Status of the updated FPY evaluation for ^{252}Cf(sf), ^{235,238}U(n,f), and ^{239}Pu(n,f)

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

CSEWG, November 3, 2022

LA-UR-22-31449

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

Evaluation methodology for fission product yields

- Combination of experimental data and model calculations through a Kalman filter optimization
  - Includes new experimental data, including recent effort to measure short-lived FPY and energy-dependent values
  - BeoH – LANL-developed, Hauser-Feshbach fission fragment decay code (e.g. PRC 103, 014615 (2021) and references therein)
  - Updated experimental FPY data with most recent structure information and updated decay data (consistency between independent and cumulative FPY with decay data)
- Covariances are calculated consistently from the Kalman filter (see talk during Wednesday's covariance session)
- R-values are not currently included in the fitting procedure but are instead being used for validation

Optimization details

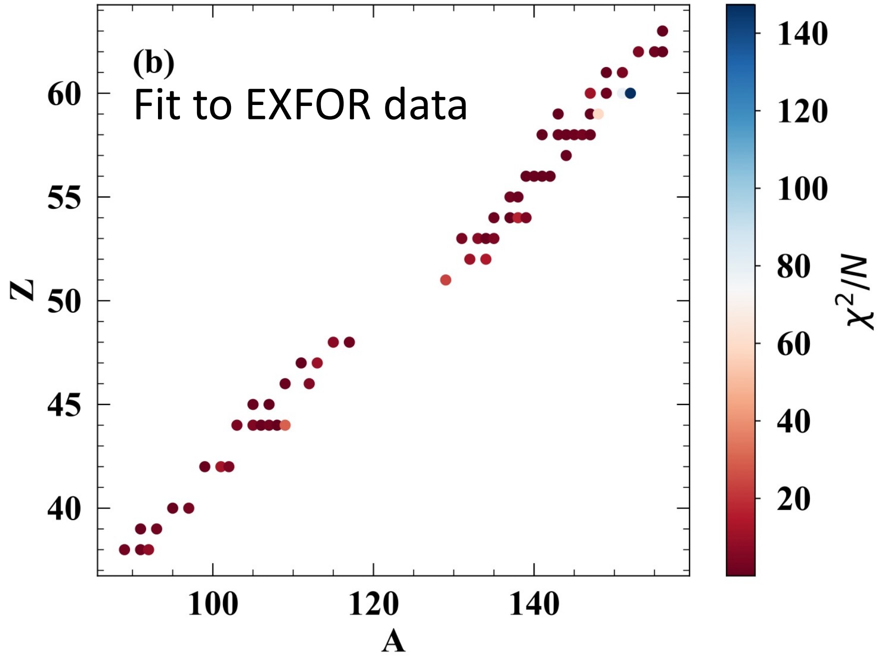
- Prompt and delayed average neutron multiplicity included in the optimization to further constrain input parameters that are not well-constrained by the cumulative fission product yields
- Currently, data from EXFOR is being used, which has been nominally curated to remove some discrepant data
  - Templates 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) 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

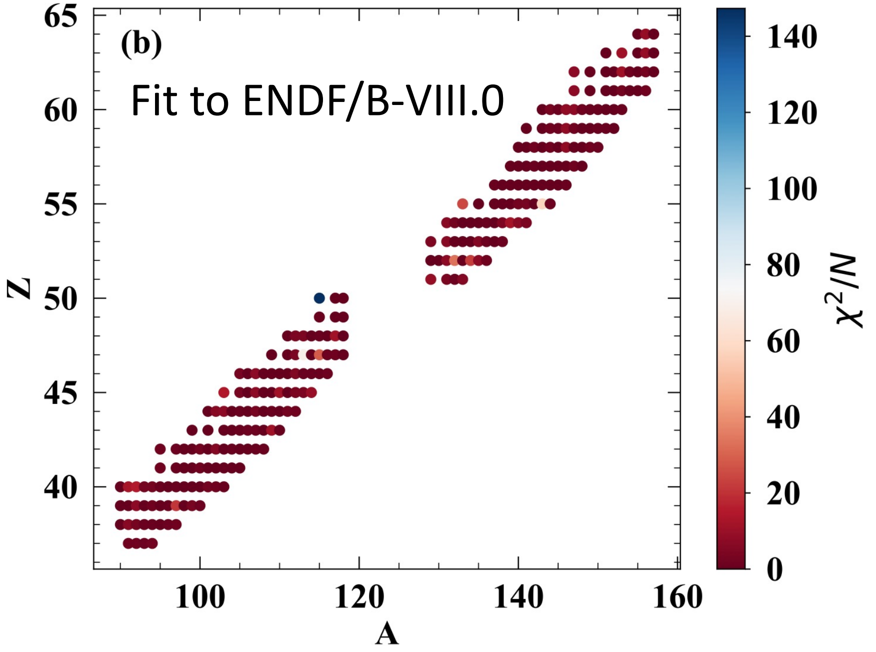
- ^{252}Cf spontaneous fission
  - Bulk fitting has been performed
  - Covariances are calculated
- ^{235}U neutron induced fission - thermal to 20 MeV
  - Bulk fitting has been performed up to 20 MeV
  - Covariances calculated up to 20 MeV
- ^{238}U neutron induced fission – thermal to 20 MeV
  - Bulk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

^{252}Cf(sf) cumulative FPY data overview (taken from EXFOR, FPY>1%)



