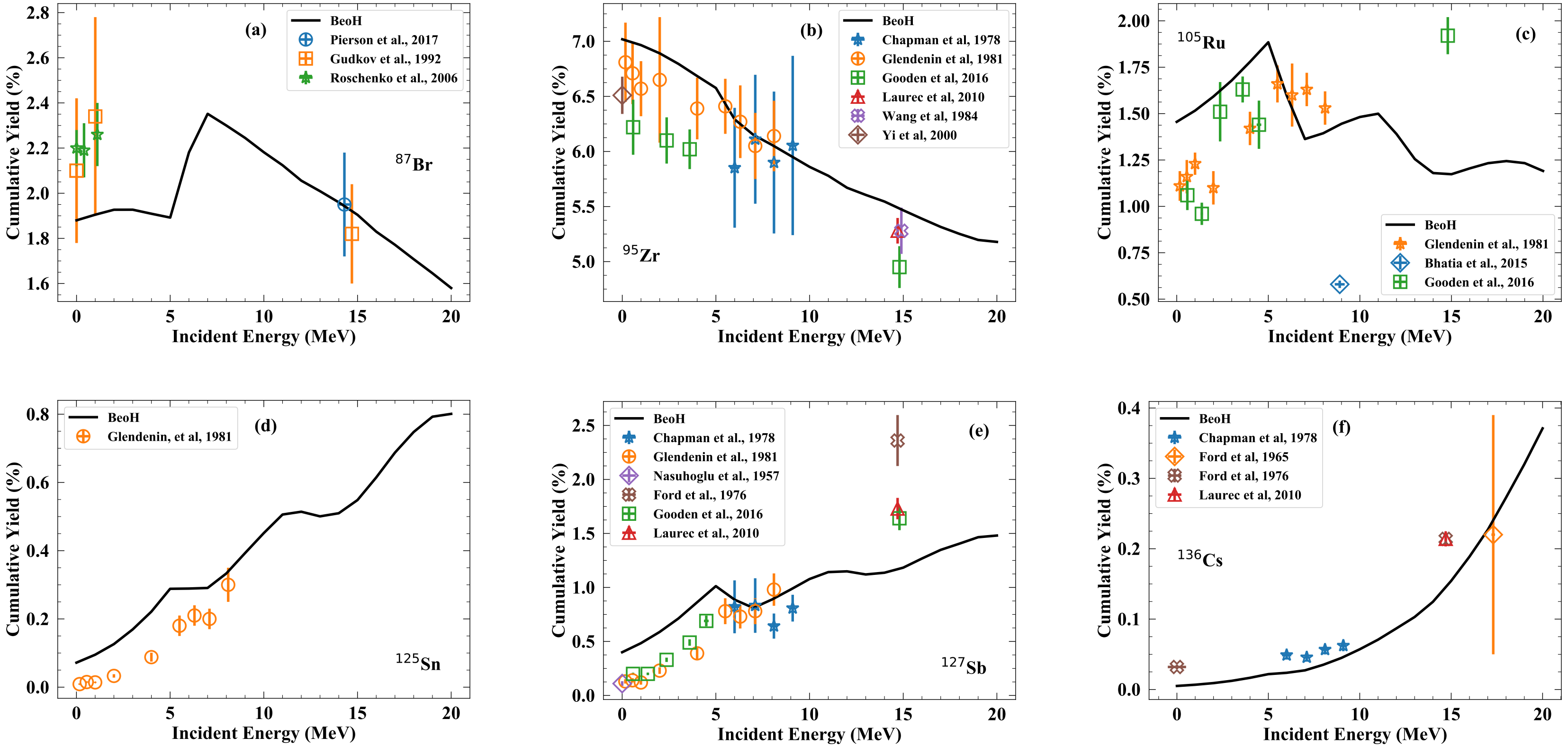
Cumulative fission product yields already show reasonable agreement without specific optimization



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General Kalman filter description

Updated parameters and parameter covariances are calculated using a linear assumption

$$\mathbf{x}_1 = \mathbf{x}_0 + \mathbb{P}\mathbb{C}^T\mathbb{V}^{-1}(\phi - f(\mathbf{x}_0))$$

$$\mathbb{P} = (\mathbb{X}^{-1} + \mathbb{C}^T\mathbb{V}^{-1}\mathbb{C})^{-1}$$

Parameter vectors

Data vector

Data covariance

Model calculation vector

Parameter covariance

Sensitivities

$$\mathbb{C}_{ij} = \frac{\Delta f_i(\mathbf{x})}{\Delta x_j}$$

Model predictions and covariance are updated

$$\Phi = f(\mathbf{x}_1) \qquad \mathbb{F} = \mathbb{C}\mathbb{P}\mathbb{C}^T$$

Optimization details

- Prompt and delayed average neutron multiplicity included in the optimization to further constrain input parameters that are not well-constrained by the cumulative fission product yields
- Currently, data from EXFOR is being used, which has been nominally curated to remove some discrepant data
  - Templates of experimental uncertainties should be used
  - BNL is sending revised FPY values based on current structure data and data that is not included in EXFOR (A. Mattera), ^{238}U(n,f) and ^{239}Pu(n,f) received already
  - BNL has shared updated decay data, which will be incorporated (A. Sonzogni)
  - Comparison against data used in previous LANL/England and Rider evaluation has to be done
- We first perform a bulk optimization to experimental cumulative FPYs (current status); next, tuning will be undertaken to ensure that our model is not too rigid to reproduce all important data (in progress)

