FPY evaluation work at LANL

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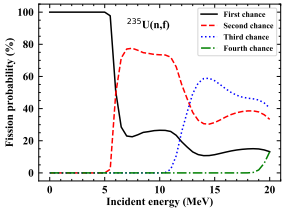
CSEWG, Nov. 17, 2021

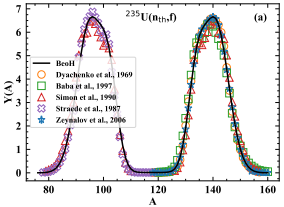
LA-UR-21-31312

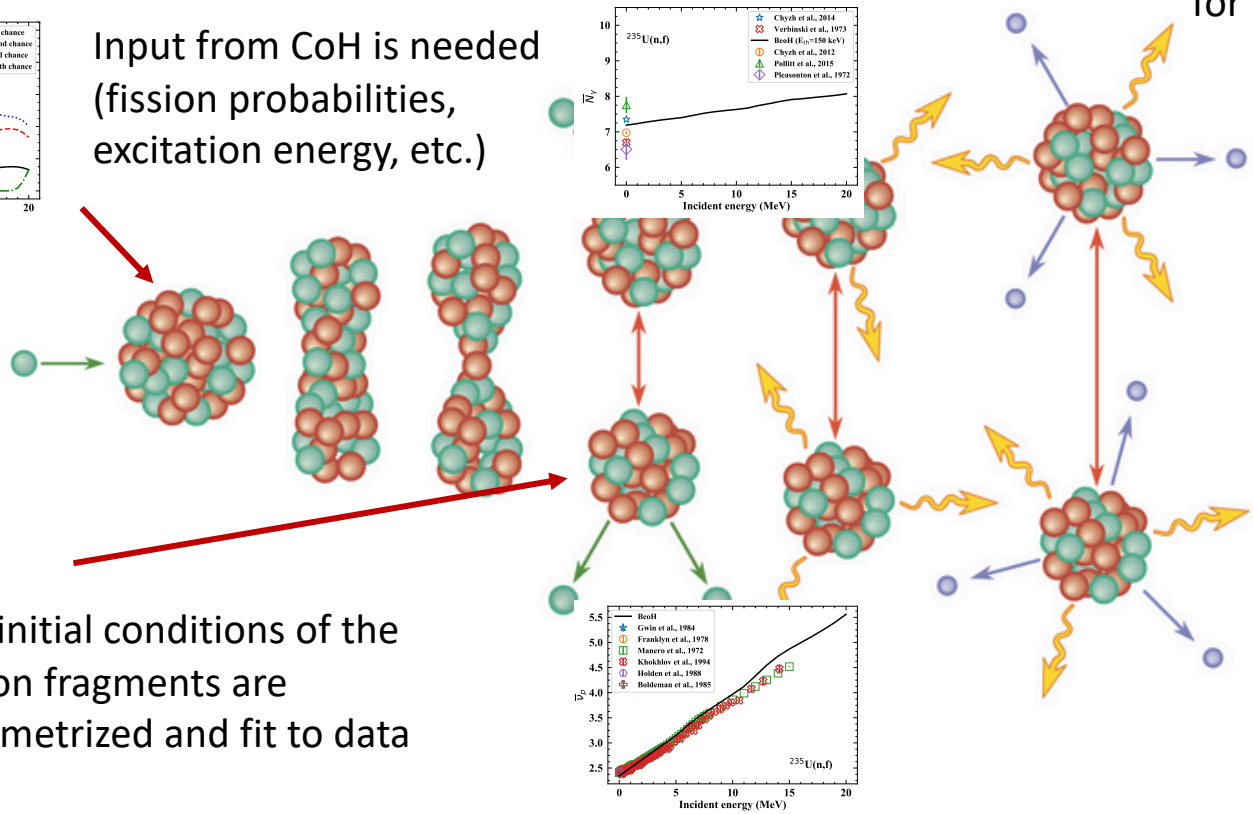
BeoH calculates prompt/delayed fission observables using the statistical Hauser-Feshbach theory

Decay data required for IFY → CFY



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

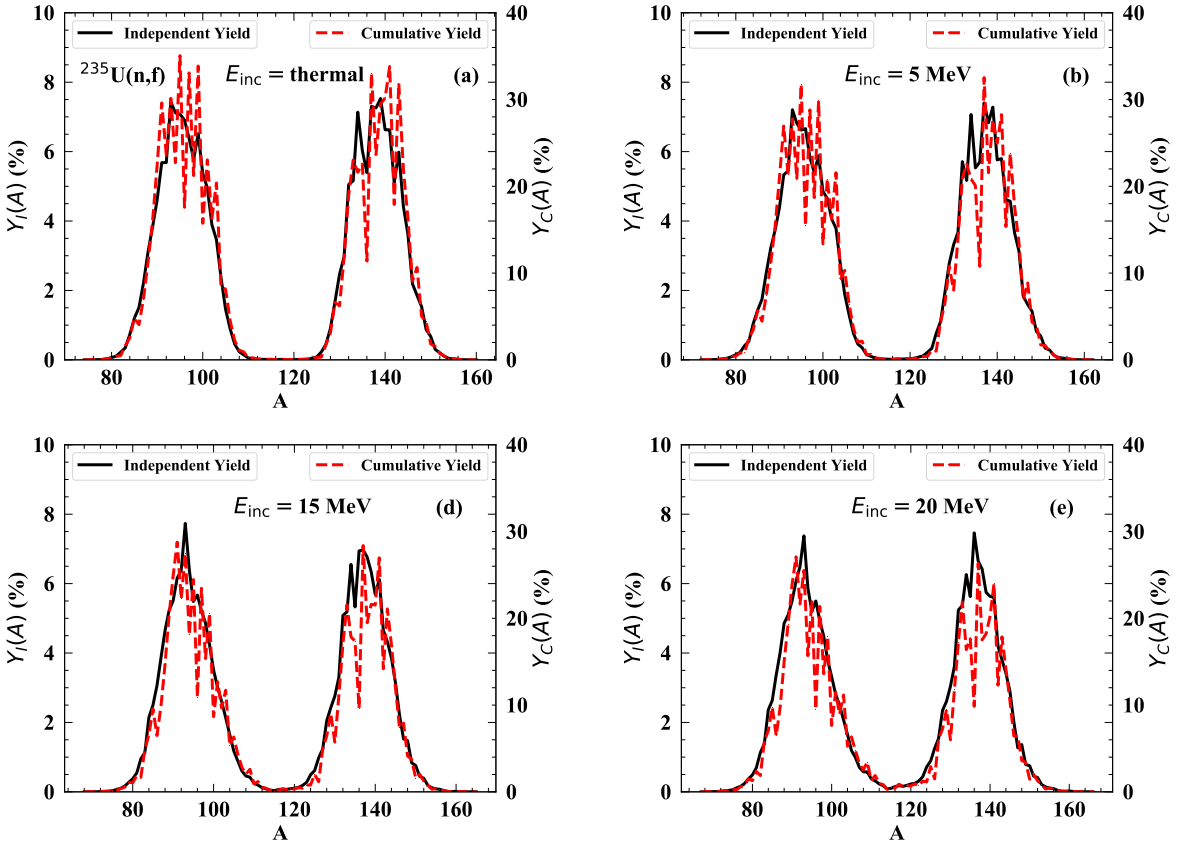




The initial conditions of the fission fragments are parametrized and fit to data

Lovell, Kawano, *et al.*, *PRC* **103** 014615 (2021)