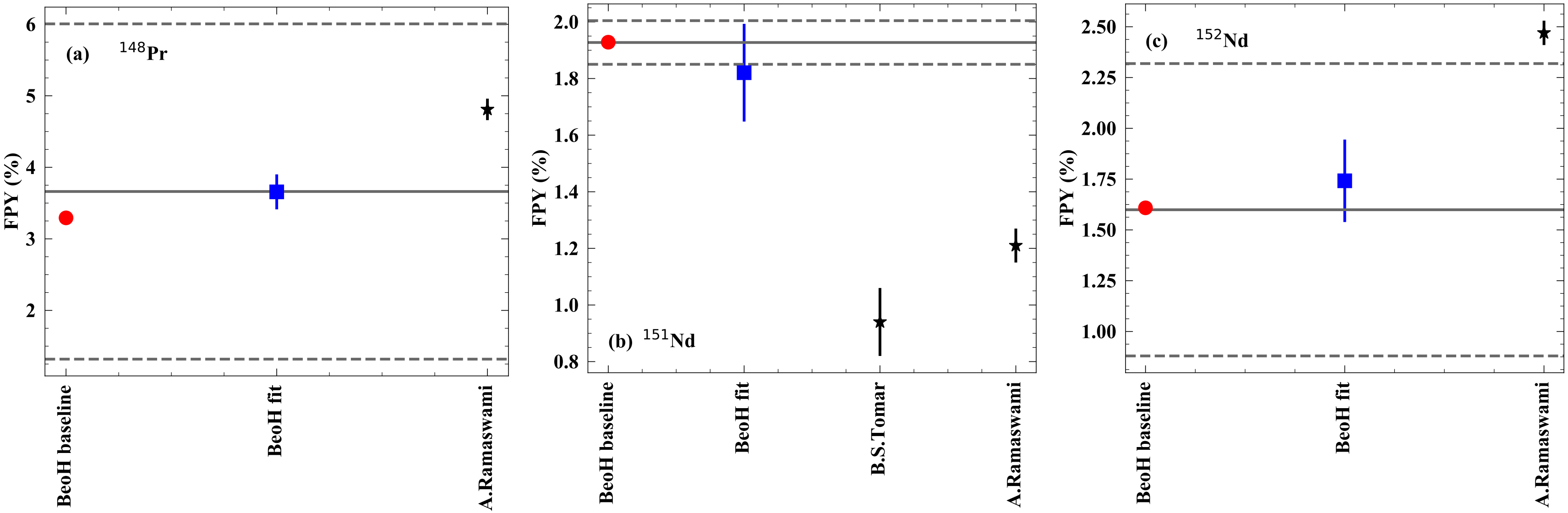
$\chi^2/N = 6.16$



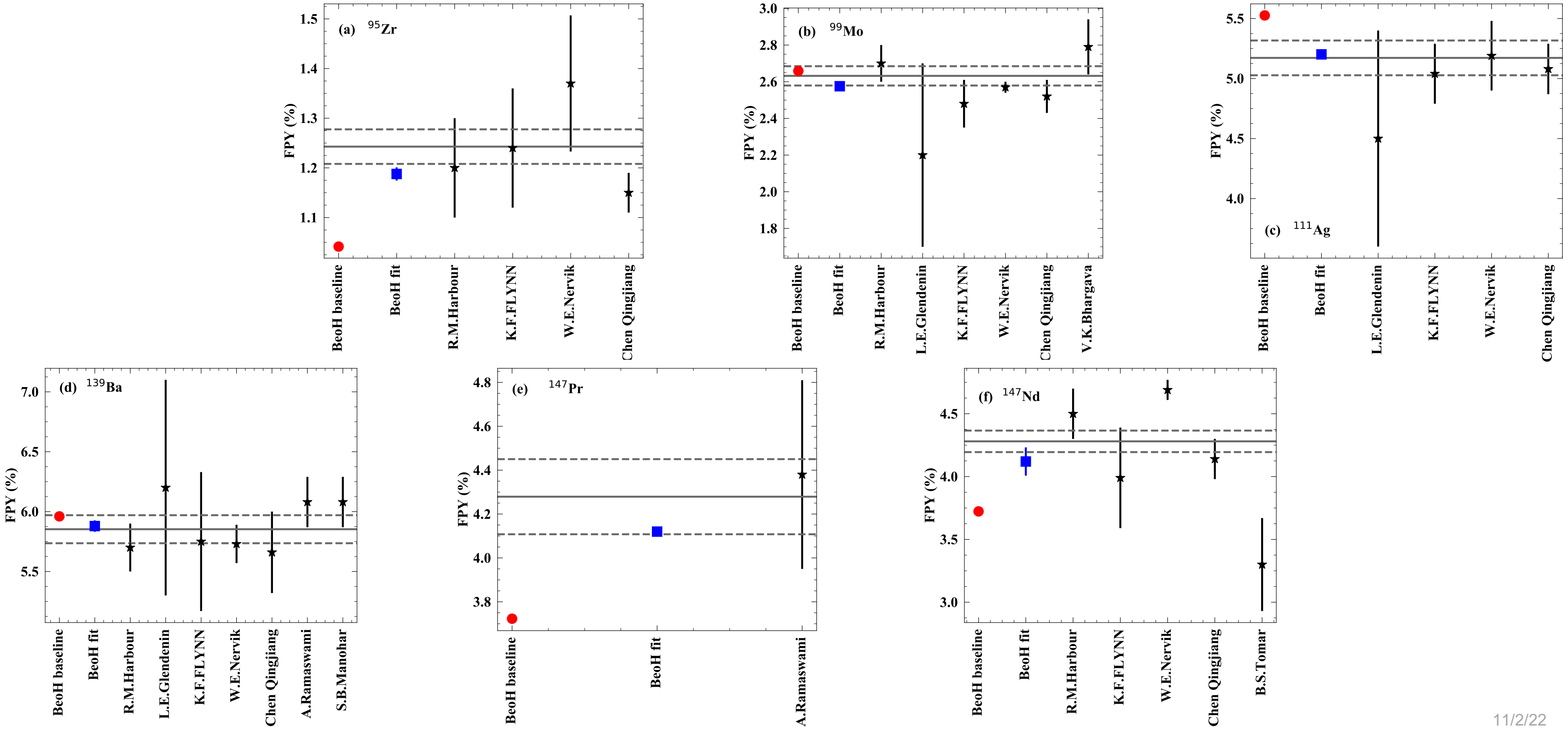
$\chi^2/N = 11.82$

The remainder of this talk focuses on fits to experimental data.

Large χ^2 values for ^{252}Cf(sf) are from a few FPYs (which agree well with ENDF/B-VIII.0 despite being fit to data)