Fission product yield evaluations under development

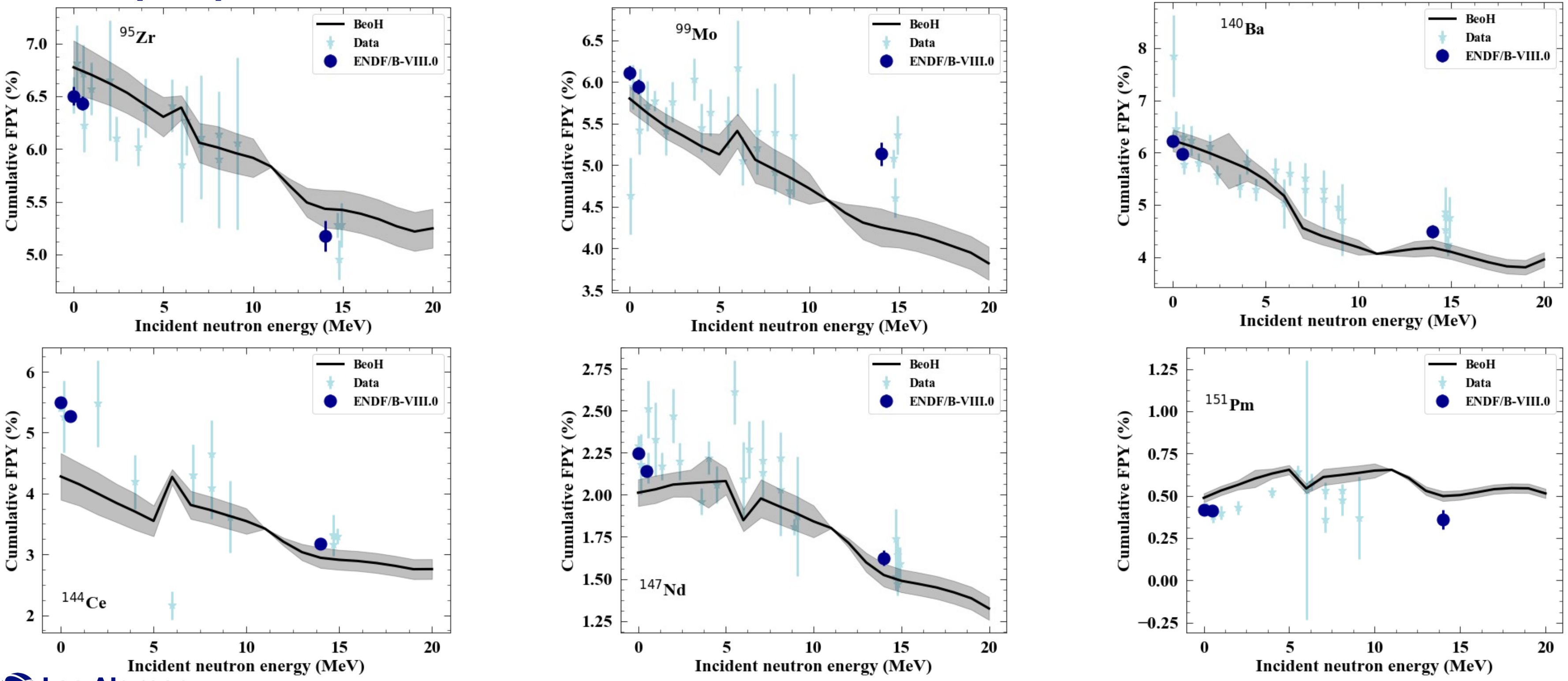
- ^{252}Cf spontaneous fission
  - Bulk fitting has been performed
  - Covariances are calculated
- ^{235}U neutron induced fission - thermal to 20 MeV
  - Bulk fitting has been performed up to 20 MeV
  - Covariances calculated up to 20 MeV
- ^{238}U neutron induced fission – thermal to 20 MeV
  - Bulk fitting has been performed up to 20 MeV
  - Covariances calculated up to 20 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.

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

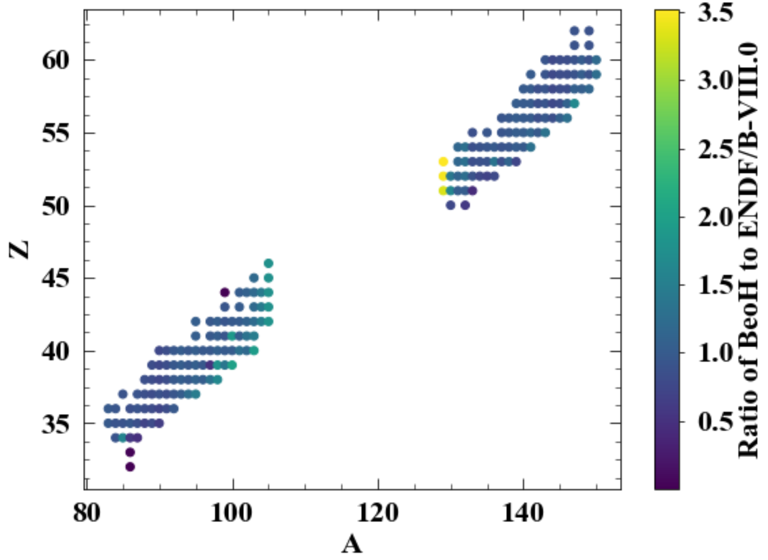
- First-chance parameters fit then fixed, second-chance parameters fit then fixed, third-chance parameters fit then fixed.
- Excitation energy sharing parameters only fit in the first-chance energy region – then kept the same for the other compounds (initial optimizations are to $\boldsymbol{\nu}$(A), 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.
- However, work is in progress to calculate sensitivities from thermal to 20 MeV to fit all energies at once (and compare to previous calculations)