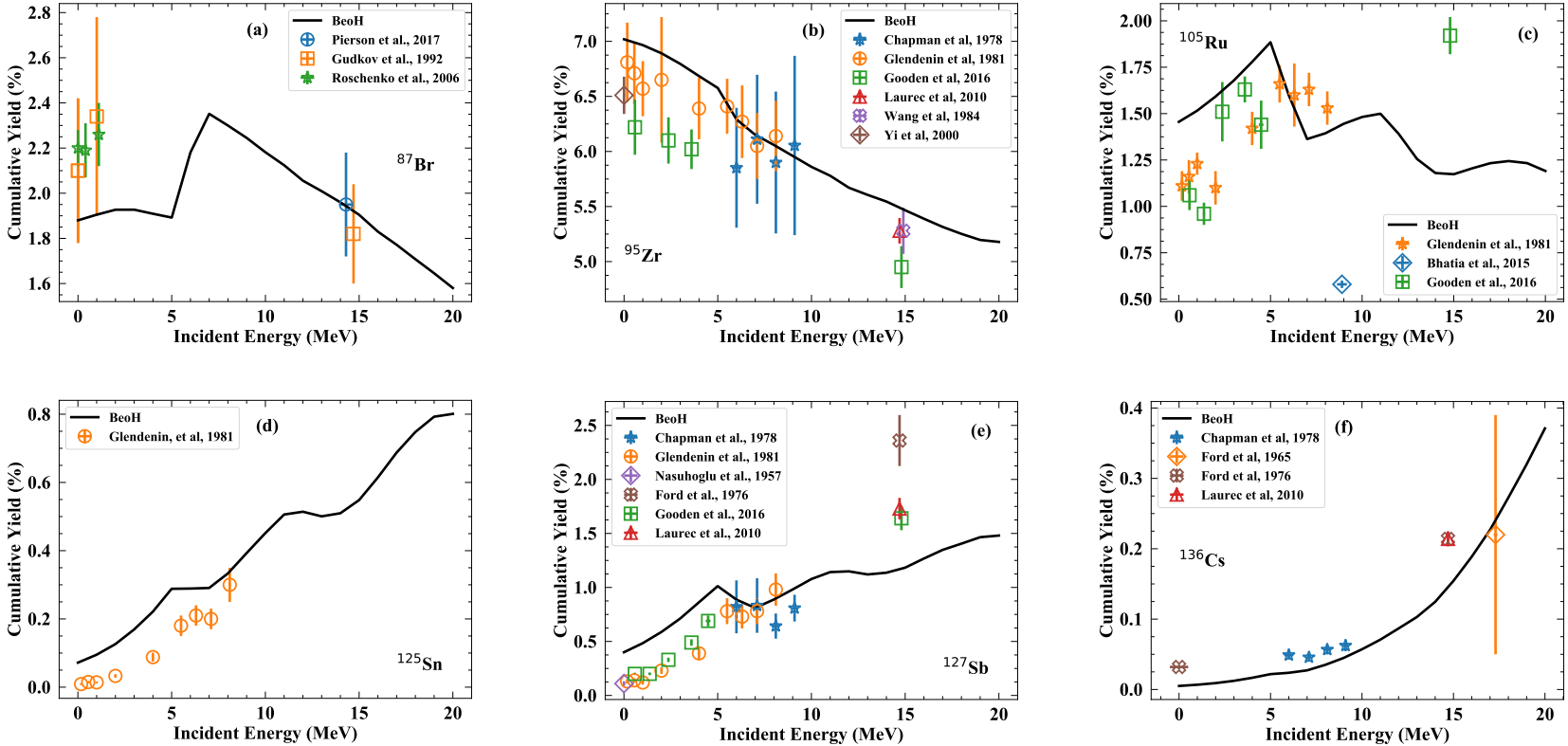
Independent and cumulative mass yields



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

Lovell, Kawano, *et al.*, *PRC* **103** 014615 (2021)

Cumulative fission product yields already show reasonable agreement without specific optimization



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A Kalman filter has been used to further optimize the fission fragment initial conditions (first-chance fission)

The mass yields before neutron emission, Wahl scaling factors, total kinetic energy, excitation energy sharing, and spin cutoff parameter are included in the optimization

^{235}U(n,f)
Prompt and delayed average neutron multiplicity
Cumulative FPYs: ^{95}Zr, ^{97}Zr, ^{99}Mo, ^{132}Te, ^{140}Ba, ^{147}Nd

^{238}U(n,f)
Prompt and delayed average neutron multiplicity
Cumulative FPYs: ^{97}Zr, ^{133}I, ^{135}Xe, ^{137}Cs, ^{140}Ba, ^{143}Ce, ^{144}Ce, ^{145}Pr, ^{147}Nd, ^{148}Nd

^{239}Pu(n,f)
Prompt and delayed average neutron multiplicity
Cumulative FPYs: ^{83}Kr, ^{85}Rb, ^{86}Kr, ^{87}Sr, ^{131}Xe, ^{132}Xe, ^{133}Xe, ^{134}Xe, ^{137}Ba, ^{142}Ce, ^{143}Pr, ^{144}Nd, ^{145}Nd, ^{146}Nd, ^{147}Nd, ^{148}Nd

The included cumulative FPYs are those with low uncertainties in the England and Rider evaluation, LA-UR-94-3106

Okumura, Kawano, *et al*., arXiv:2102.01015 [nucl-th] 1 Feb 2021, in press JNST, LA-UR-21-20820

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

Model calculation vector

Data covariance

Parameter covariance

Sensitivities

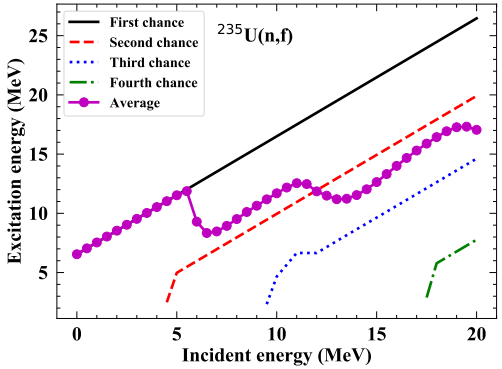
$$\mathbb{C}_{ij} = \frac{\Delta f_i(\mathbf{x})}{\Delta x_j}$$

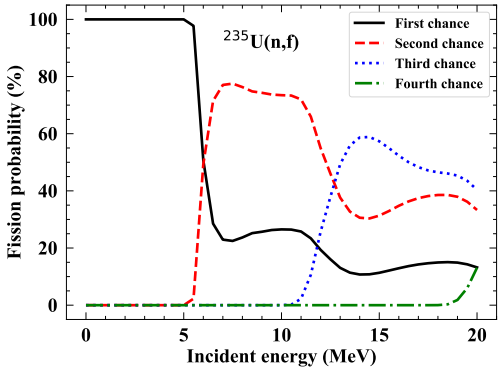
Model predictions and covariance are updated

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

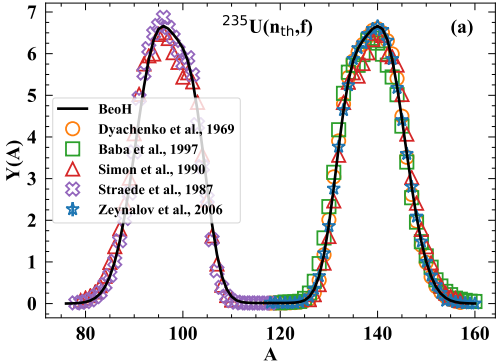
A variety of inputs are needed for BeoH calculations

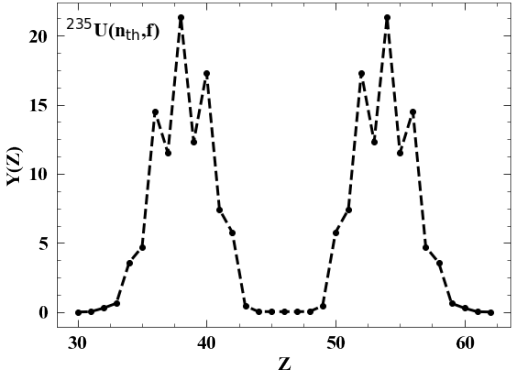
Information on the compound nucleus – from CoH

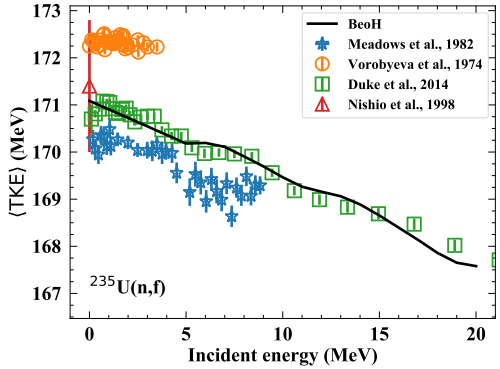




Fission fragment initial conditions are parametrized (mass, charge, TKE, spin, parity distributions) and taken as free parameters in the FPY optimization