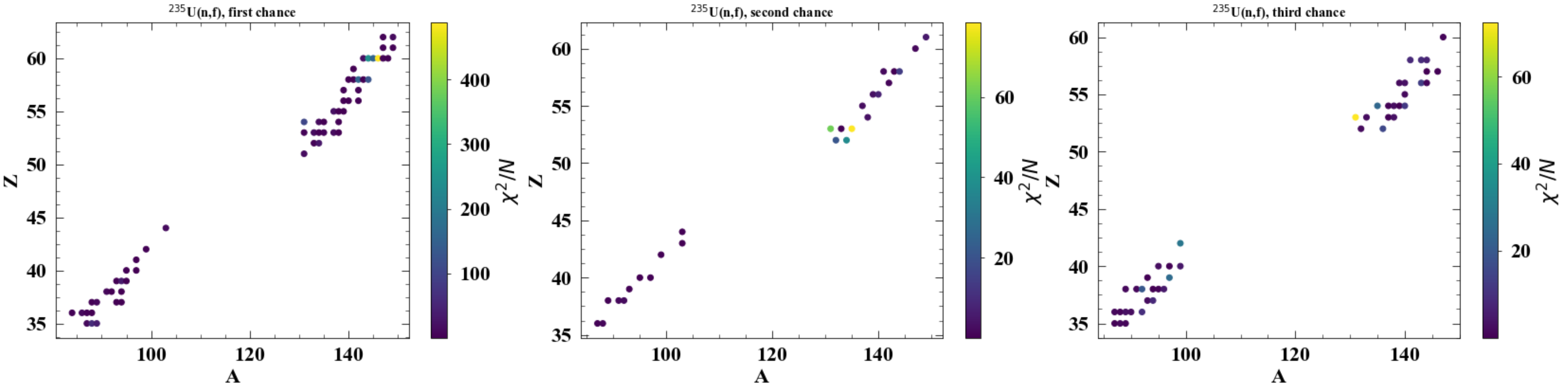
Overall, reasonable agreement between data, ENDF/B-VIII.0, and present work mean cumulative FPY values



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.

^{235}U(n,f) cumulative FPY data overview (taken from EXFOR, FPY>1%)