Select cumulative FPYs up from thermal to 20 MeV for $^{235}U(n,f)$

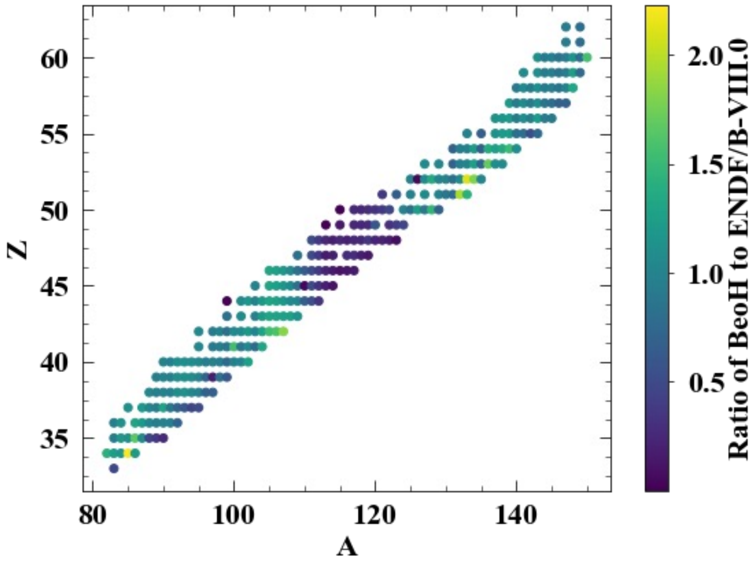


Reasonable agreement with the current ENDF evaluation

E_{inc} = thermal

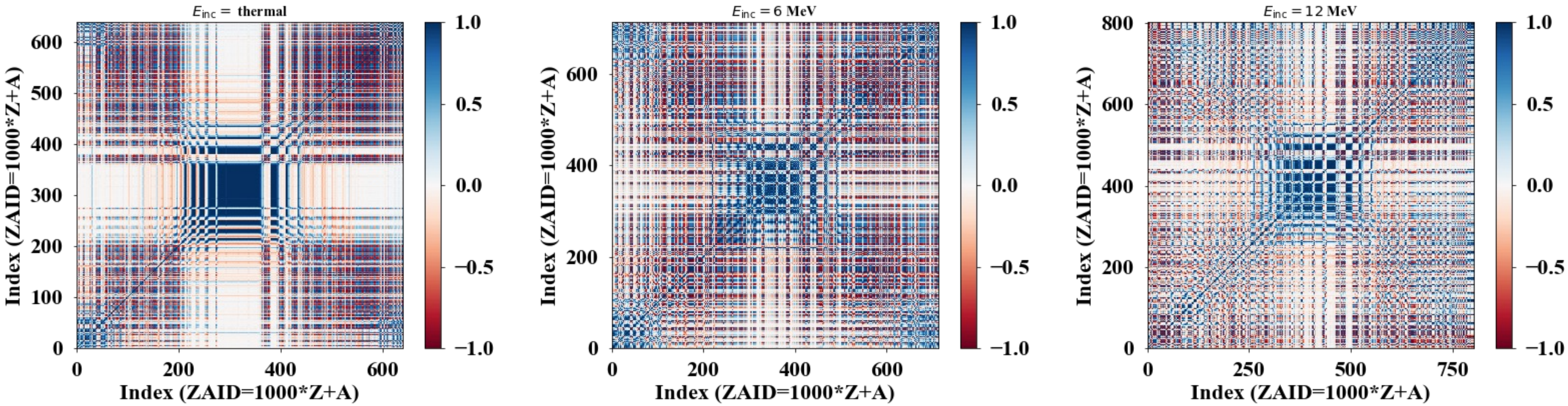


E_{inc} = 14 MeV



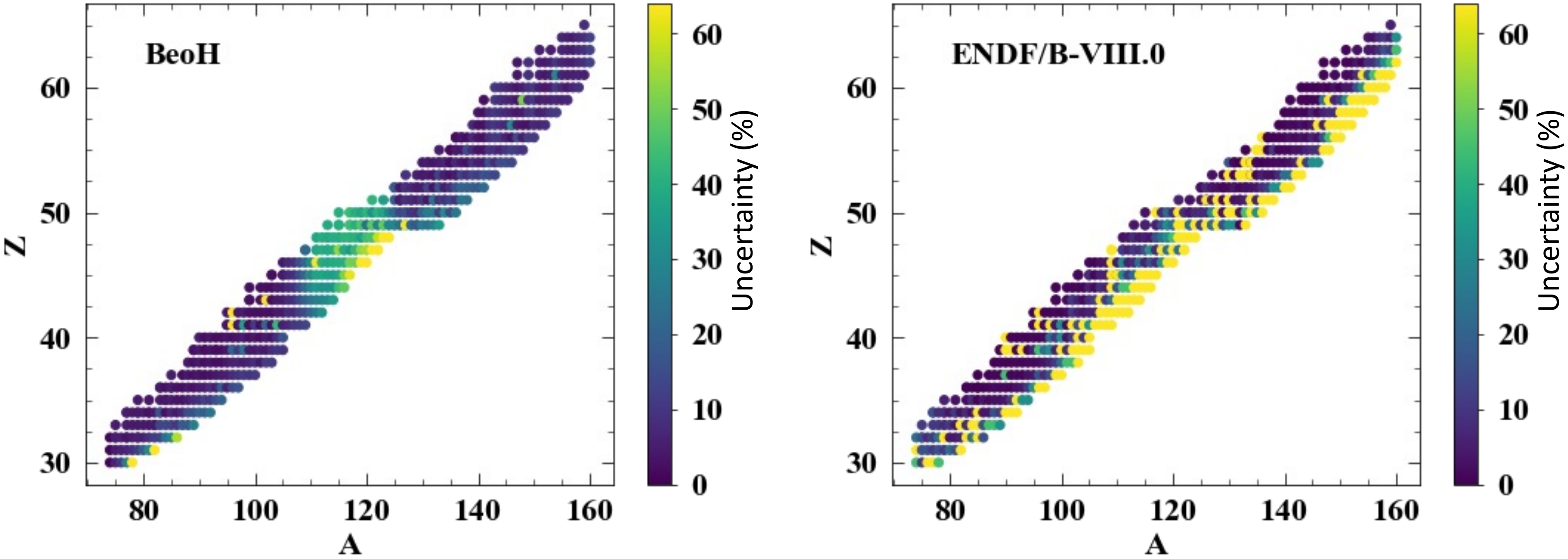
We only plot cumulative FPYs where the ENDF value is > 0.5%.