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

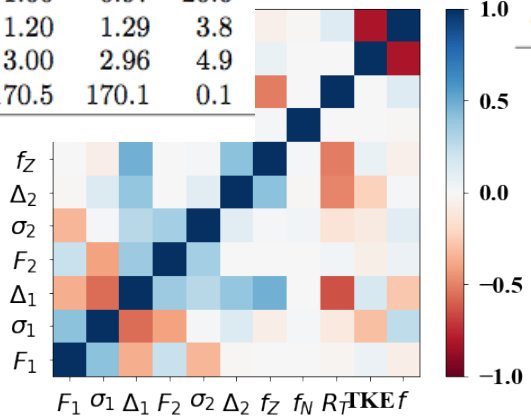
Excitation energy shared based on a ratio of temperatures (constant or mass dependent)

$$R_T = \frac{T_L}{T_H}$$

Model parameters are updated with uncertainties and correlations

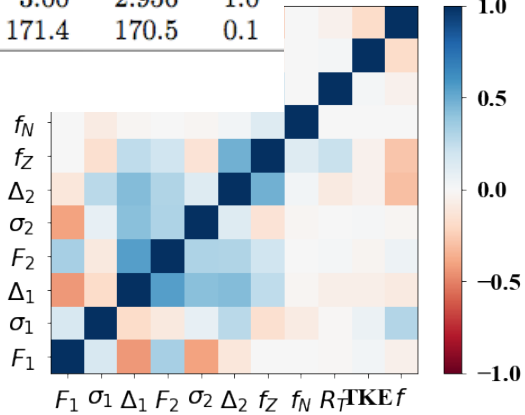
$^{235}U(n_{th},f)$

	pri	post	% change
F_1	0.793	0.824	4.3
σ_1	4.83	5.05	1.4
Δ_1	23.0	23.1	0.5
F_2	0.205	0.197	4.7
σ_2	2.73	2.92	3.1
Δ_2	15.6	15.2	0.7
f_{Z0}	1.00	1.78	6.6
f_{N0}	1.00	0.97	20.6
R_{T0}	1.20	1.29	3.8
f_J	3.00	2.96	4.9
TKE	170.5	170.1	0.1



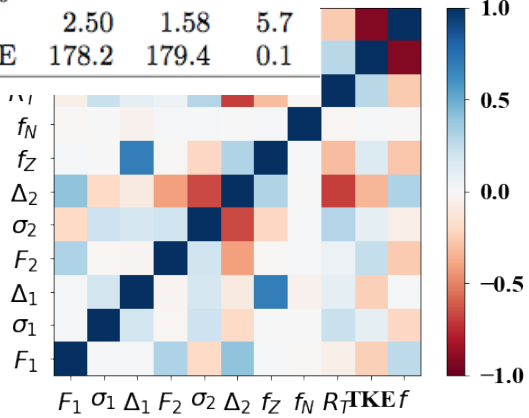
$^{238}U(n_{1\ MeV},f)$

	pri	post	% change
F_1	0.587	0.625	3.6
σ_1	5.405	5.580	1.4
Δ_1	22.879	23.128	0.5
F_2	0.413	0.380	4.4
σ_2	3.459	3.326	2.6
Δ_2	15.515	15.584	0.7
f_{Z0}	1.00	2.386	5.3
f_{N0}	1.00	0.736	52.8
R_{T0}	1.30	1.327	1.0
f_J	3.00	2.956	1.0
TKE	171.4	170.5	0.1



$^{239}Pu(n_{th},f)$

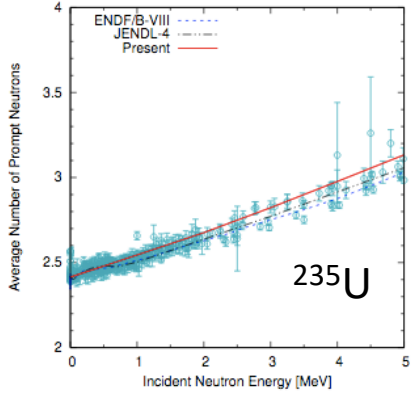
	pri	post	% change
F_1	0.234	0.248	4.1
σ_1	3.51	3.26	5.2
Δ_1	14.9	14.1	1.8
F_2	0.765	0.718	4.6
σ_2	6.06	6.58	0.5
Δ_2	20.8	20.1	0.5
f_{Z0}	1.00	2.58	4.4
f_{N0}	1.00	0.93	21.3
R_{T0}	1.20	1.30	2.4
f_J	2.50	1.58	5.7
TKE	178.2	179.4	0.1

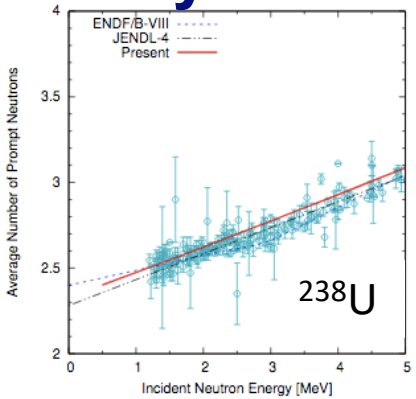


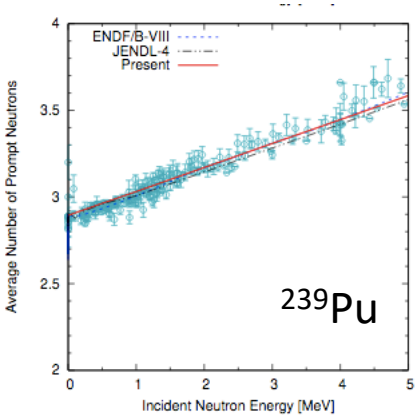
$$\mathbb{F} = \mathbb{C}\mathbb{P}\mathbb{C}^T$$

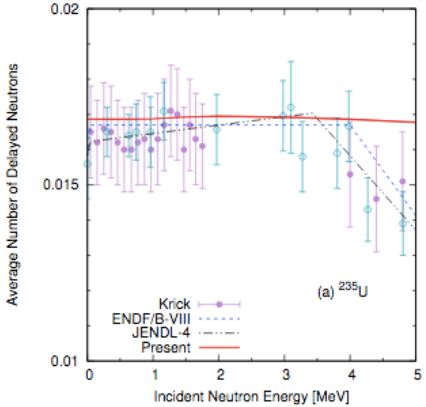
Okumura, Kawano, *et al.*, arXiv:2102.01015 [nucl-th] 1 Feb 2021, in press JNST, LA-UR-21-20820

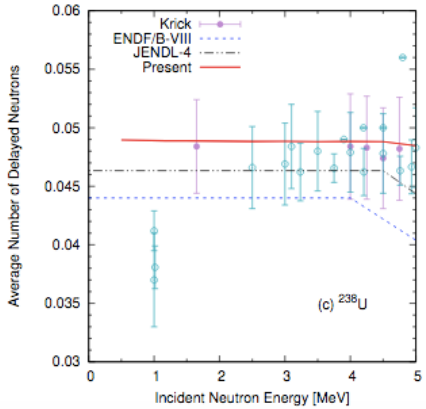
Prompt and delayed neutron multiplicities are reproduced simultaneously

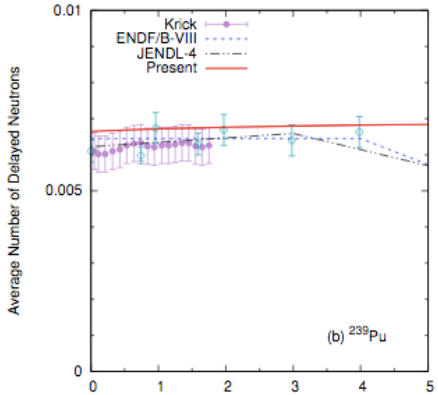












Okumura, Kawano, *et al.*, arXiv:2102.01015 [nucl-th] 1 Feb 2021, in press JNST, LA-UR-21-20820

