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# Overview of an energy-dependent fission product yield evaluation

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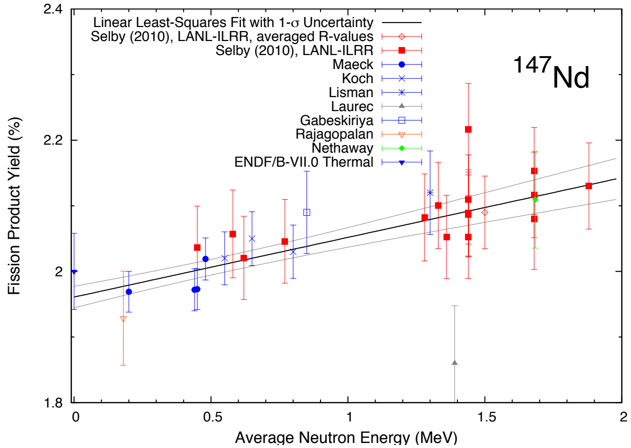
# The time is ripe for an updated fission product yield evaluation

The current FPY ENDF evaluation is based on the 1989 evaluation of England and Rider, energies are limited to thermal, fast, and 14 MeV.

A denser energy grid requires a more predictive model than has been used previously combined with high-quality experimental data across a range of energies.

A LANL led, NA-22 funded project will provide an updated FPY evaluation incorporating recent model developments and new experimental data.

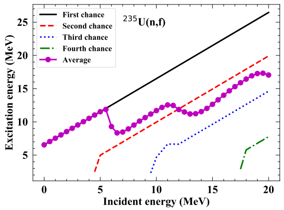
In 2010, Chadwick, et al. updated the energy-dependence for $^{239}$Pu only (with an energy point added at 2 MeV)

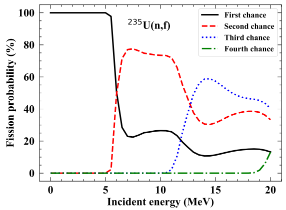


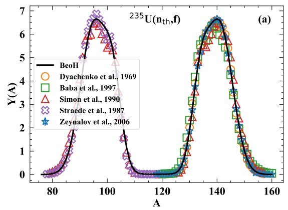

Chadwick, Kawano, et al., *Nucl. Data Sheets* **111**, 2923 (2010)

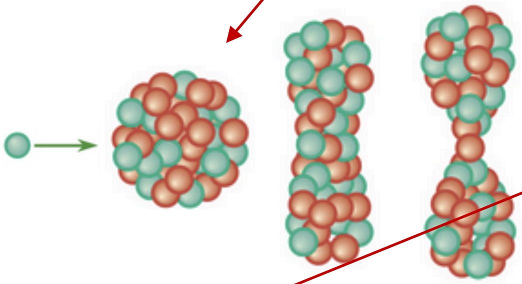
# BeoH calculates prompt/delayed fission observables using the statistical Hauser-Feshbach theory

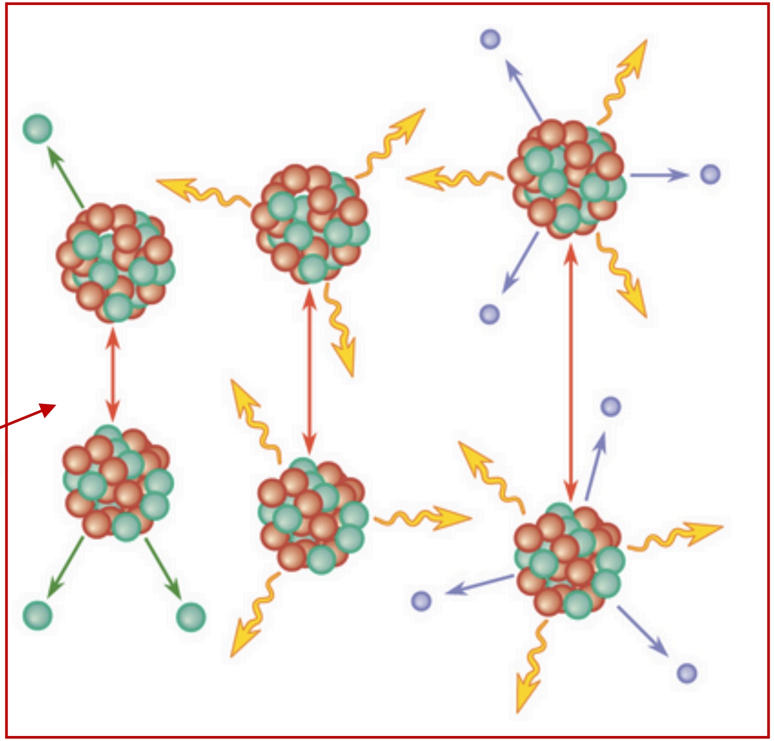
Input from CoH is needed (fission probabilities, excitation energy, etc.)