The discrepancy grows away from the peaks of the distribution.

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

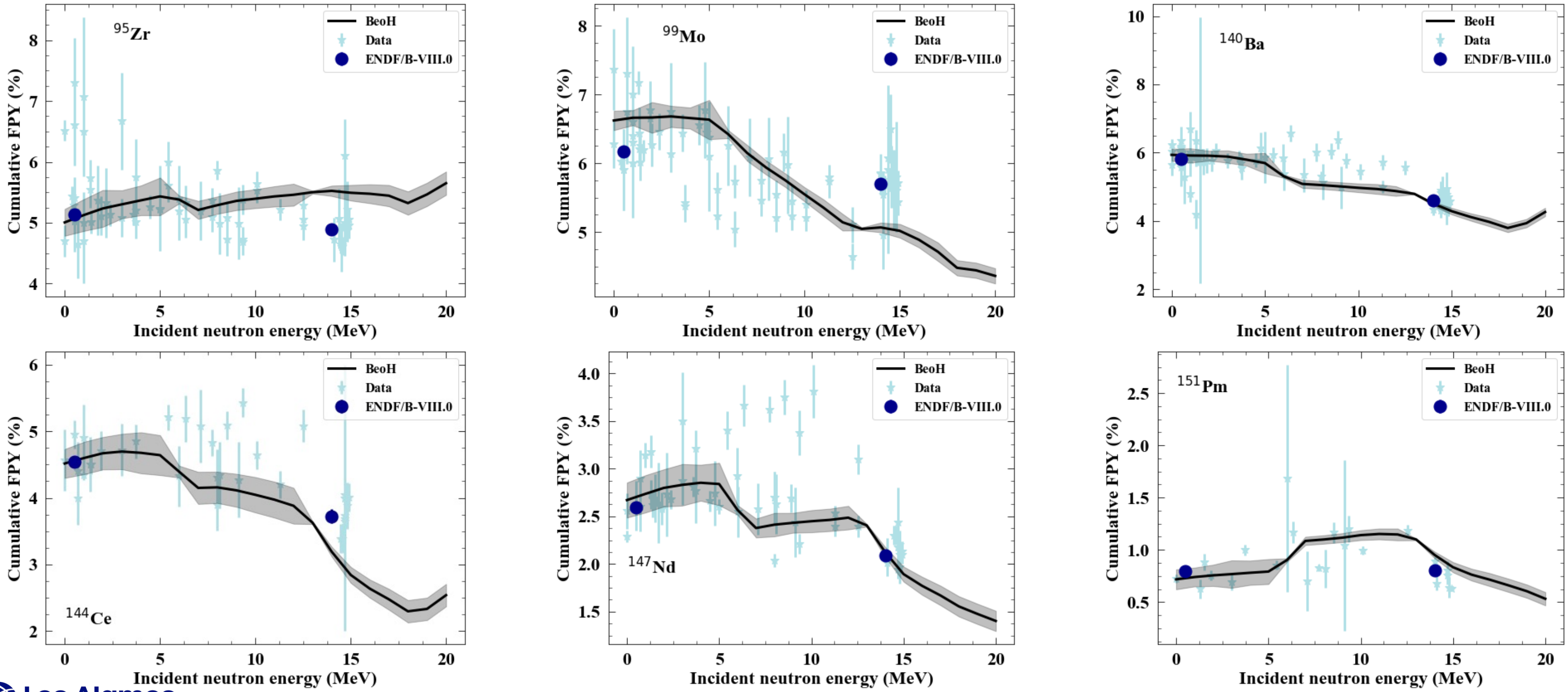


Because parameters in the fourth-chance energy region are currently not fit, we currently use the covariance matrix from the highest energy point in the third-chance region for the covariances up to 20 MeV.