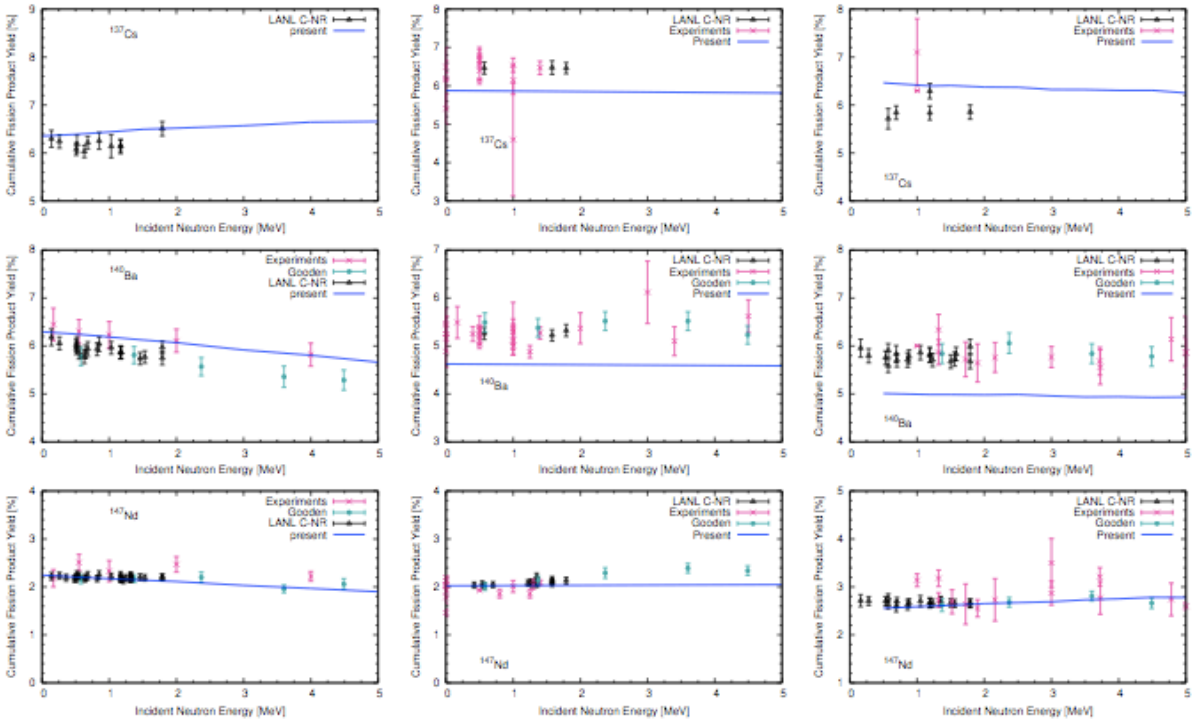
A variety of cumulative fission product yields can also be reproduced

^{235}U ^{239}Pu ^{238}U

^{137}Cs

^{140}Ba

^{147}Nd



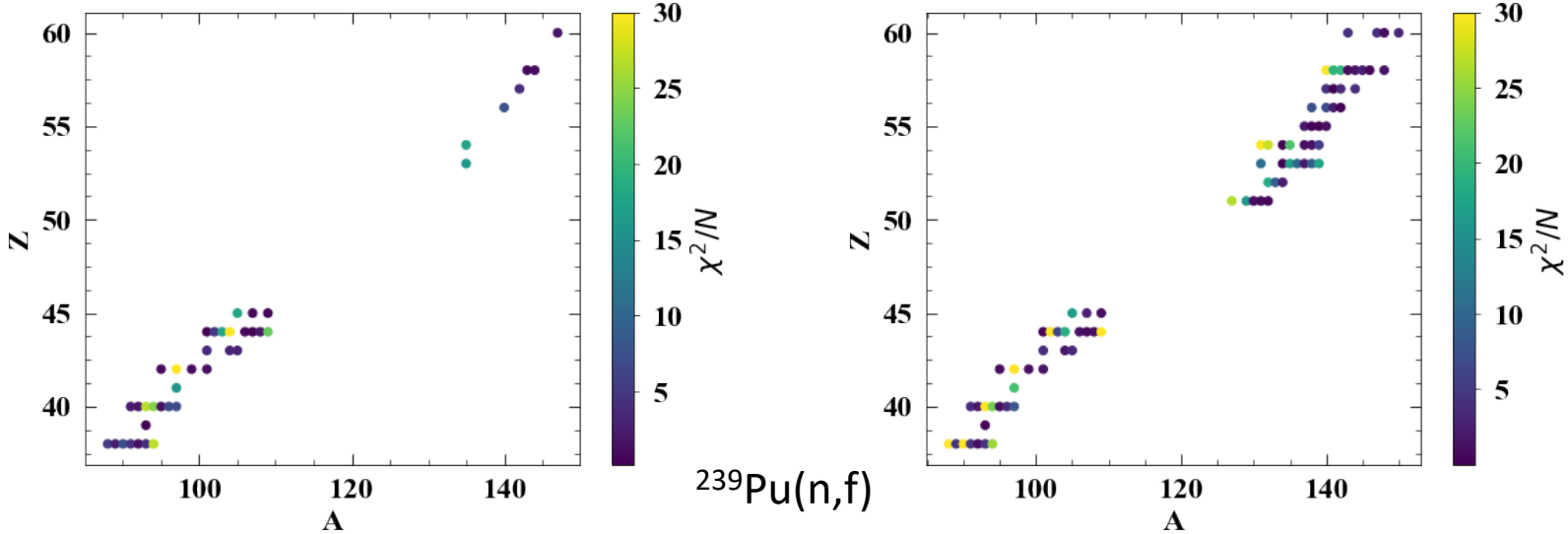
Mean values **and** covariances (not shown) are calculated

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

Okumura, Kawano, *et al*., arXiv:2102.01015 [nucl-th] 1 Feb 2021, in press JNST, LA-UR-21-20820

A stepped approach is being used to include the bulk of the experimental data into the optimization

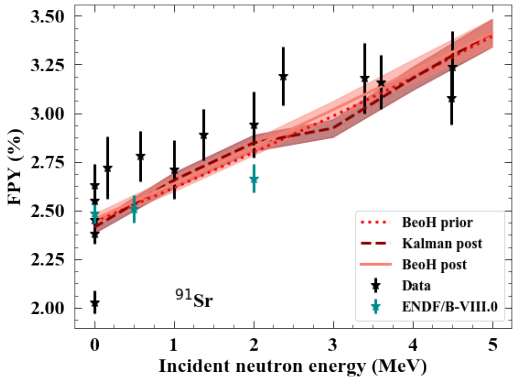
1) including a handful of important-to-model nuclei, 2) nuclei with good energy dependence [up to E_{inc}=5 MeV], 3) light nuclei, 4) heavy nuclei

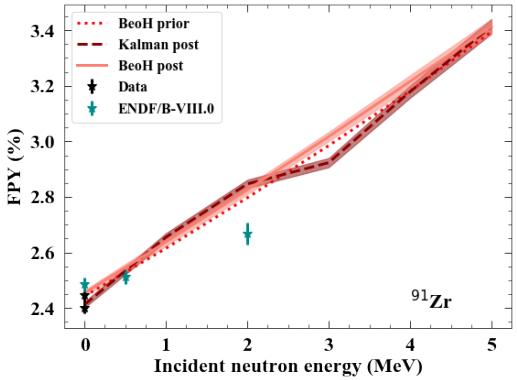


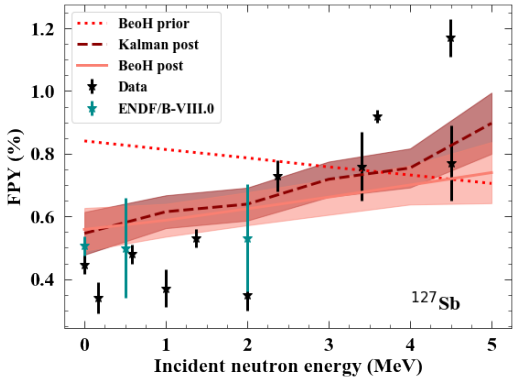
^{239}Pu(n,f)

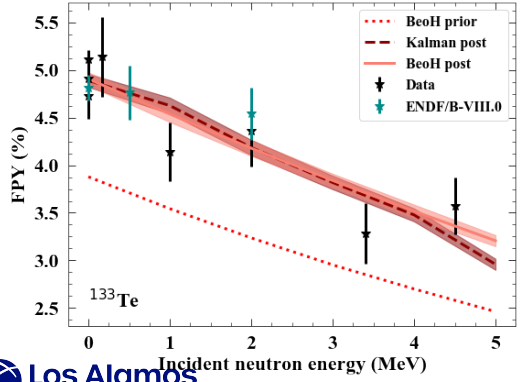
Note: this optimization currently only includes experimental cumulative FPY data, not R-values, other ratio data, or the current ENDF/B-VIII.0 values

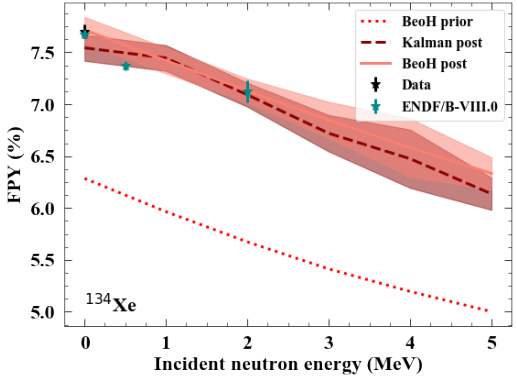
Many FPYs show reasonable agreement with experimental data for light and heavy nuclei