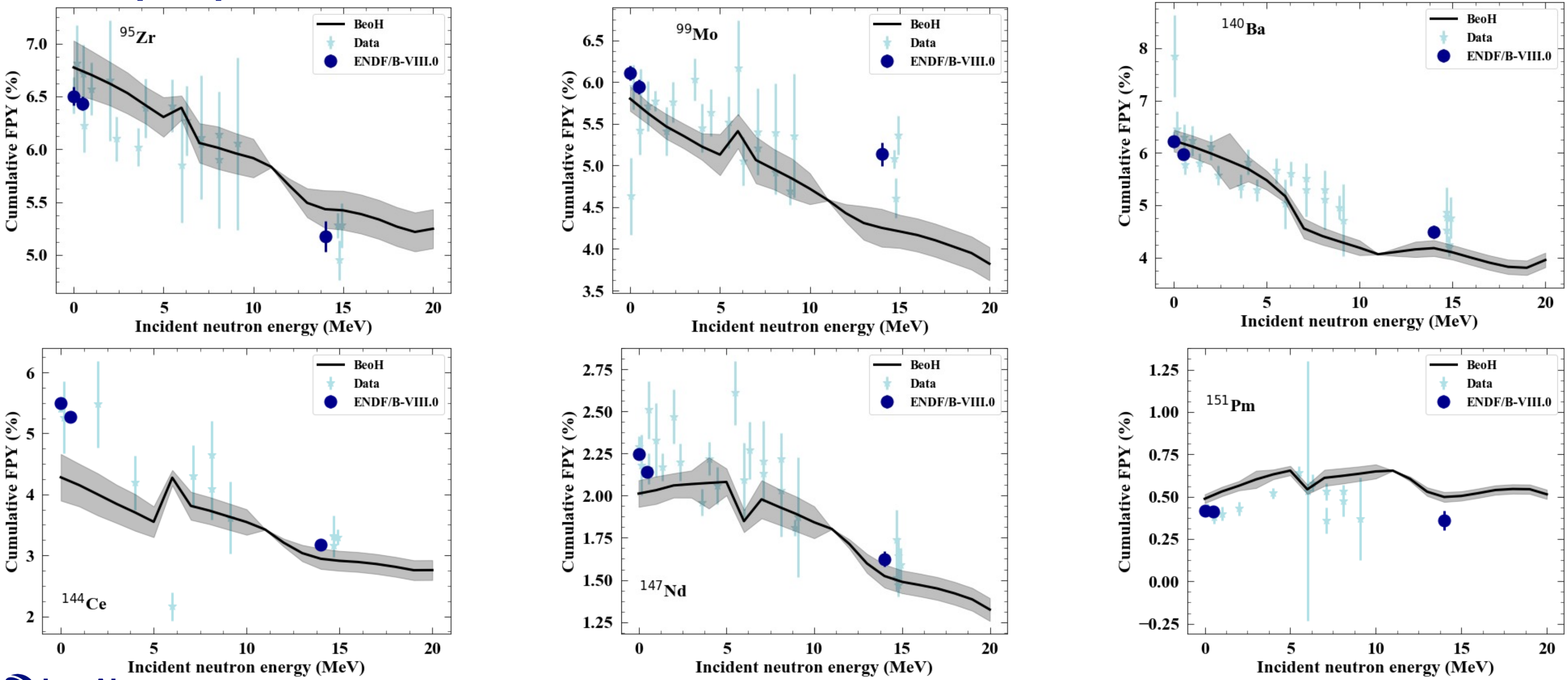


First chance
$\chi^2/N = 15.02$

Second chance
$\chi^2/N = 7.00$

Third chance
$\chi^2/N = 7.83$

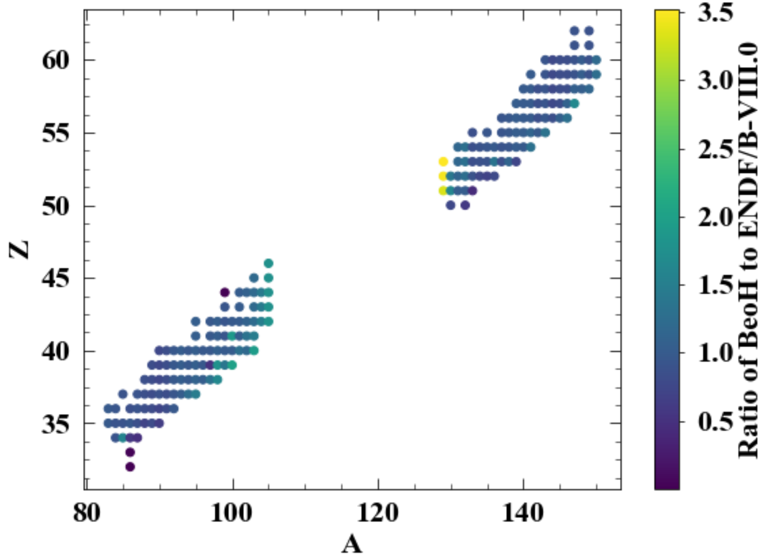
Select cumulative FPYs up from thermal to 20 MeV for $^{235}U(n,f)$