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

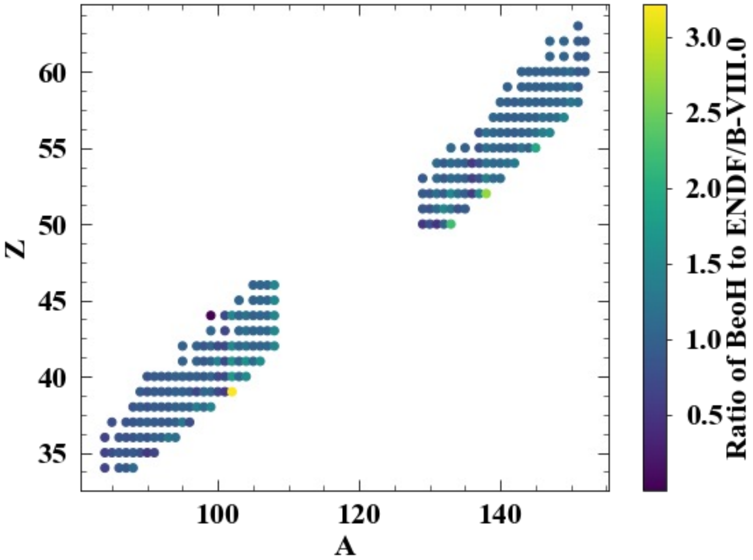


Select cumulative FPYs up from thermal to 20 MeV for ^{238}U(n,f)