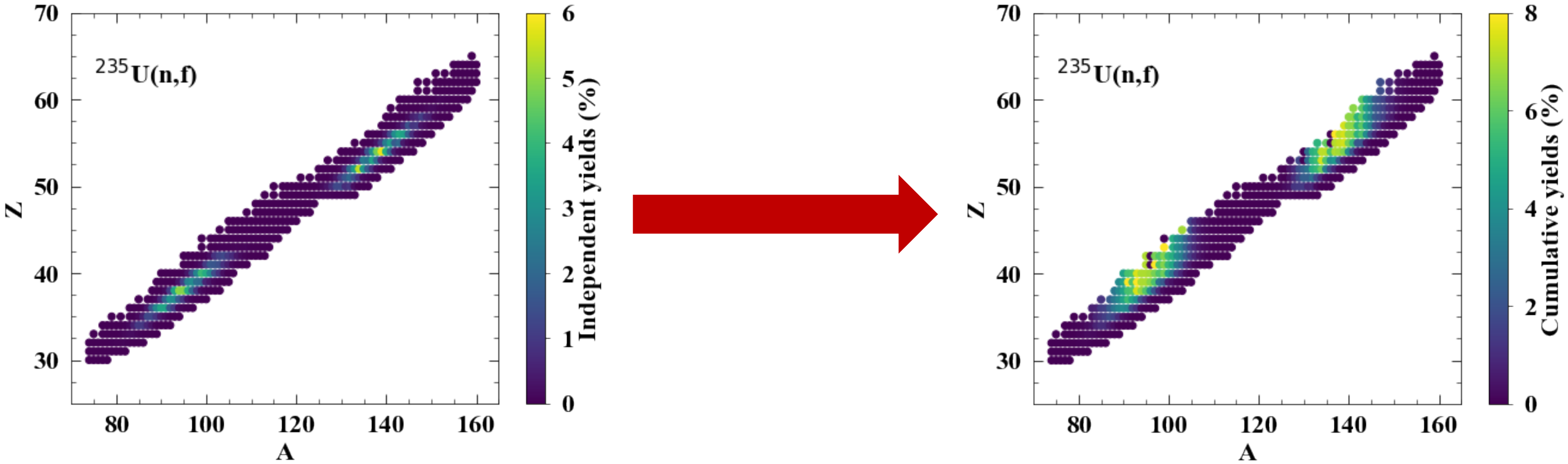
The initial conditions of the fission fragments are parametrized and fit to experimental data where available (mass, charge, kinetic energy, spin, parity)

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

# 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.

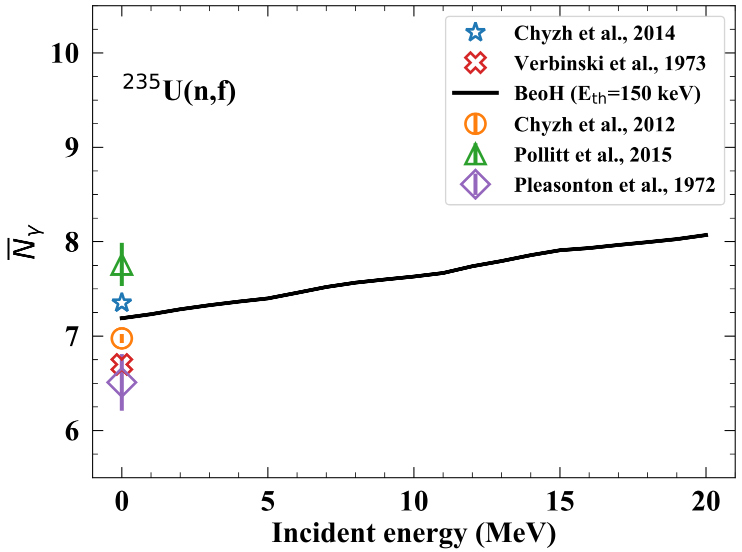
Then, a time-independent calculation is performed, using decay data library information (from ENDF/B-VIII.0) to calculate the cumulative yields from the independent yields.  Isomeric states are kept track of for the independent and cumulative yields.



