Fission Product Yield Modeling and Evaluation

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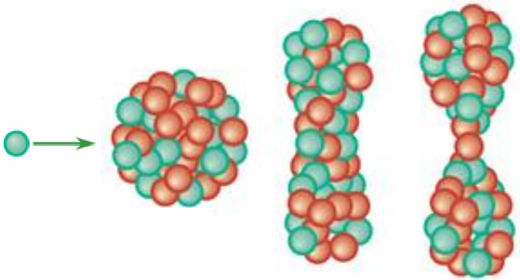
Significant developments have gone into theoretical and experimental FPY values, leads to new evaluation effort

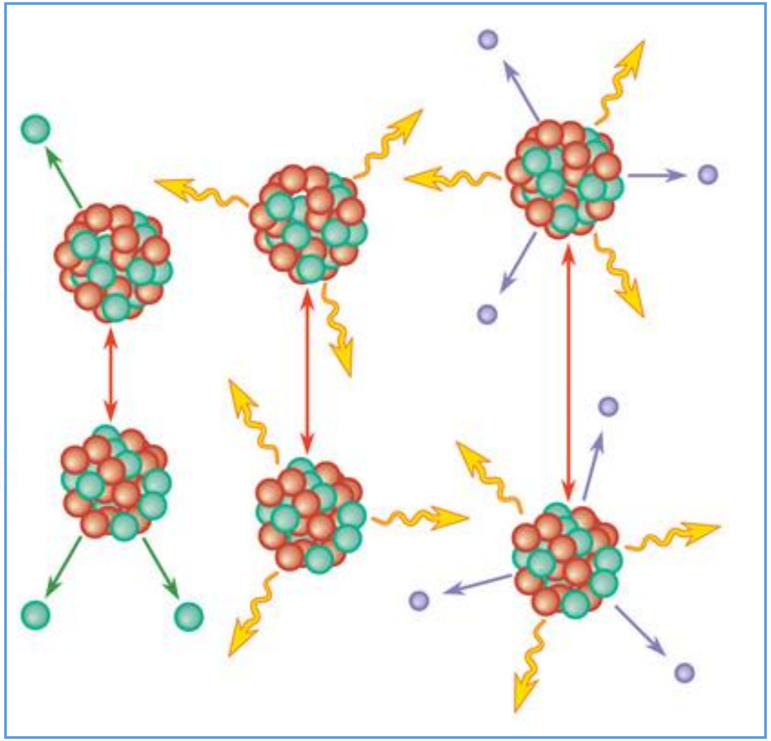
- Last US evaluation is from England and Rider in 1994, LA-UR-94-3106
- Only one update has been performed, a 2010 update to include a 2 MeV point in ^{239}Pu(n,f) by Chadwick, *et al*. (NDS 111, 2923) to develop an energy dependence around the fast region
  - Otherwise, fission product yields are only given for thermal, fast, and 14 MeV neutrons
- Since then, significant experimental efforts have gone into measuring energy-dependent FPYs, especially between 1 MeV and 14 MeV
- Significant theoretical modeling effort has been made for consistent fission modeling (FPYs connected to prompt quantities and fission initial conditions)
- A multi-institutional effort will provide energy-dependent FPYs from thermal to 20 MeV for ^{235,238}U, ^{239}Pu, and spontaneous fission of ^{252}Cf including full covariances.

BeoH can be used to calculate prompt and delayed multi-chance fission observables

BeoH – the LANL-developed (T. Kawano) deterministic fission fragment decay code – has been extended for multi-chance fission calculations.

The decay of fission fragments is followed through both prompt and delayed emission.





In this way, low-yield observables are calculated to the same accuracy as high-yield observables.

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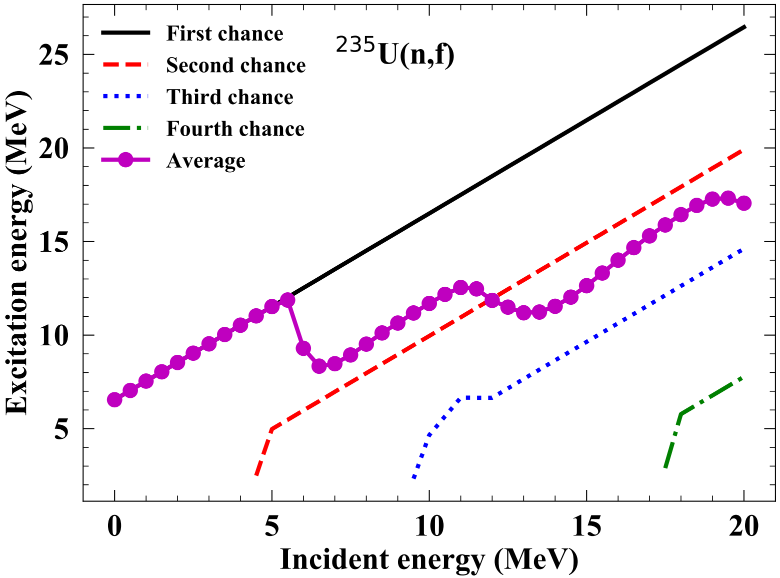
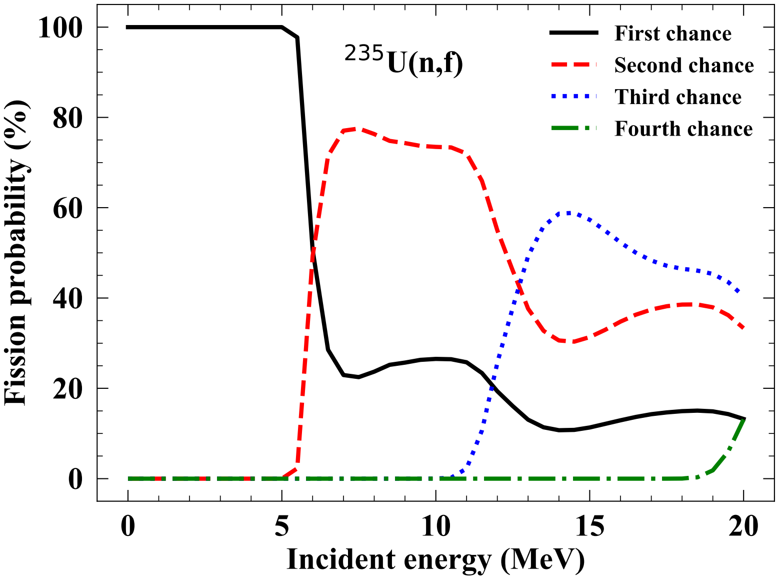
Pre-scission calculations are taken from CoH