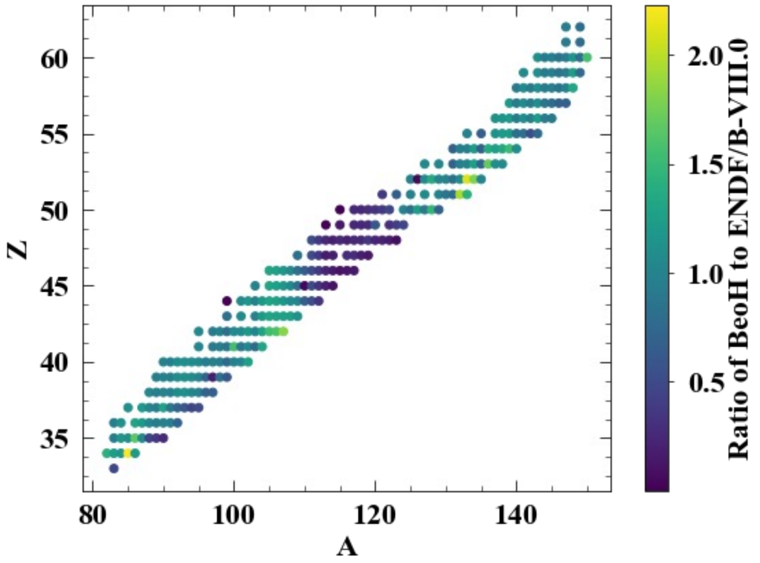
Los Alamos NATIONAL LABORATORY

Reasonable agreement with the current ENDF evaluation

E_{inc} = thermal



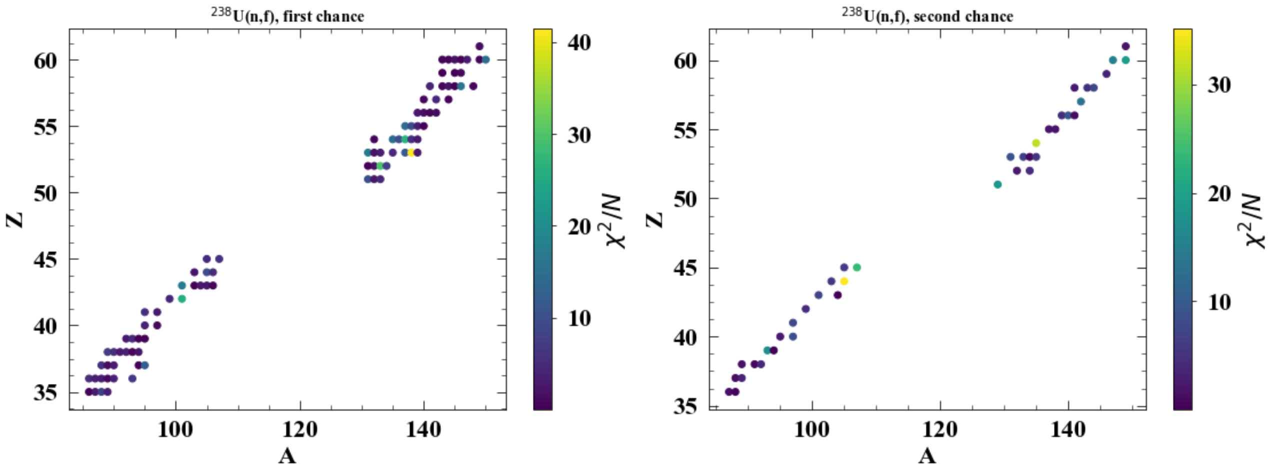
E_{inc} = 14 MeV



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

Los Alamos NATIONAL LABORATORY

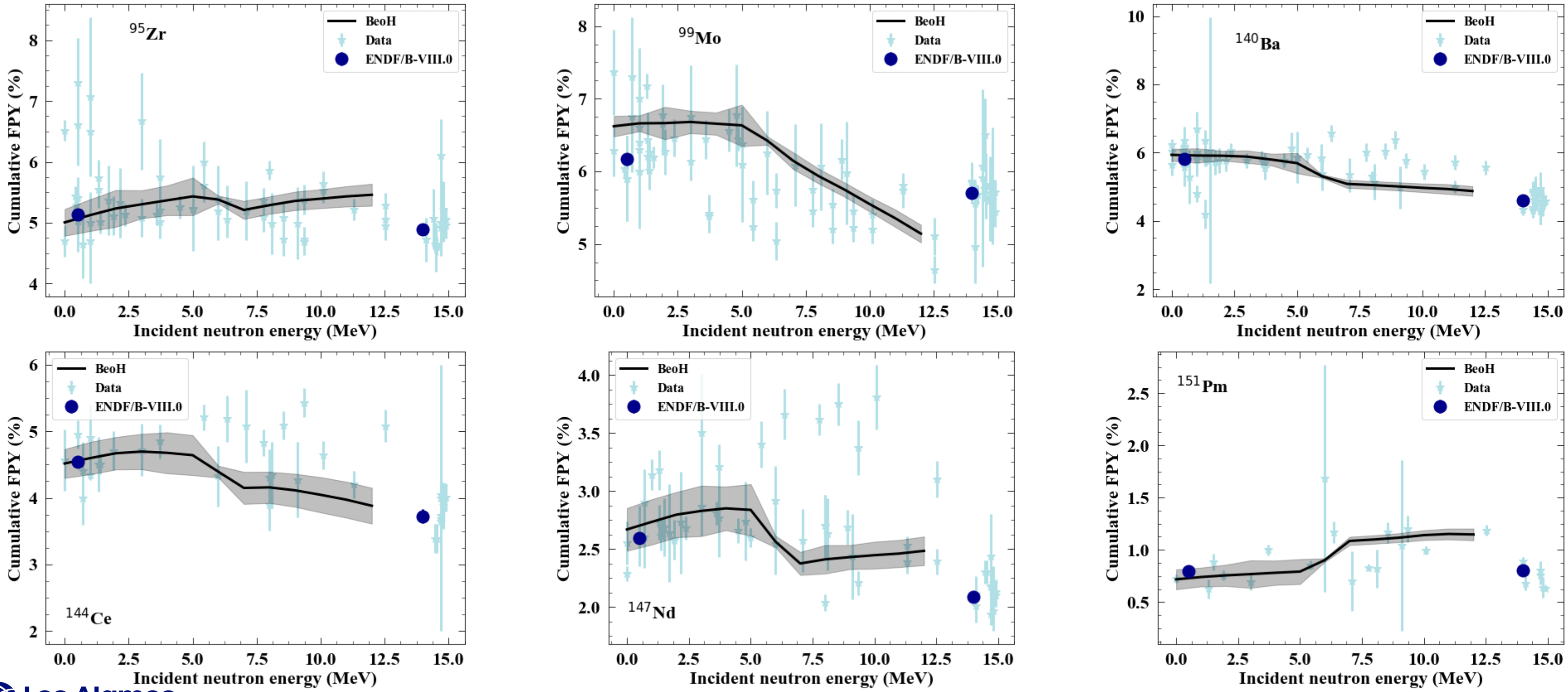
^{238}U(n,f) cumulative FPY data overview (taken from EXFOR, FPY>1%)