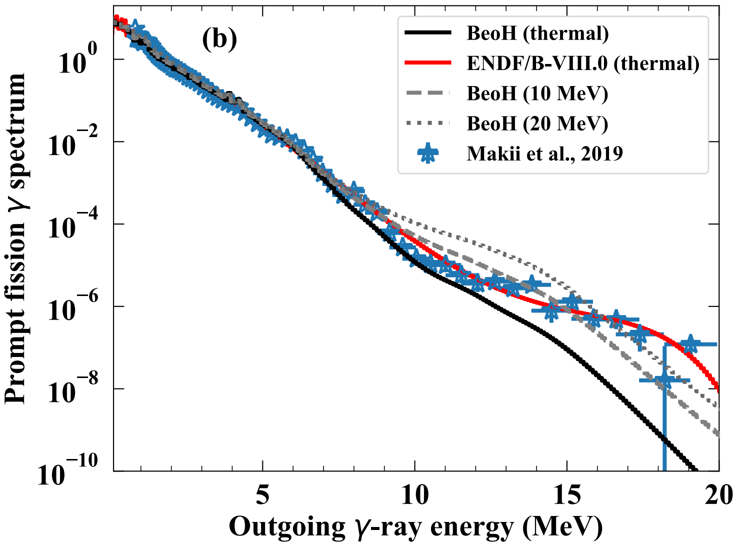

Lovell, Kawano, *et al.*, *PRC* **103** 014615 (2021)

# Prompt gamma-ray observables can be calculated

Average prompt $\gamma$-ray multiplicity




Prompt $\gamma$-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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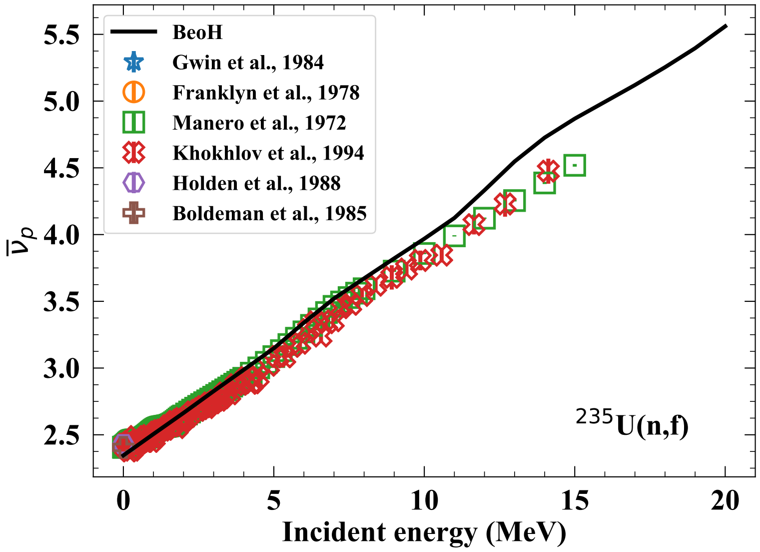
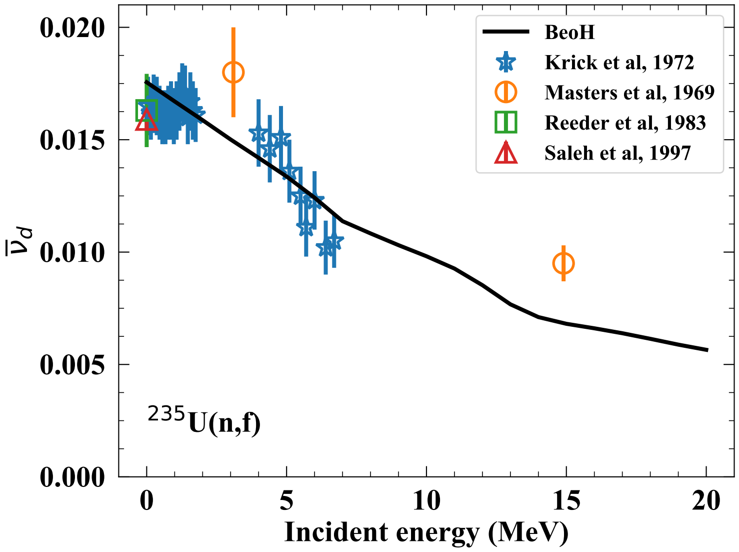
# Prompt and delayed neutron observables can be calculated