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)



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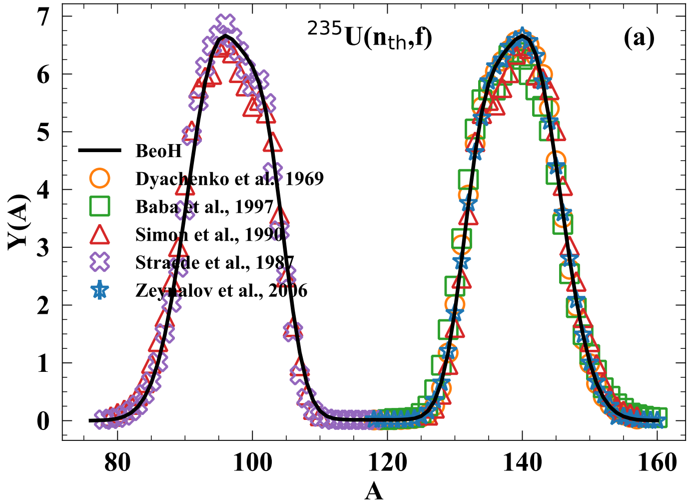
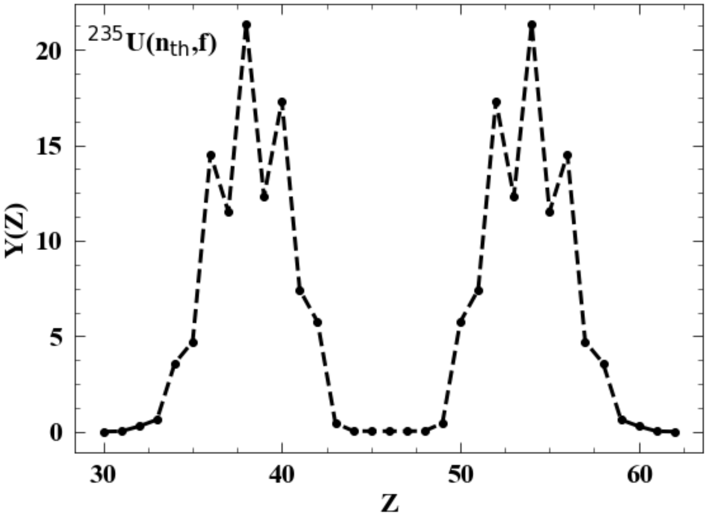
Fission fragment initial conditions are parametrized and fit to available experimental data, Y(A,Z,TKE,J,π)

Mass distributions, 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.).



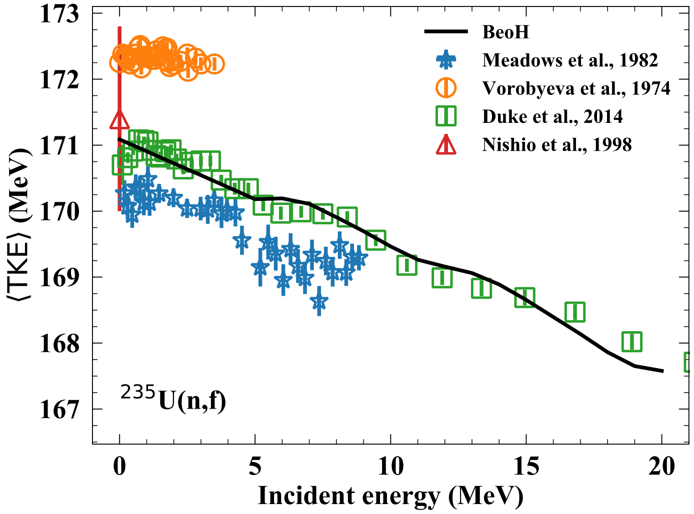


The Wahl systematics are used to calculate the charge distribution, Y(Z|A).