First chance
$\chi^2/N = 5.22$

Second chance
$\chi^2/N = 7.05$

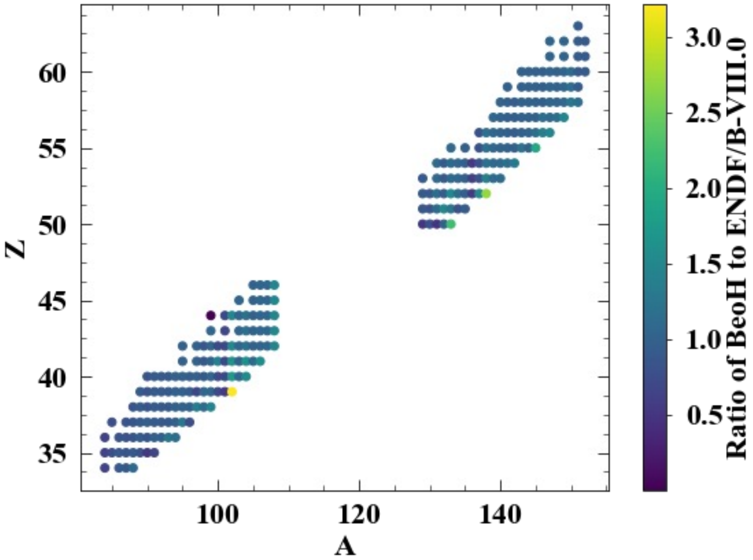
Select cumulative FPYs up from thermal to 12 MeV for $^{238}U(n,f)$



Los Alamos NATIONAL LABORATORY

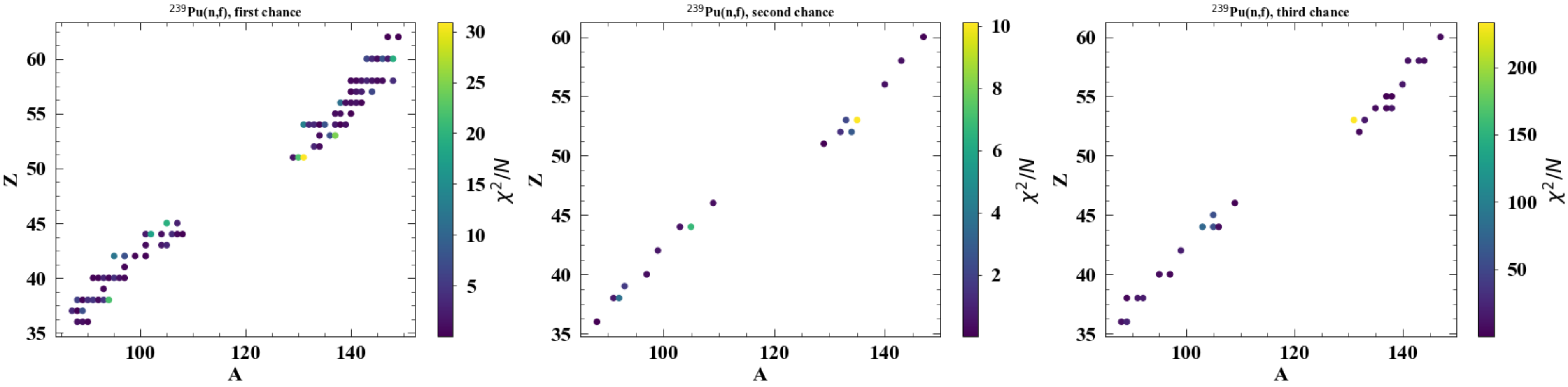
Reasonable agreement with the current ENDF evaluation

E_{inc} = 0.5 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) cumulative FPY data overview (taken from EXFOR, FPY>1%)