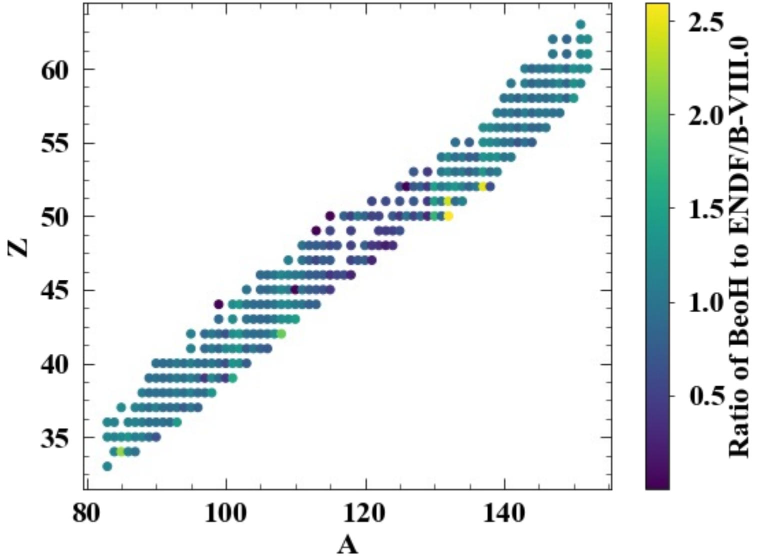


Reasonable agreement with the current ENDF evaluation

E_{inc} = 0.5 MeV

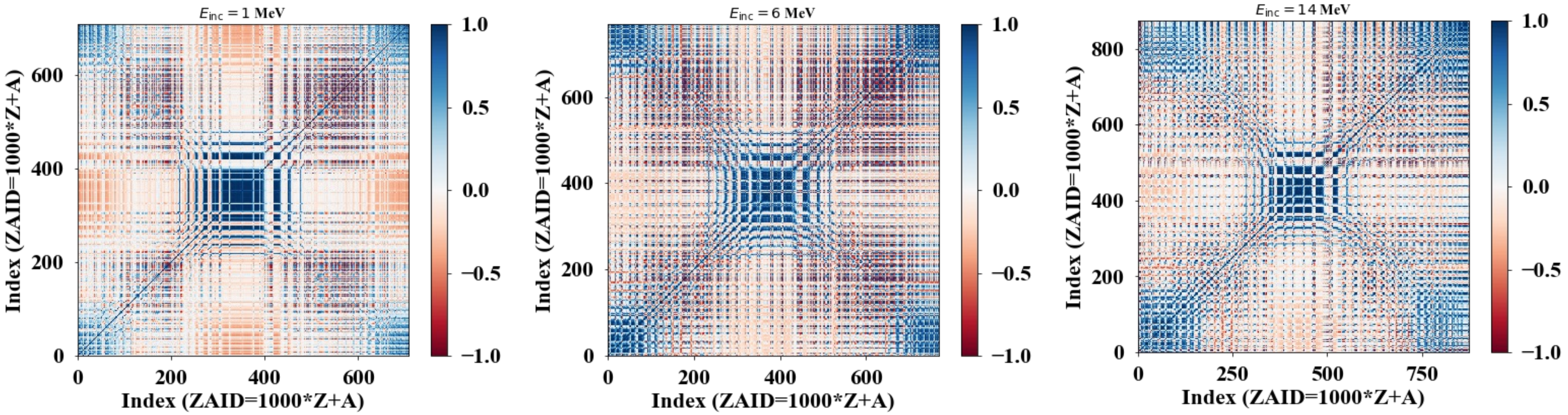


E_{inc} = 14 MeV



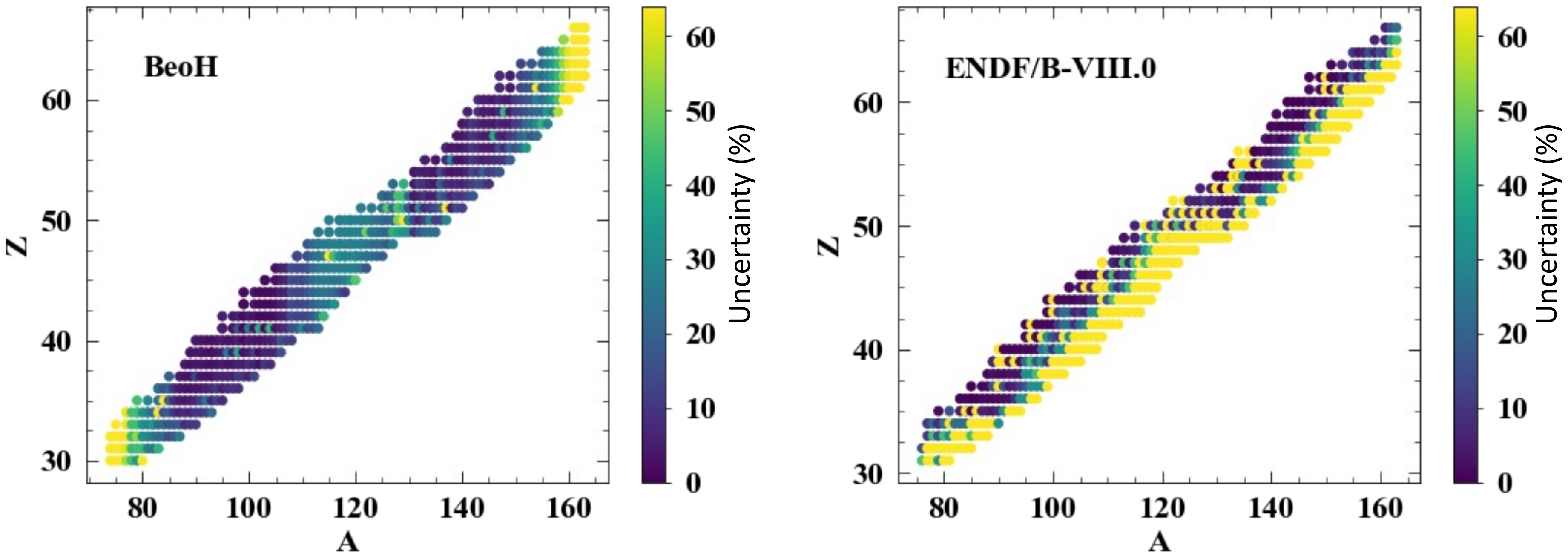
We only plot cumulative FPYs where the ENDF value is > 0.5%.
The discrepancy grows away from the peaks of the distribution.