Fission fragment initial conditions are parametrized and fit to available experimental data, Y(A,Z,TKE,J,π)

<TKE>(E_{inc}) is linear for each chance fission and can include an optional slope change at low incident neutron energies.

<TKE>(A) is Gaussian, with the means and widths fit to data as a function to mass.



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.

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

Positive and negative parities are taken to be equally probable.

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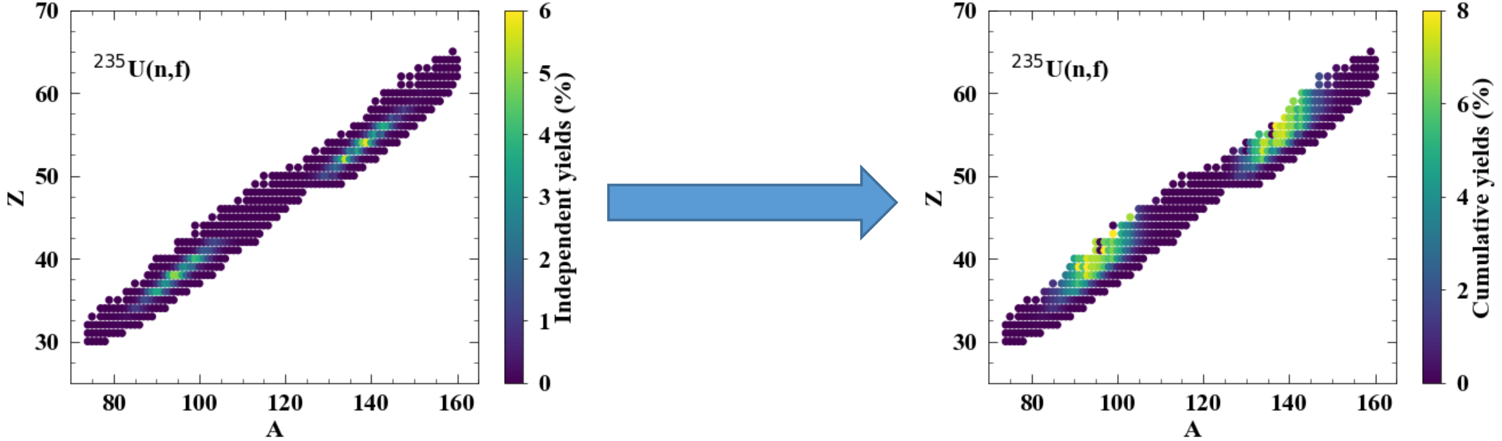
Calculating independent and cumulative yields

Once the initial conditions of each fragment are determined, the Hauser-Feshbach statistical decay is performed for each excited 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. We keep track of the isomeric states for the independent and cumulative yield calculations.



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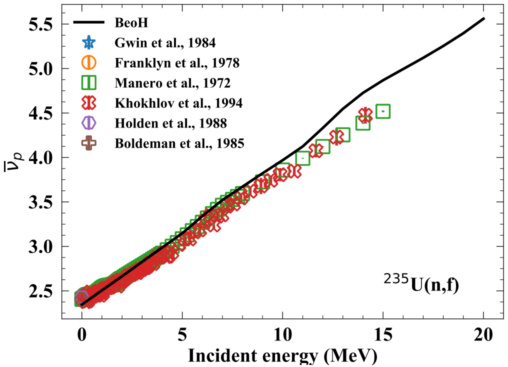
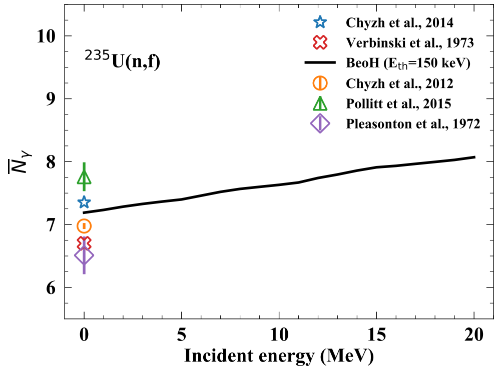
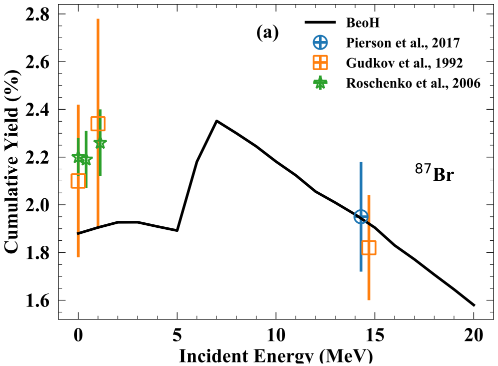
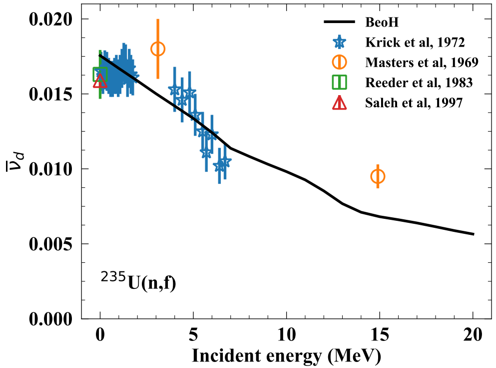
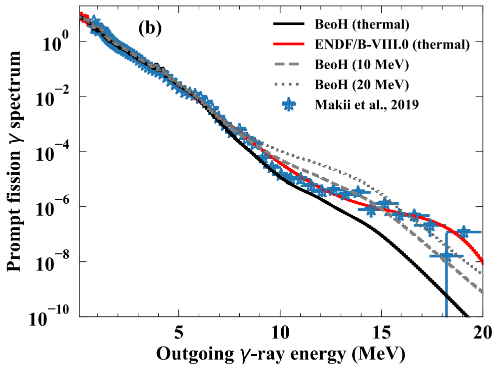
Prompt and delayed observables can be calculated consistently