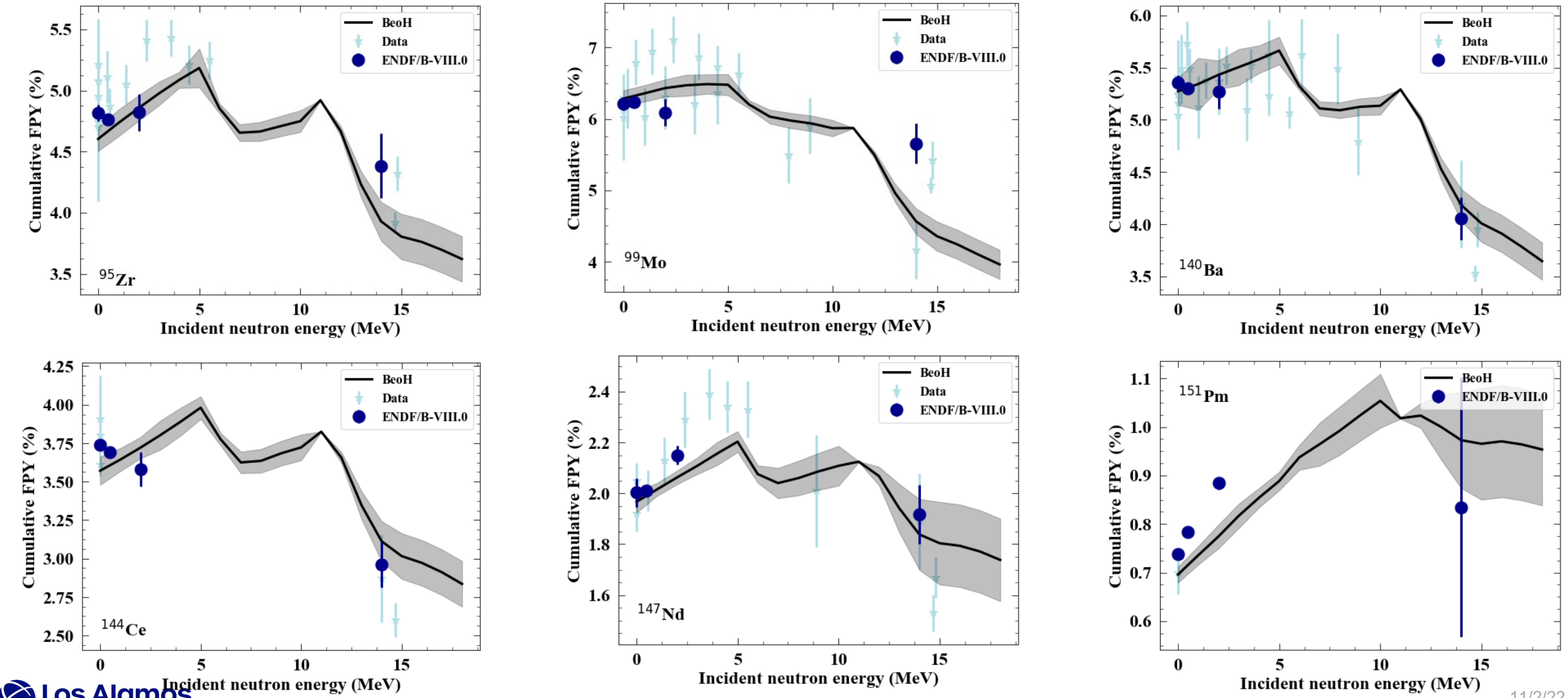


First chance
$\chi^2/N = 3.49$

Second chance
$\chi^2/N = 2.14$

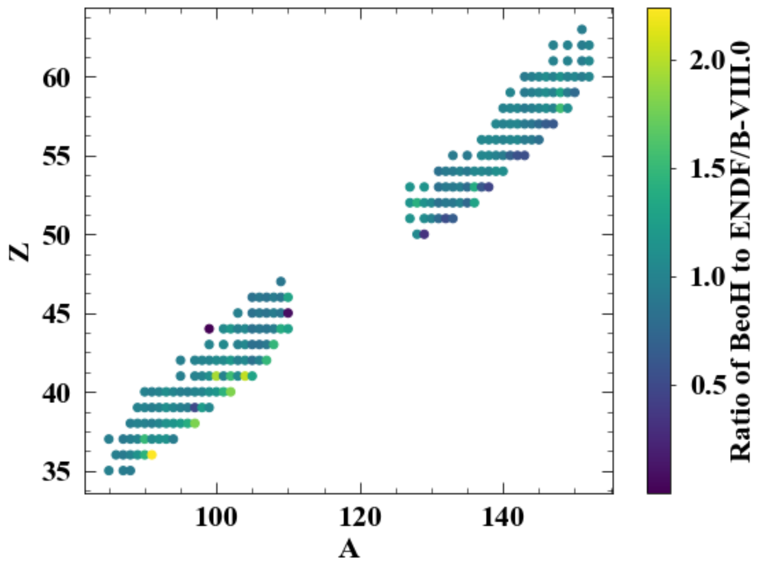
Third chance
$\chi^2/N = 21.65$

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

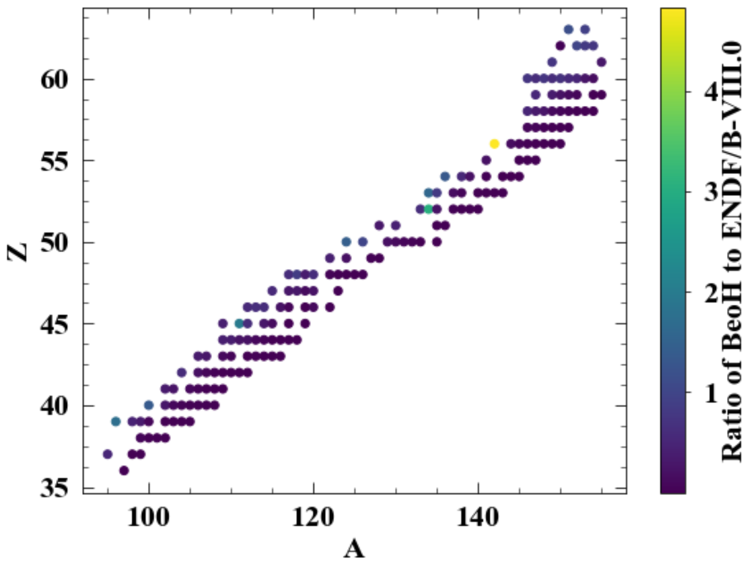


Reasonable agreement with the current ENDF evaluation

E_{inc} = thermal

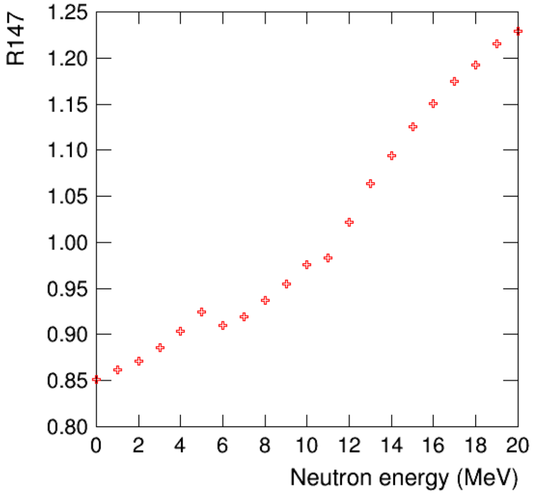


E_{inc} = 14 MeV



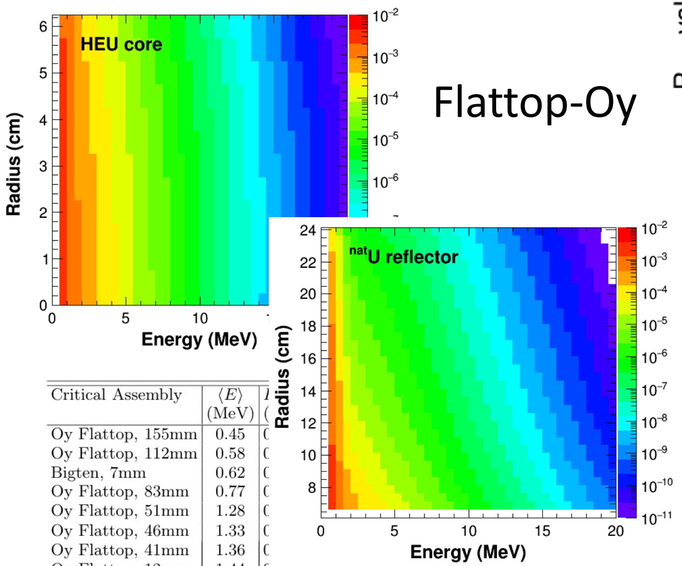
We only plot cumulative FPYs where the ENDF value is > 0.5%.
The discrepancy grows away from the peaks of the distribution.

A process has been set up to validate select cumulative FPYs with critical assemblies



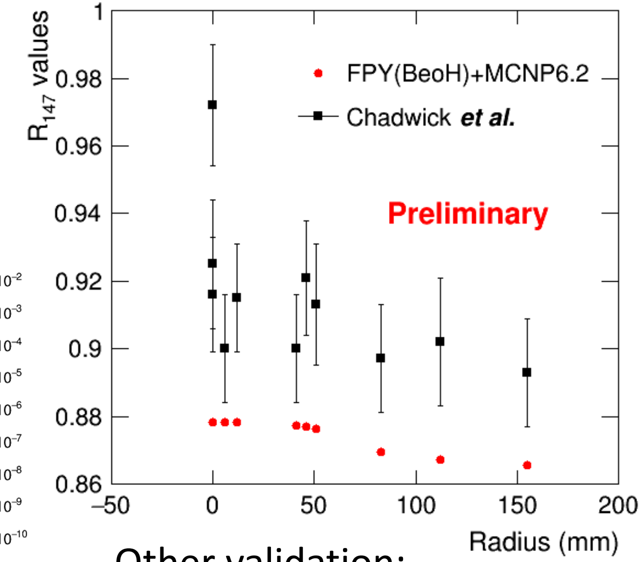
$$R_{147} = \frac{Y_{147}(\mathrm{Pu})}{Y_{147}(\mathrm{U_{th}})} \frac{Y_{99}(\mathrm{U_{th}})}{Y_{99}(\mathrm{Pu})}$$

Pu calcs from BeoH; $\mathrm{U_{th}}$ from ENDF



Flattop-Oy

Critical Assembly	⟨E⟩ (MeV)	[illegible]	[illegible]
Oy Flattop, 155mm	0.45	[illegible]	[illegible]
Oy Flattop, 112mm	0.58	[illegible]	[illegible]
Bigten, 7mm	0.62	[illegible]	[illegible]
Oy Flattop, 83mm	0.77	[illegible]	[illegible]
Oy Flattop, 51mm	1.28	[illegible]	[illegible]
Oy Flattop, 46mm	1.33	[illegible]	[illegible]
Oy Flattop, 41mm	1.36	[illegible]	[illegible]
Oy Flattop, 12mm	1.44	[illegible]	[illegible]
Oy Flattop, 6mm	1.44	0.896 ± 3.3%	0.900 ± 1.78%
Oy Flattop, center	1.44	0.968 ± 3.3%	0.972 ± 1.89%
Oy Flattop, center	1.44	0.929 ± 2.7%	0.925 ± 2.04%