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

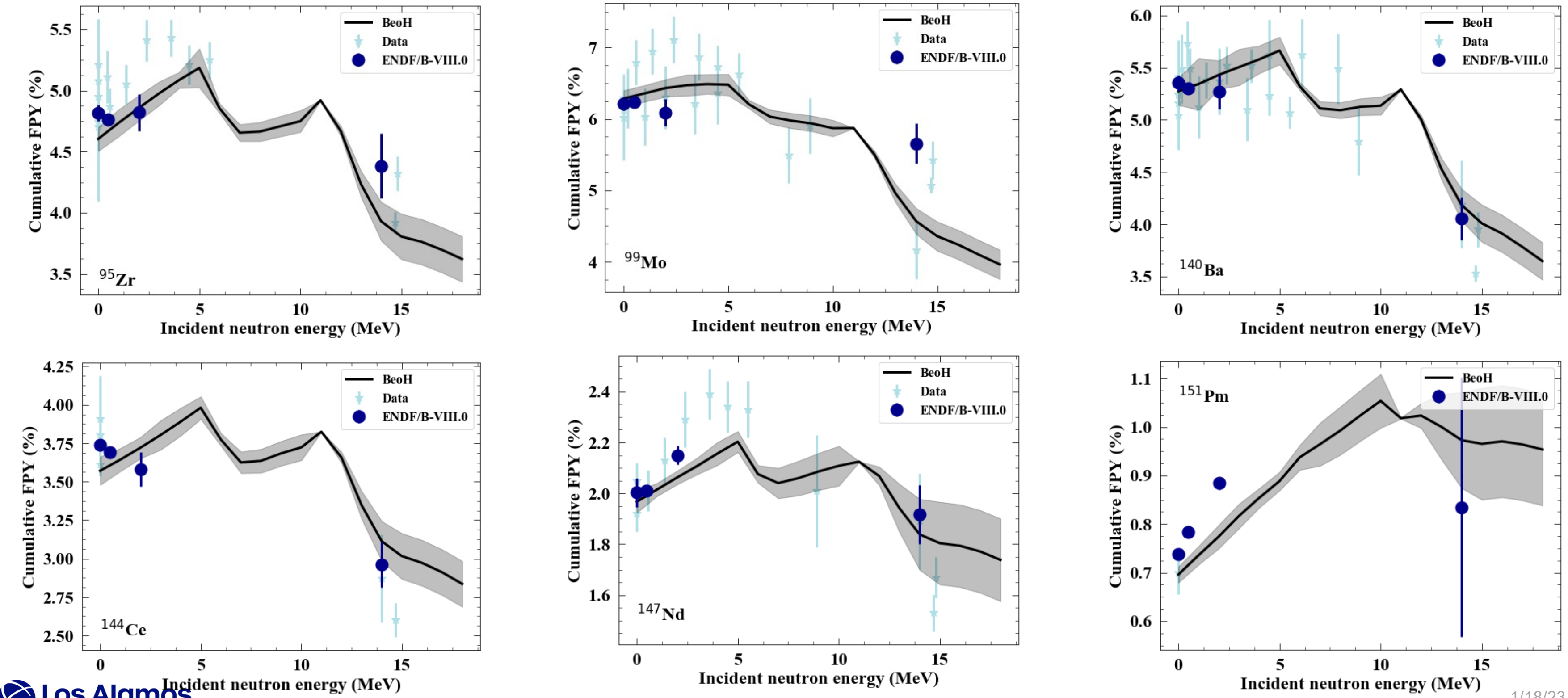


Because parameters in the fourth-chance energy region are currently not fit, we currently use the covariance matrix from the highest energy point in the third-chance region for the covariances up to 20 MeV.