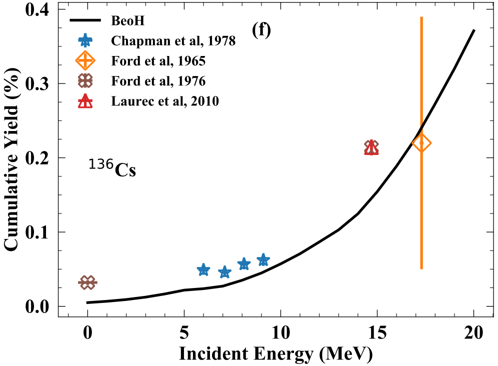












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Results here are not optimized to experimental data

A Kalman filter optimization is being used to evaluate FPYs and produce covariances

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

Model calculation vector

Data covariance

Parameter covariance

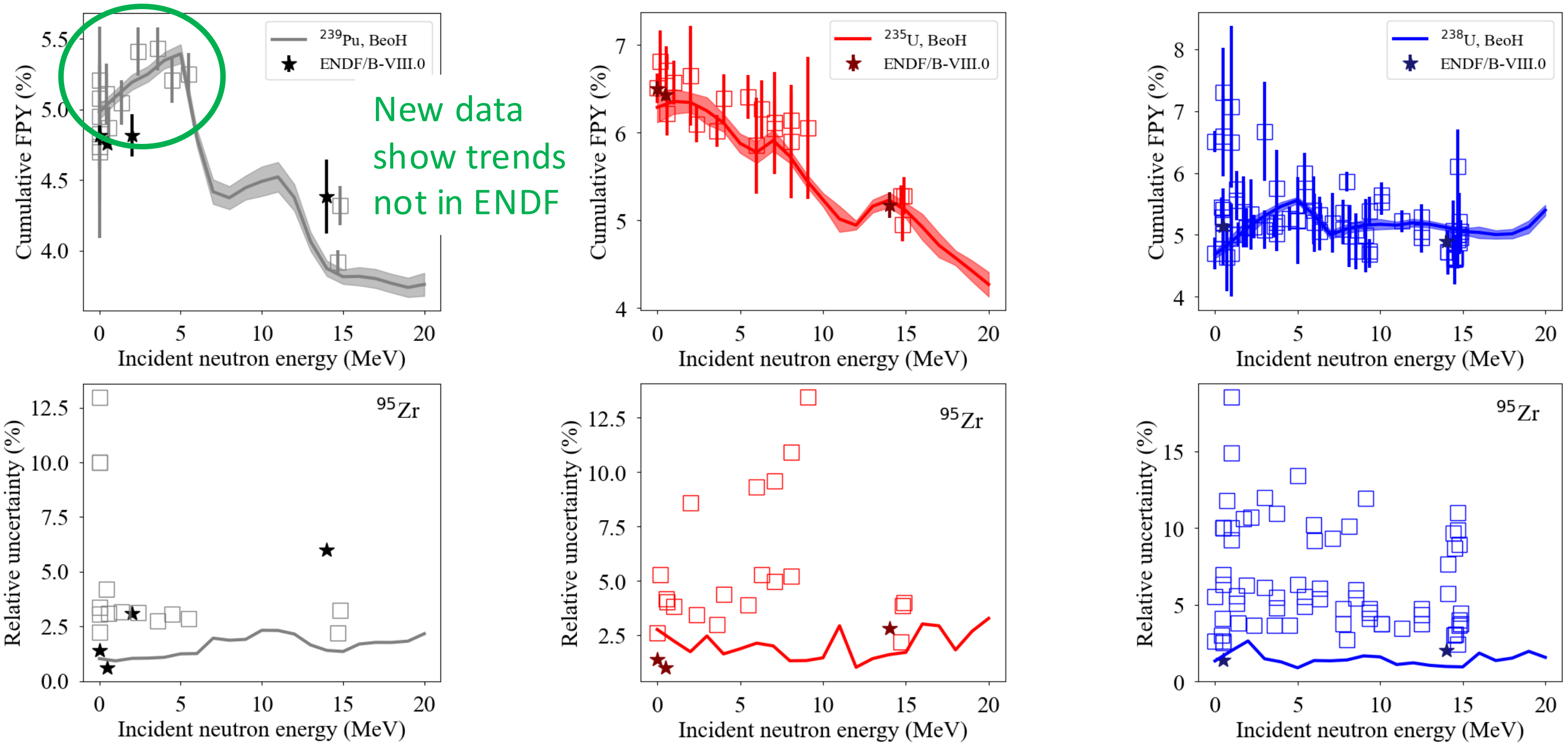
Sensitivities

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

Model predictions and covariance are updated

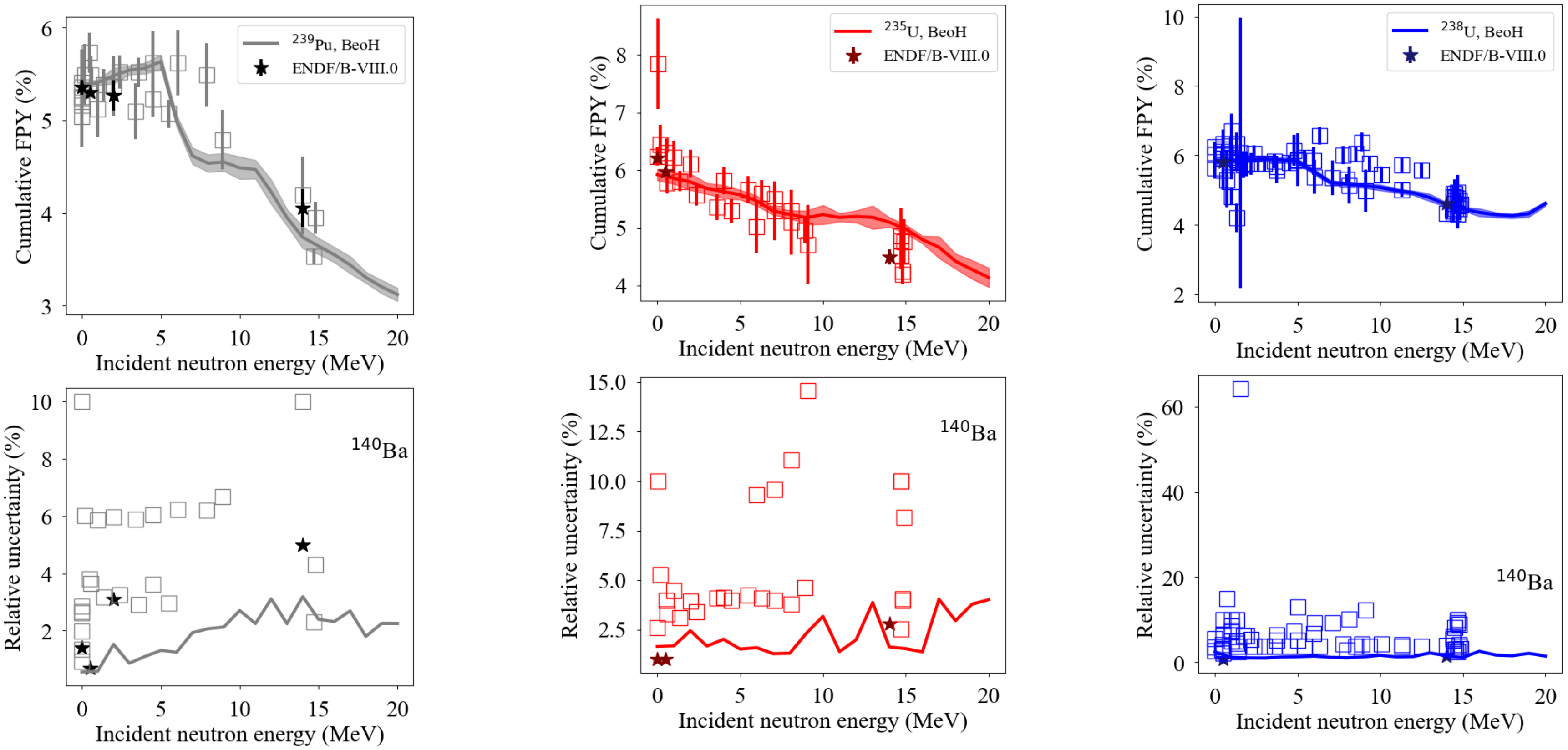
$$\Phi = f(\mathbf{x}_1) \qquad \mathbb{F} = \mathbb{C}\mathbb{P}\mathbb{C}^T$$