Oy Flattop, center	1.44	0.899 ± 2.7%	0.916 ± 1.88%
Pu Flattop, center	1.68	0.895 ± 2.7%	0.912 ± 2.70%
Pu Flattop, center	1.68	0.927 ± 2.7%	0.944 ± 1.78%
Pu Flattop, center	1.68	– –	0.928 ± 1.77%
Pu Jezebel, center	1.88	0.927 ± 3.3%	0.934 ± 2.32%
Average *R*-value			0.916 ± 0.8%



Other validation:
Remaining critical assemblies
SOFIA integrated results
Dosimetry

M.B. Chadwick, et al., NDS 111, 2923 (2010)

Los Alamos NATIONAL LABORATORY

Figures from G. Rusev (LANL)

Covariance format is up for discussion (2 main options)

- Create an MF 38 format (like MF 35) for covariances; move FPY uncertainties out of MF 8 into MF 38 only
  - Pros: consistent with other covariance files, could essentially use the format for MF 35 (little to no new development)
  - Cons: applications that use the current format will have to update to take uncertainties from a new file
- Extend the MF 8 format to include correlations as well as uncertainties
  - Pros: applications can keep their current way of reading uncertainties
  - Cons: new format will have to be developed
- Cross correlations between incident energies would not be included

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)
- Third-chance calculations for ^{238}U(n,f) are being finished
- Tweaking of BeoH Y(A) shape underway to account for stiffness in the model that currently doesn't consistently calculate important FPYs
- 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