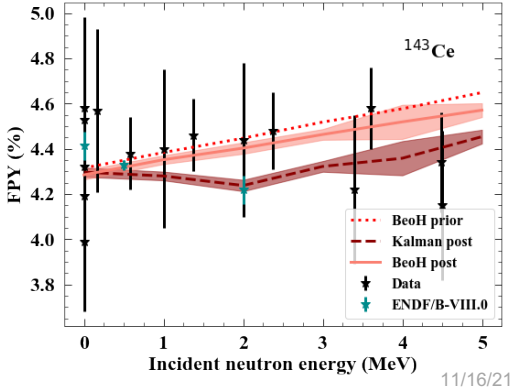








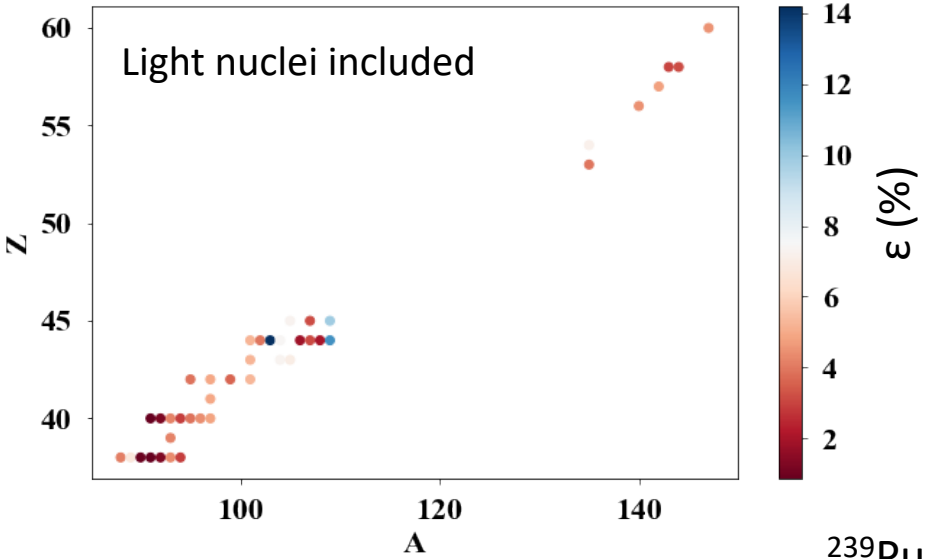


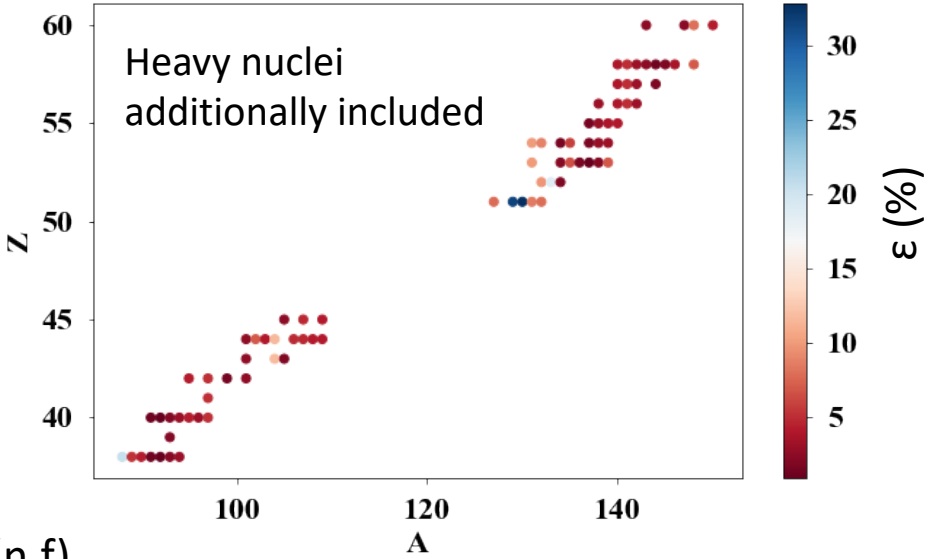


Non-linearities in the model can lead to significant differences between the Kalman and BeoH posteriors

The majority of FPYs match reasonably well between Kalman and BeoH (linear assumption is okay), but BeoH may still not describe data

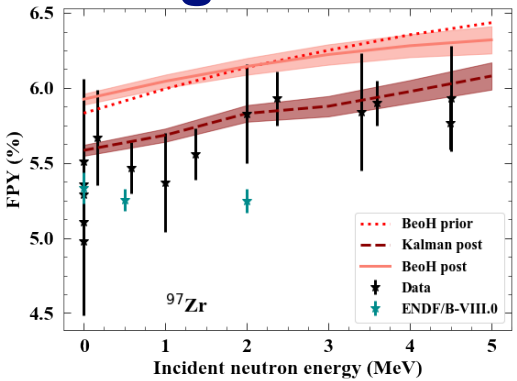
$$\varepsilon = \frac{1}{N}\sum_{i=1}^{N}\frac{|o^{\mathrm{BeoH}} - o^{\mathrm{Kalman}}|}{o^{\mathrm{BeoH}}}$$





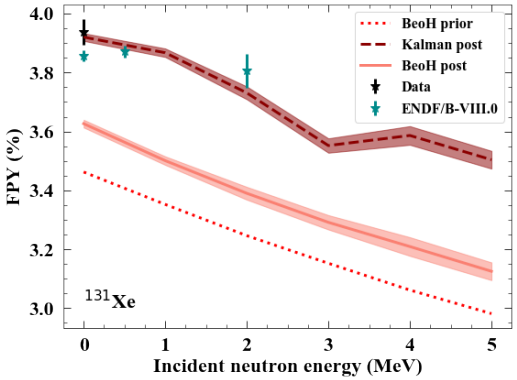
^{239}Pu(n,f)

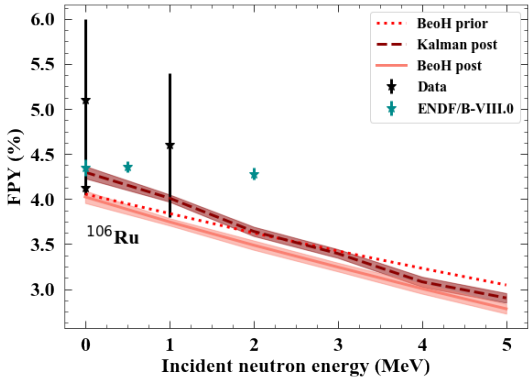
Differences between Kalman and BeoH could be mitigated through several means



Potential challenges:

- Calculations are not run with a low enough Y(A,Z) threshold → missing contributions to cumulative yields and sensitivities
- Sensitivities are EXTREMELY non-linear and should be calculated much closer to the best fit parameter set



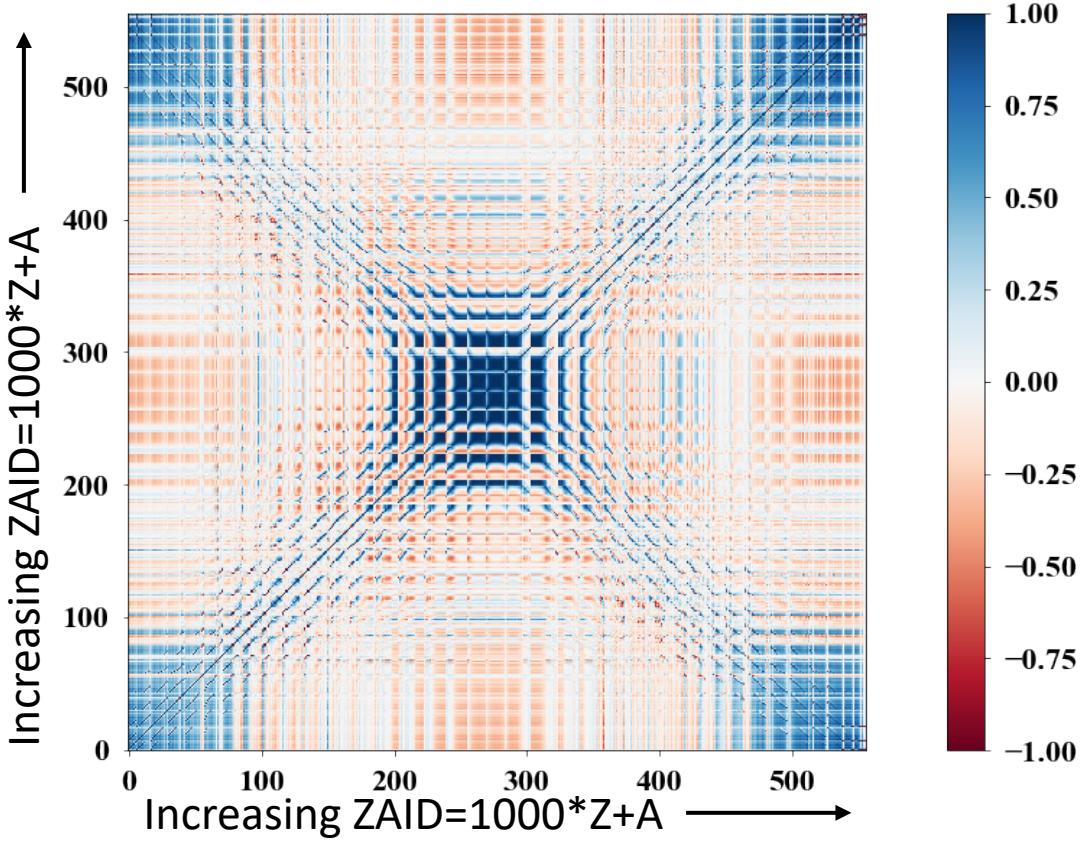


- Small uncertainties on the data pull to hard on the optimization (FPY templates exist, Neudecker, et al., LA-UR-19-31156)

Ultimately, we may have to put a correction on top of the BeoH calculations to ensure we reproduce important FPYs.