Cumulative FPYs for ^{95}Zr from the major actinides



New data show trends not in ENDF

Cumulative FPYs for ^{140}Ba from the major actinides



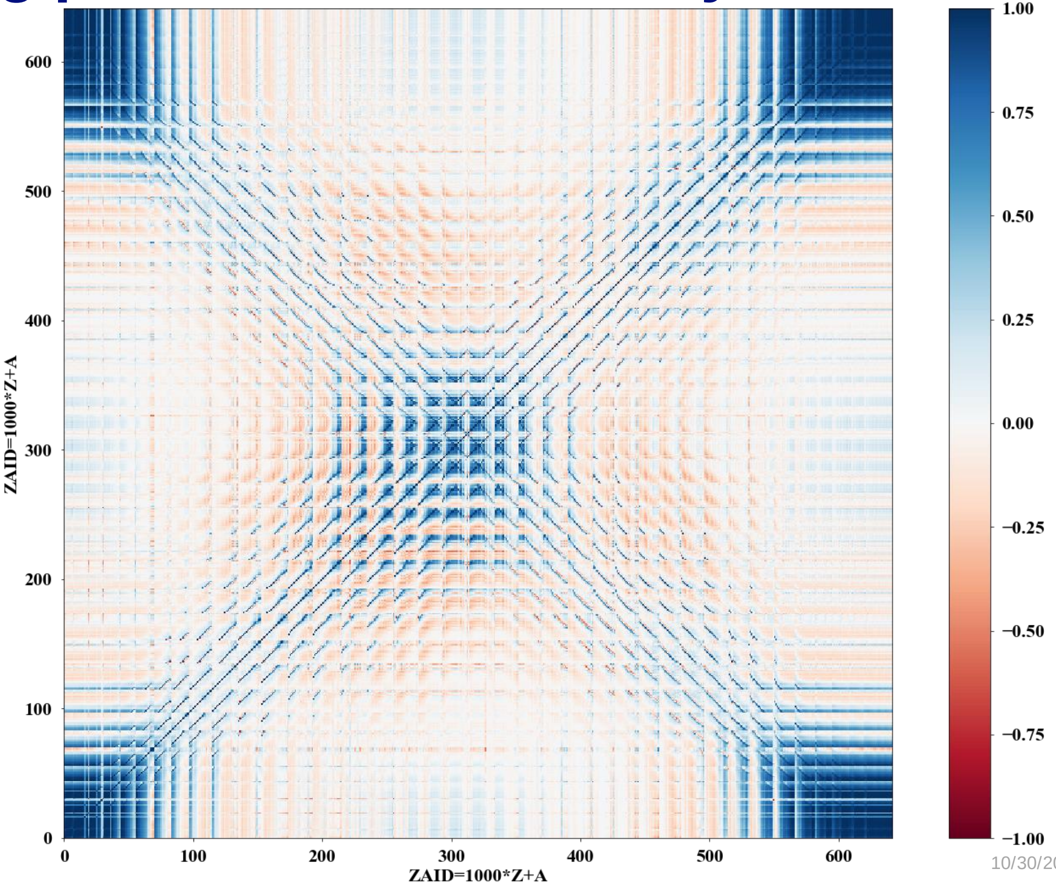
Covariances are being produced consistently

Example correlation matrix for cumulative FPYs from ^{252}Cf(sf).

Cumulative FPYs are largely uncorrelated but we see blocks of higher correlations.

See A.E. Lovell, *et al., EPJ Web of Conferences* **281**, 00018 (2023) for details.

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

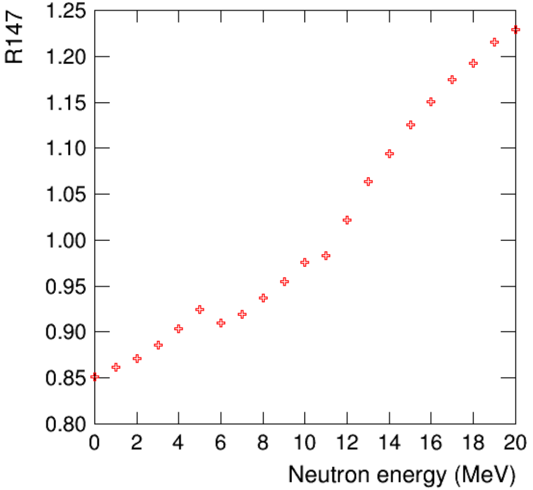


Validation is being performed for the new FPYs using R-values from critical assembly measurements

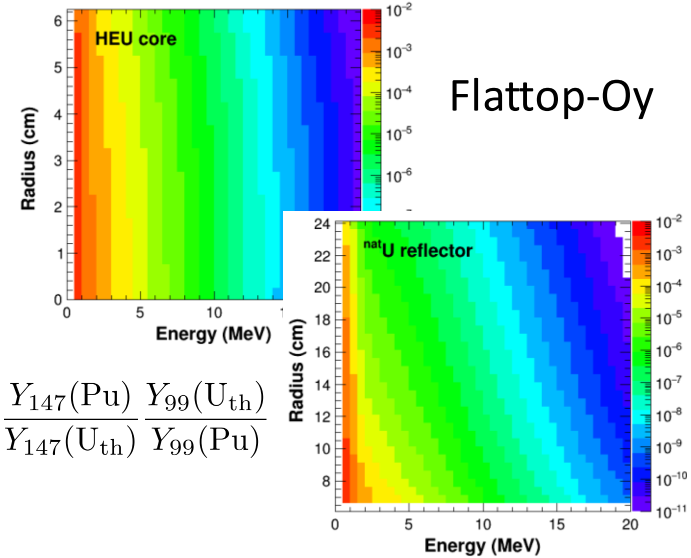
Historic measurements have been adjusted for energy causing fission