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

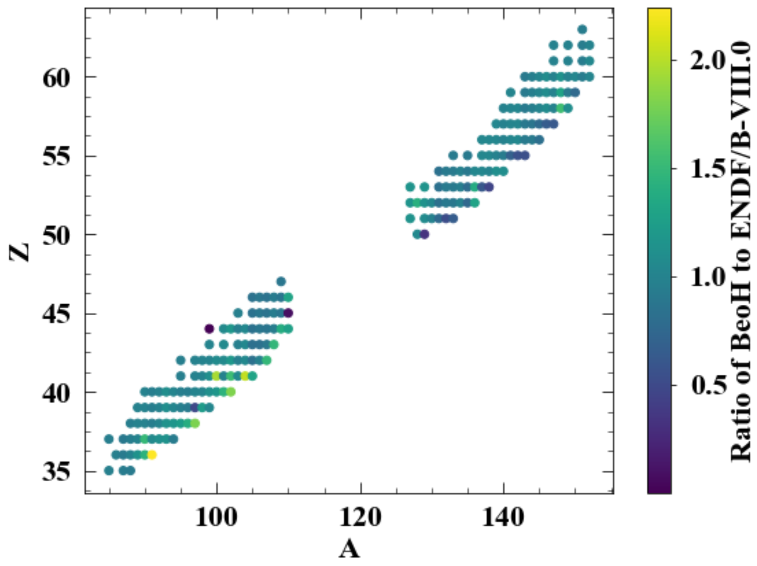


Select cumulative FPYs up from thermal to 20 MeV for $^{239}Pu(n,f)$

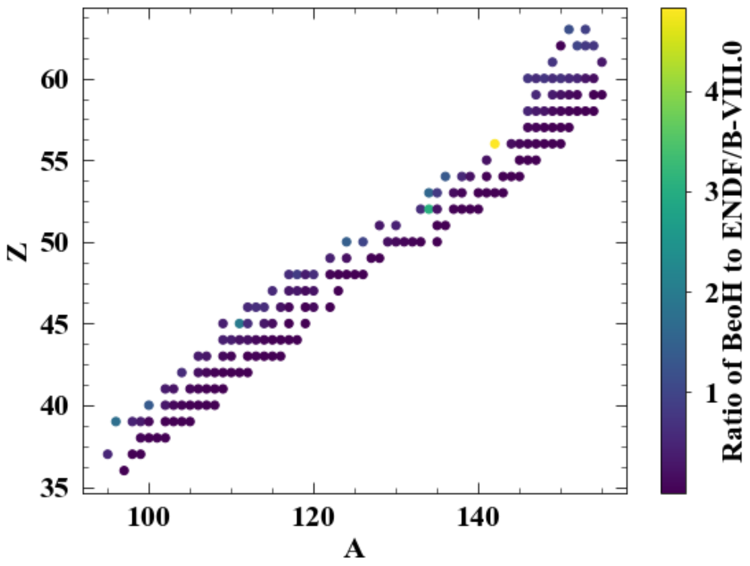


Reasonable agreement with the current ENDF evaluation

E_{inc} = thermal

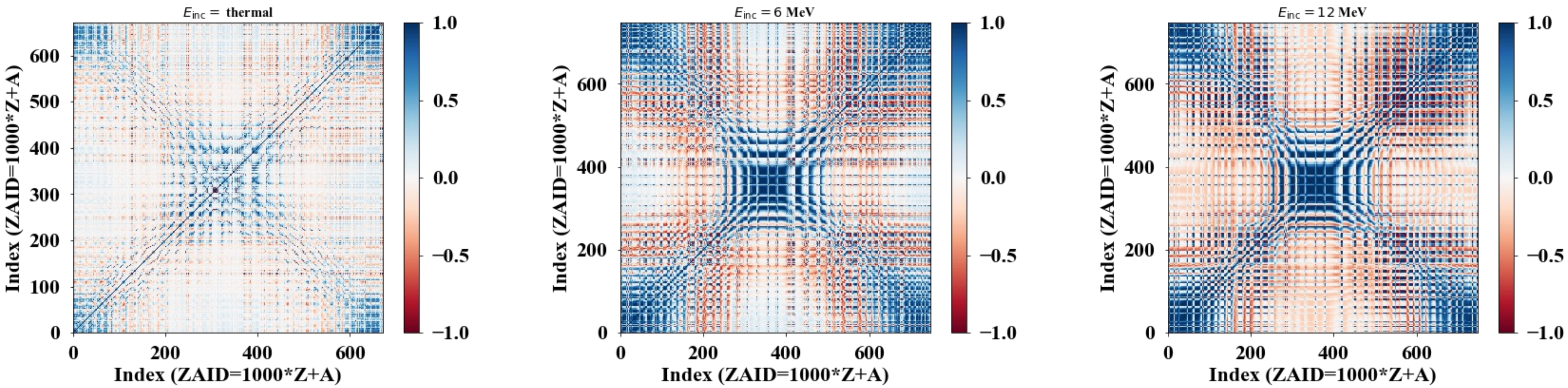


E_{inc} = 14 MeV



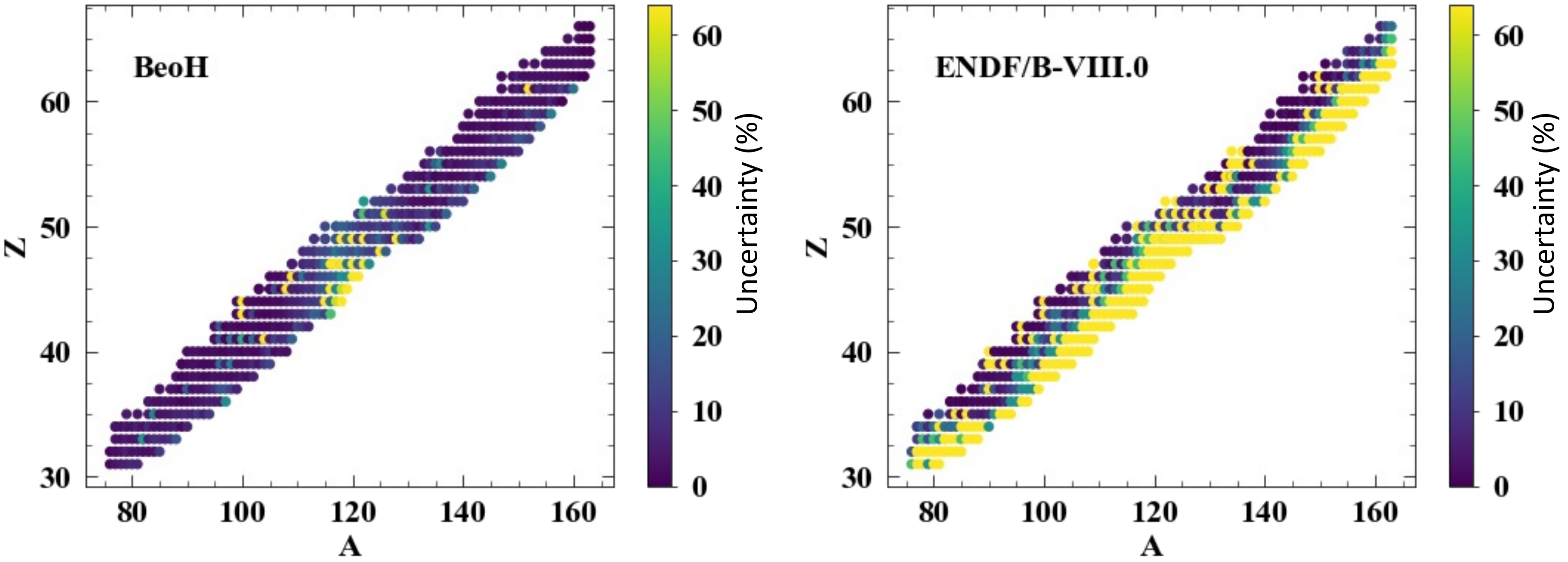
We only plot cumulative FPYs where the ENDF value is > 0.5%.
The discrepancy grows away from the peaks of the distribution.

^{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



Conclusions and path forward

- Independent and cumulative FPYs are being re-evaluated, with covariances, for ^{252}Cf(sf), ^{235,238}U(n,f), and ^{239}Pu(n,f)
- Tweaking of BeoH Y(A) shape underway to account for stiffness in the model that currently doesn't consistently calculate important FPYs
- Currently, only considering covariances at single incident energies (no cross-energy correlations included)
- More work on the database and uncertainties:
  - Updated FPY values from BNL
  - Updated decay data from BNL
  - Comparing database from England and Rider evaluation with current fitted data
  - Template of expected experimental uncertainties
  - Calculating R values of critical assemblies, other validation needed