Correlations between cumulative (and independent) fission product yields can be calculated

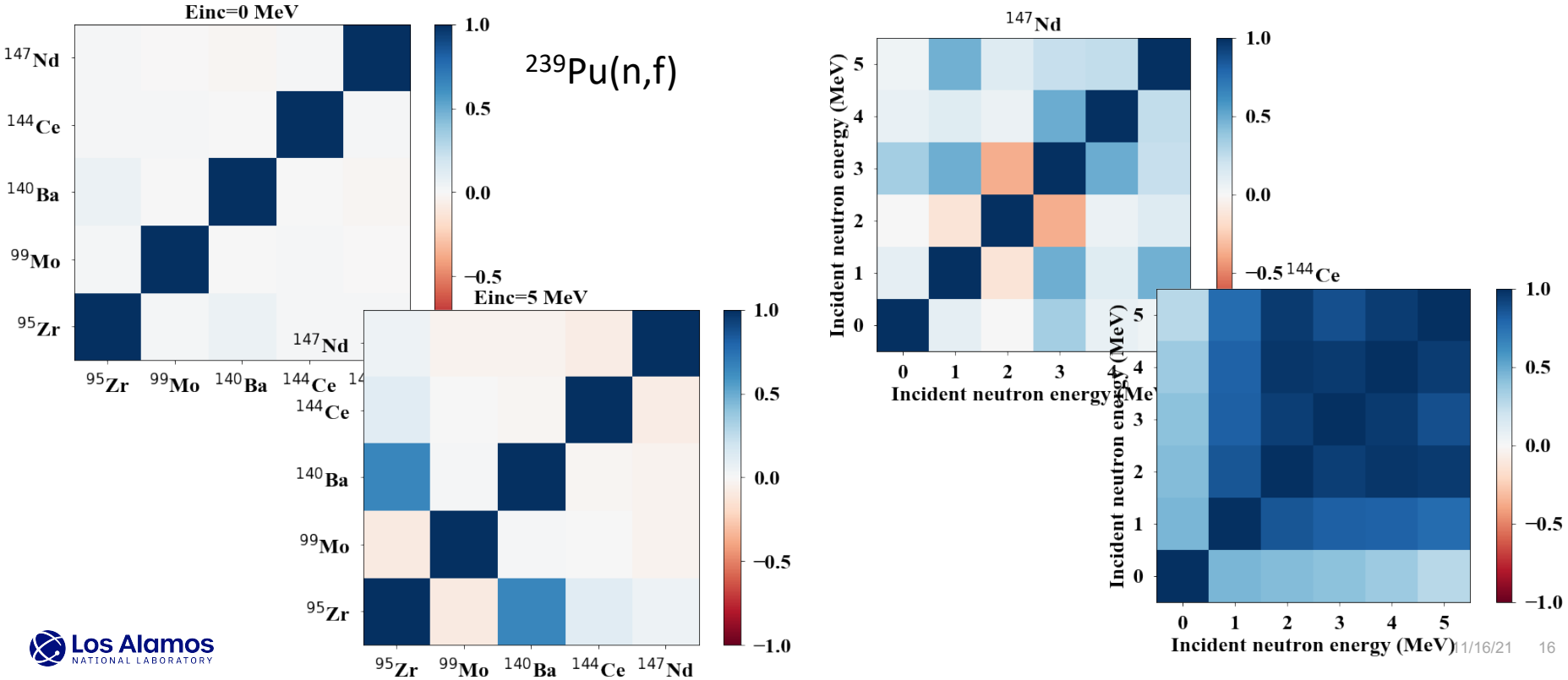
$^{239}Pu(n_{th},f)$



The inclusion of a mass-dependence excitation energy sharing term greatly reduces the correlations between FPYs (updated from mini-CSEWG).

The Kalman filter can be further be extended to include the energy-dependent parameters

Giving us access to correlations between FPYs and across energies



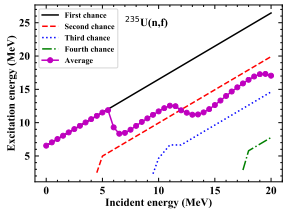
Summary

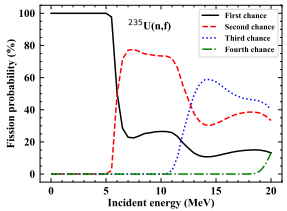
- The Hauser-Feshbach fission fragment decay code, BeoH is being used to consistently calculate independent and cumulative fission product yields, simultaneously with other prompt and delayed observables.
- A Kalman filter has been implemented to adjust parameters describing the fission fragment initial conditions to prompt and delayed average neutron multiplicity and certain thermal cumulative fission product yields with low reported uncertainty in the England and Rider evaluation, for first-chance fission (up to 5 MeV).
- First-chance fission for ^{239}Pu is currently being studied in detail to include the bulk of the experimental cumulative FPY data in the optimization. Discrepancies between Kalman, BeoH, and data need to be addressed either through modeling or additional corrections. Methods will be extended beyond first-chance fission.
- Covariance across the FPYs are being constructed (more during covariance session).
- ^{235}U, ^{238}U, and ^{239}Pu for first-chance fission are in good shape; initial calculations for ^{252}Cf have been started, and input for ^{237}Np is being prepared.

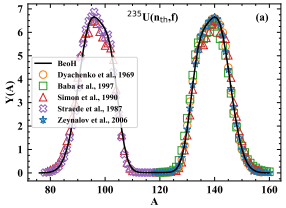
BeoH calculates prompt/delayed fission observables using the statistical Hauser-Feshbach theory

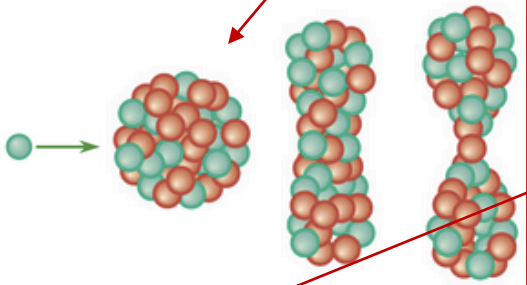
Input from CoH is needed (fission probabilities, excitation energy, etc.)