Critical Assembly	⟨E⟩ (MeV)	R (Ford-Norris) (dimensionless)	R (Updated) (dimensionless)
Oy Flattop, 155mm	0.45	0.889 ± 3.3%	0.893 ± 1.77%
Oy Flattop, 112mm	0.58	0.898 ± 3.3%	0.902 ± 2.06%
Bigten, 7mm	0.62	0.883 ± 3.3%	0.886 ± 1.86%
Oy Flattop, 83mm	0.77	0.894 ± 3.3%	0.897 ± 1.82%
Oy Flattop, 51mm	1.28	0.908 ± 3.3%	0.913 ± 1.94%
Oy Flattop, 46mm	1.33	0.917 ± 3.3%	0.921 ± 1.85%
Oy Flattop, 41mm	1.36	0.896 ± 3.3%	0.900 ± 1.79%
Oy Flattop, 12mm	1.44	0.910 ± 3.3%	0.915 ± 1.78%
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%

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



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

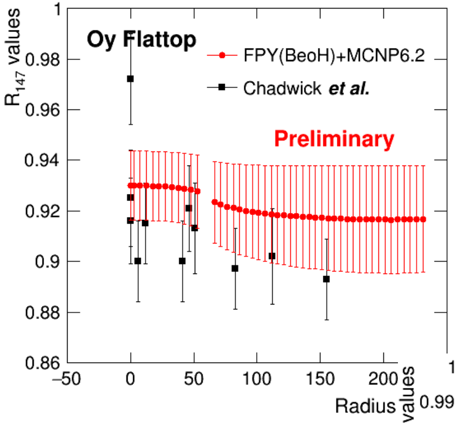


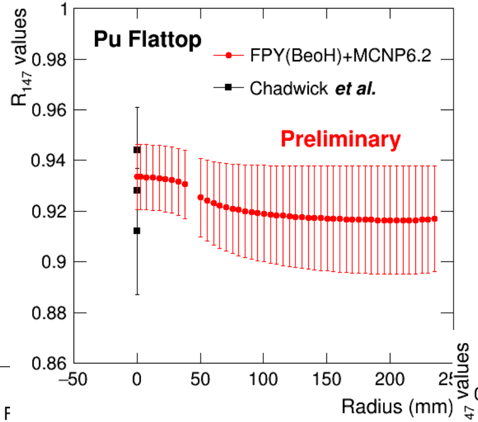
Flattop-Oy

R-values are calculated and folded with flux simulations from MCNP

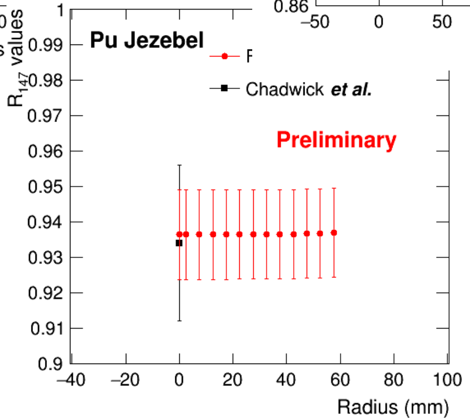
Other validation:
Remaining critical assemblies
SOFIA integrated results
Dosimetry

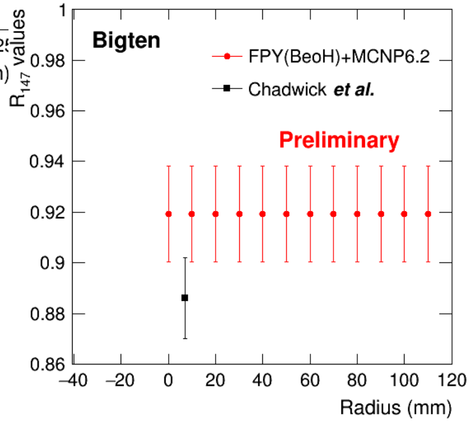
Validation using various assemblies is being performed





Correlations are not yet included in the uncertainty calculations – uncertainties will likely decrease





R-values show good agreement with data trends, and give valuable feedback on FPY magnitudes