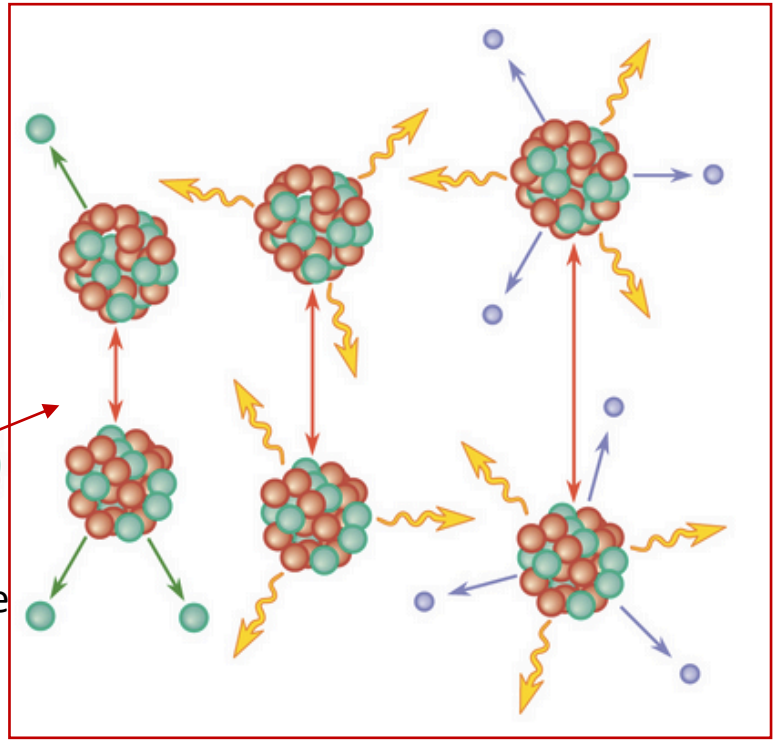
Decay data required for IFY → CFY











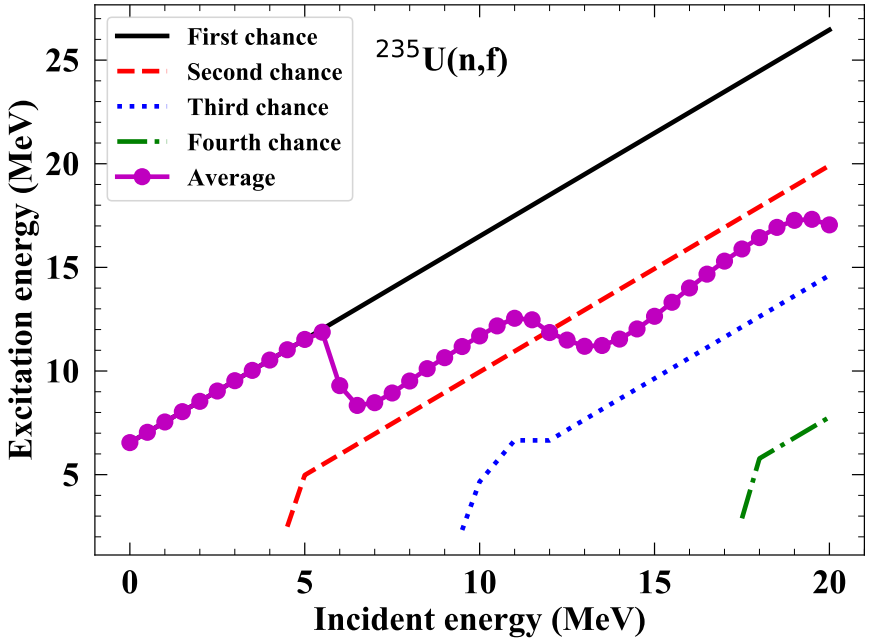
The initial conditions of the fission fragments are parametrized and fit to data (mass, charge, kinetic energy, spin, parity)

Lovell, Kawano, *et al.*, *PRC* **103** 014615 (2021)

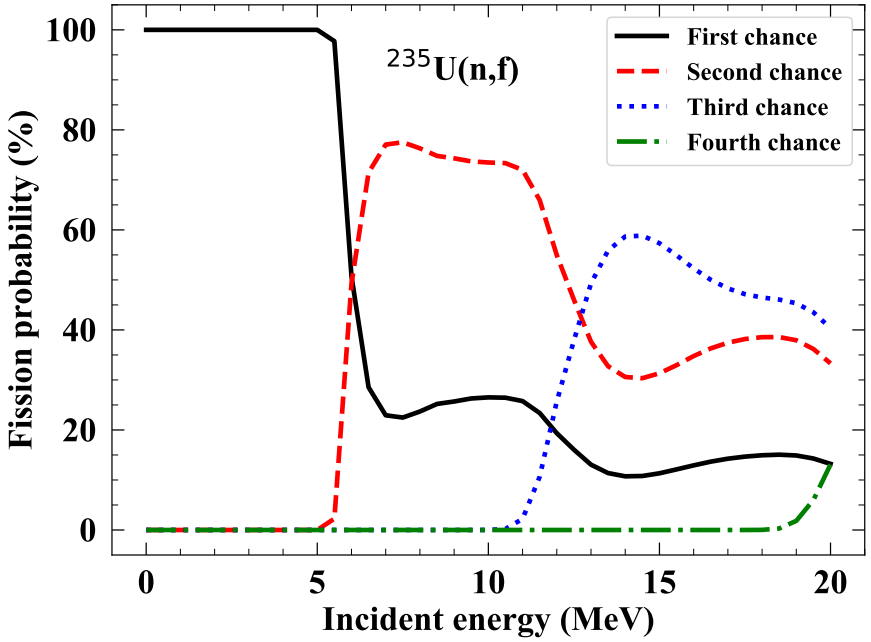
Pre-decay quantities are calculated with CoH

Most probable excitation energy causing fission

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

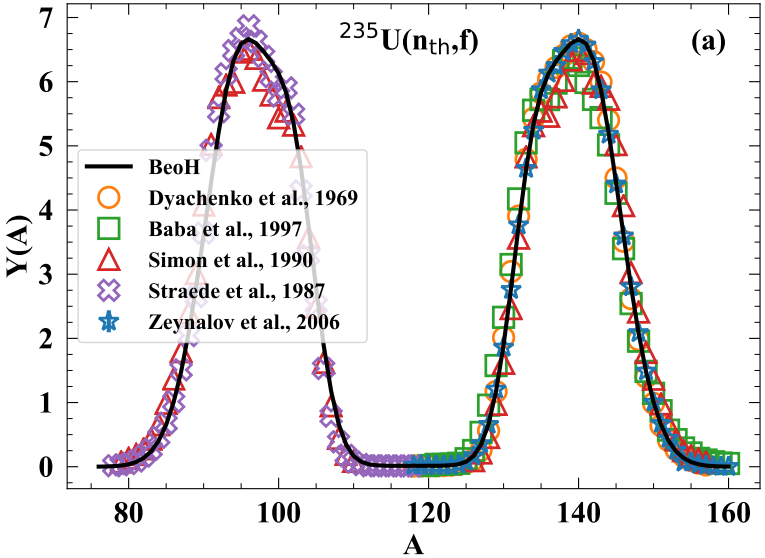


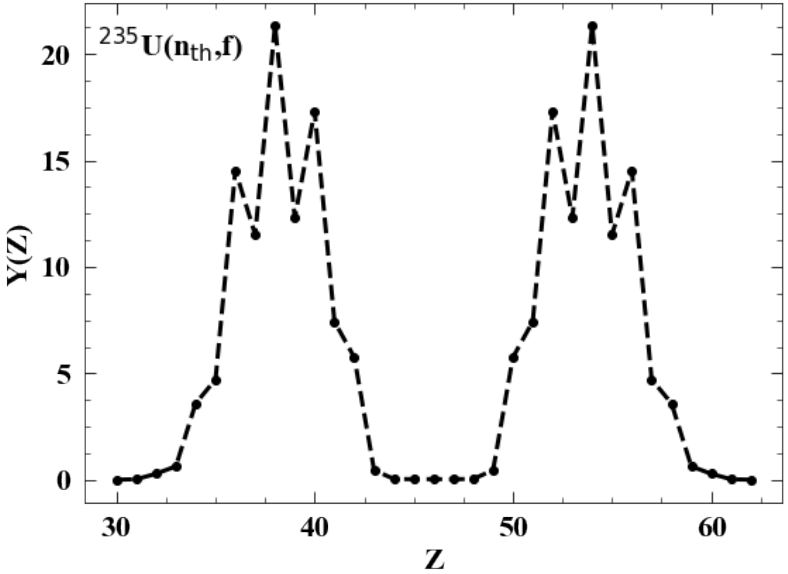
Fission probabilities (fission barriers and level densities can be fit to cross sections)



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.).



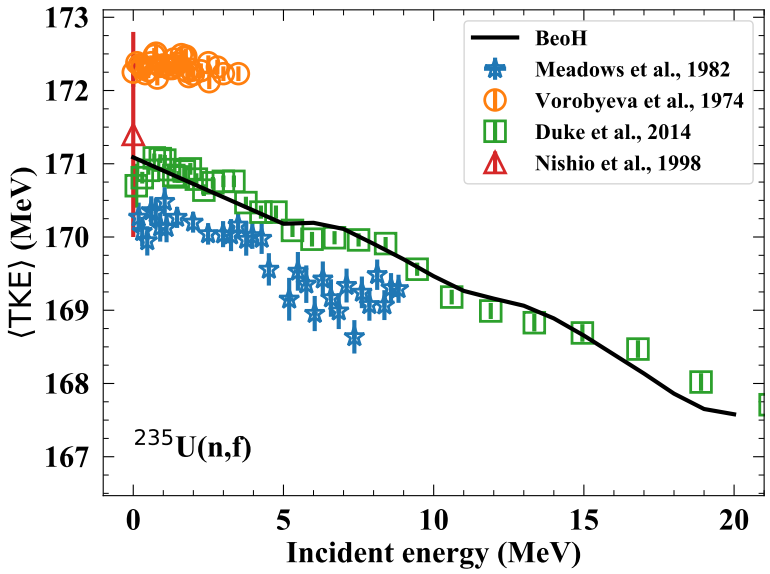


The Wahl systematics are used to calculate the charge distribution, Y(Z|A).