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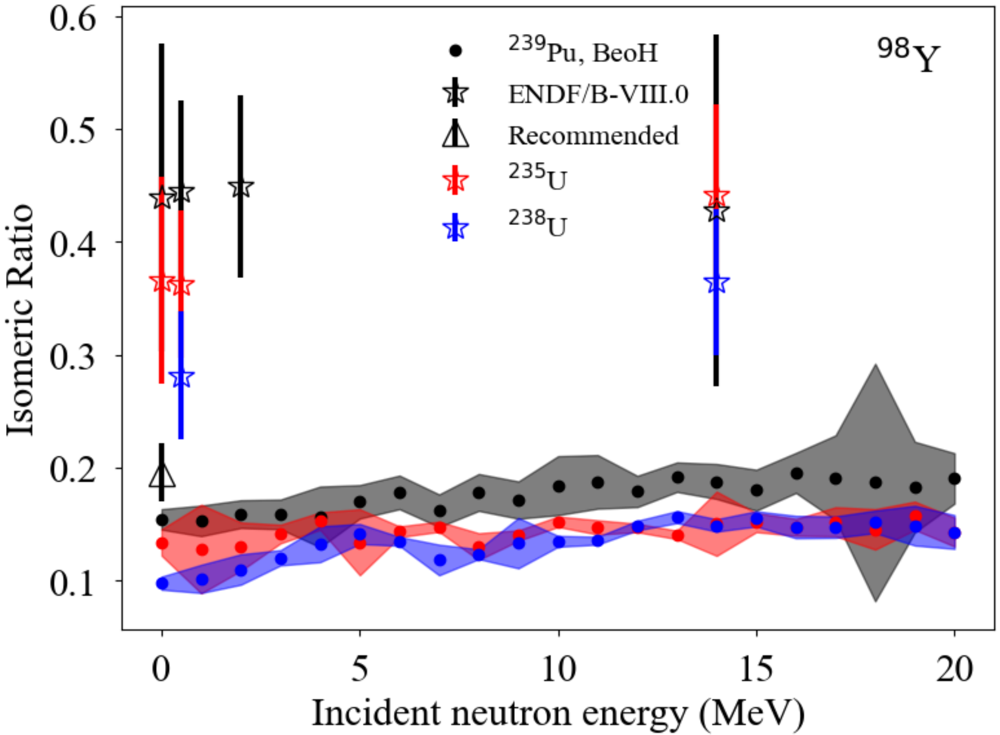
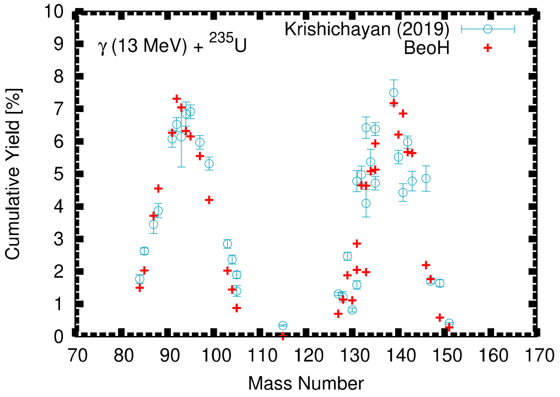
Investigation of isomeric ratios is underway

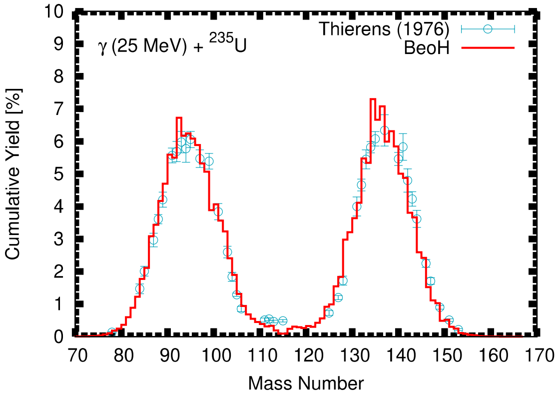


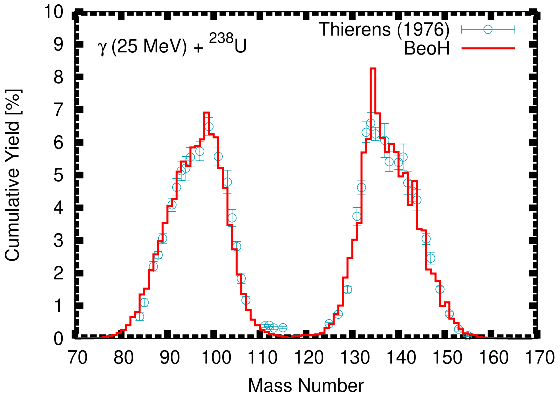
Our calculated isomeric ratios are often lower than evaluations/data; however, there are indications that the Madland-England treatment is over-simplified. Differences between theory and data can point to needed nuclear structure information.

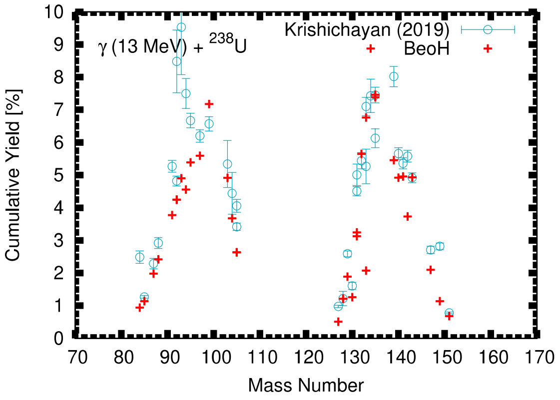
"Recommended": C.J. Sears, *et al.*, *NDS* **173**, 118 (2021)

Extension to FPY calculations for photofission









Conclusions and outlook

- Significant efforts in modeling and experiment have allowed for new, energy-dependent calculations and evaluations of independent and cumulative fission product yields, consistent with prompt and delayed observables.
- The update to multi-chance fission of the fission fragment decay code BeoH has provided these types of calculations for the first time.
- Calculations have been performed for major actinides from thermal to 20 MeV incident neutron energies, and covariances are being produced.
- We are investigating isomeric ratios, which show some significant differences when comparing the present calculations and recent data to the ENDF evaluations.
- The calculations are being extended to minor isotopes, and we are able to calculate photofission observables within the same framework.