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.



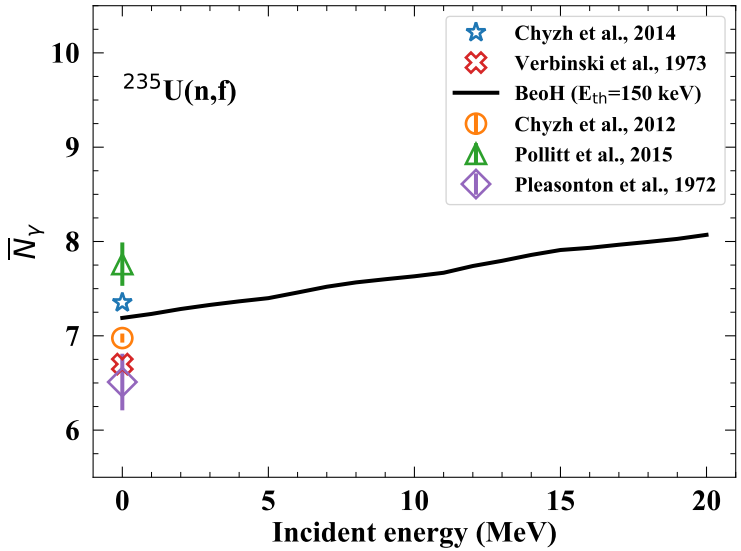
The spin distribution is proportional to the available states in the level density formula, with an adjustable scaling factor on the spin cut-off parameter, f.

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

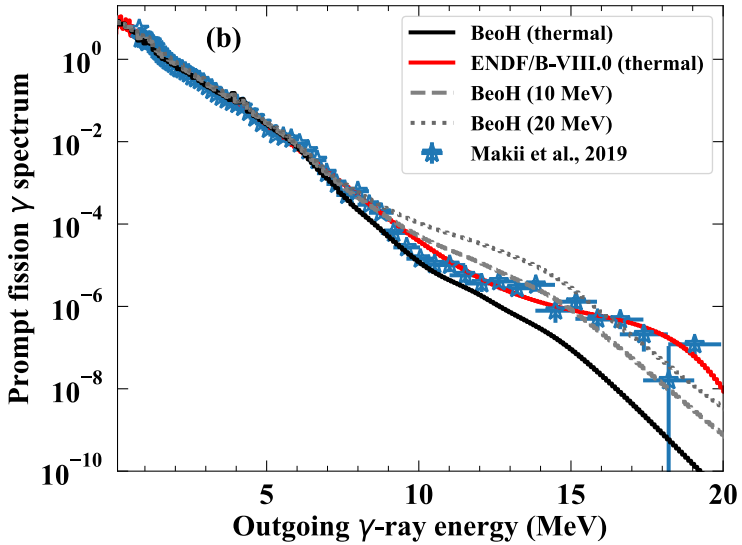
Positive and negative parities are taken to be equally probable.

Prompt gamma-ray observables can be calculated

Average prompt γ-ray multiplicity



Prompt γ-ray energy spectrum



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

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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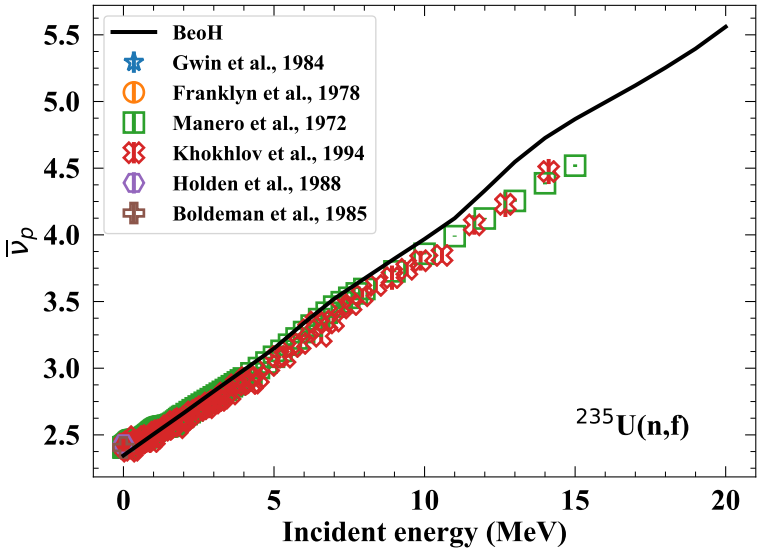
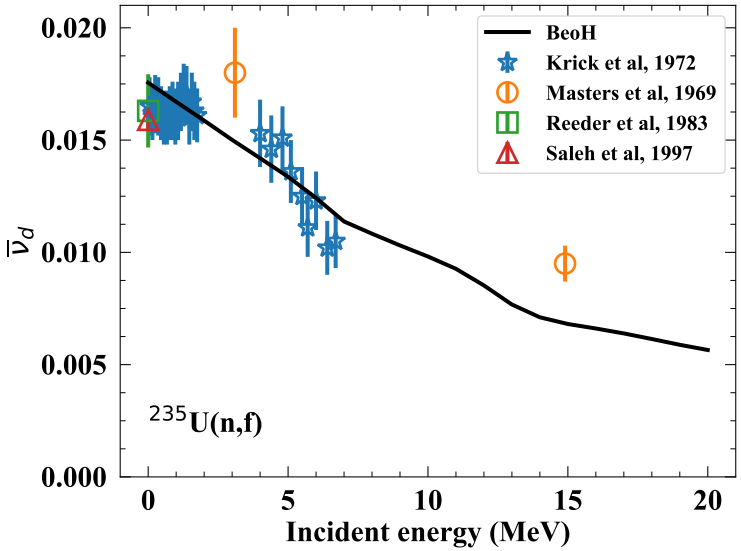
Prompt and delayed neutron observables can be calculated

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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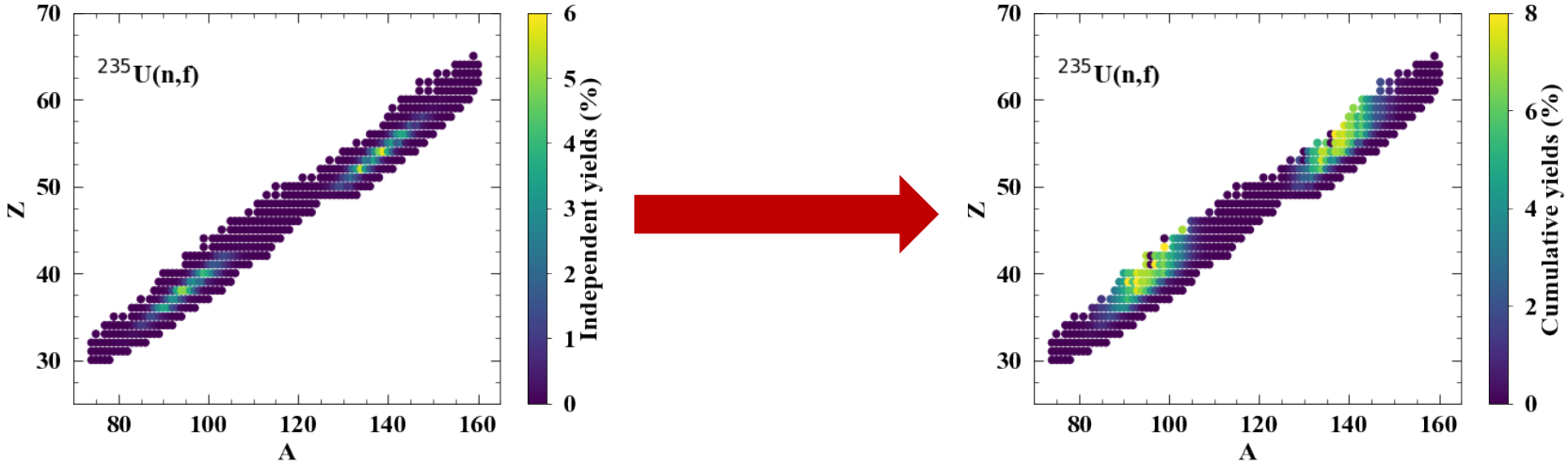
Independent yields to cumulative yields

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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