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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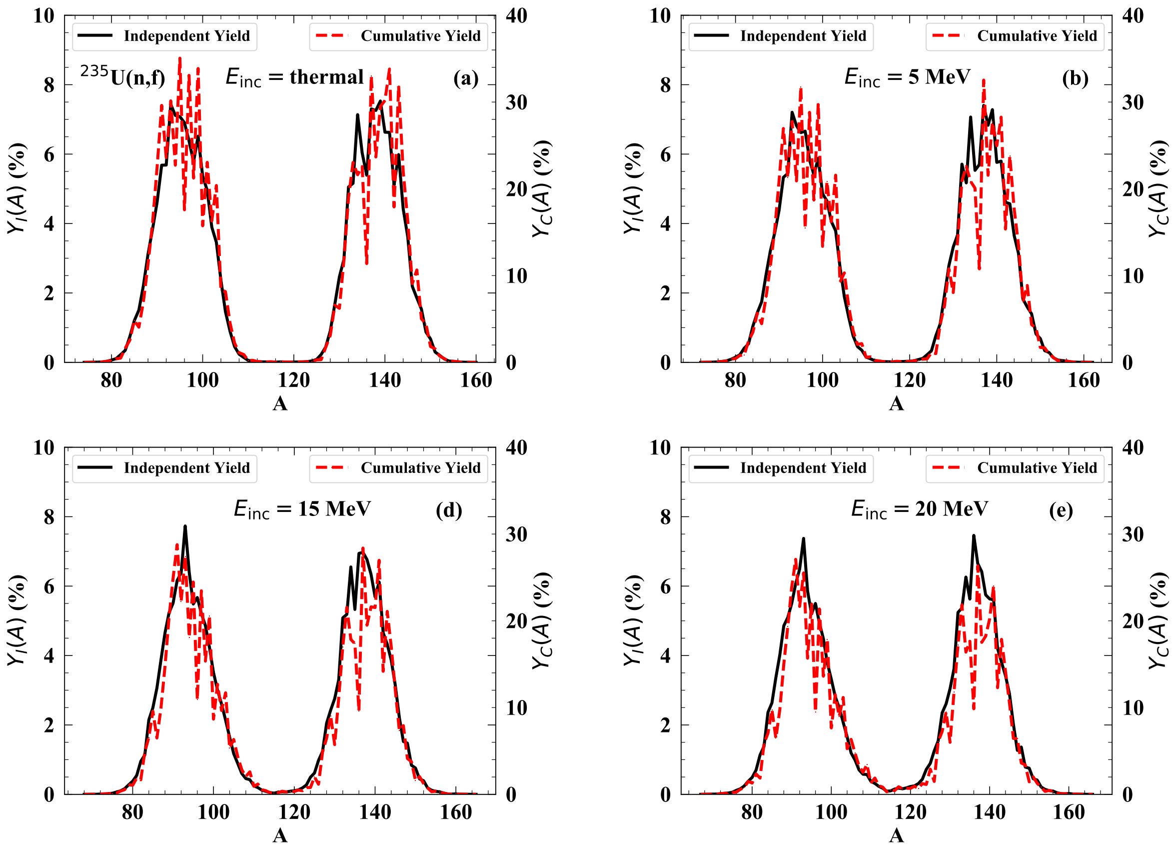
# Independent and cumulative mass yields




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

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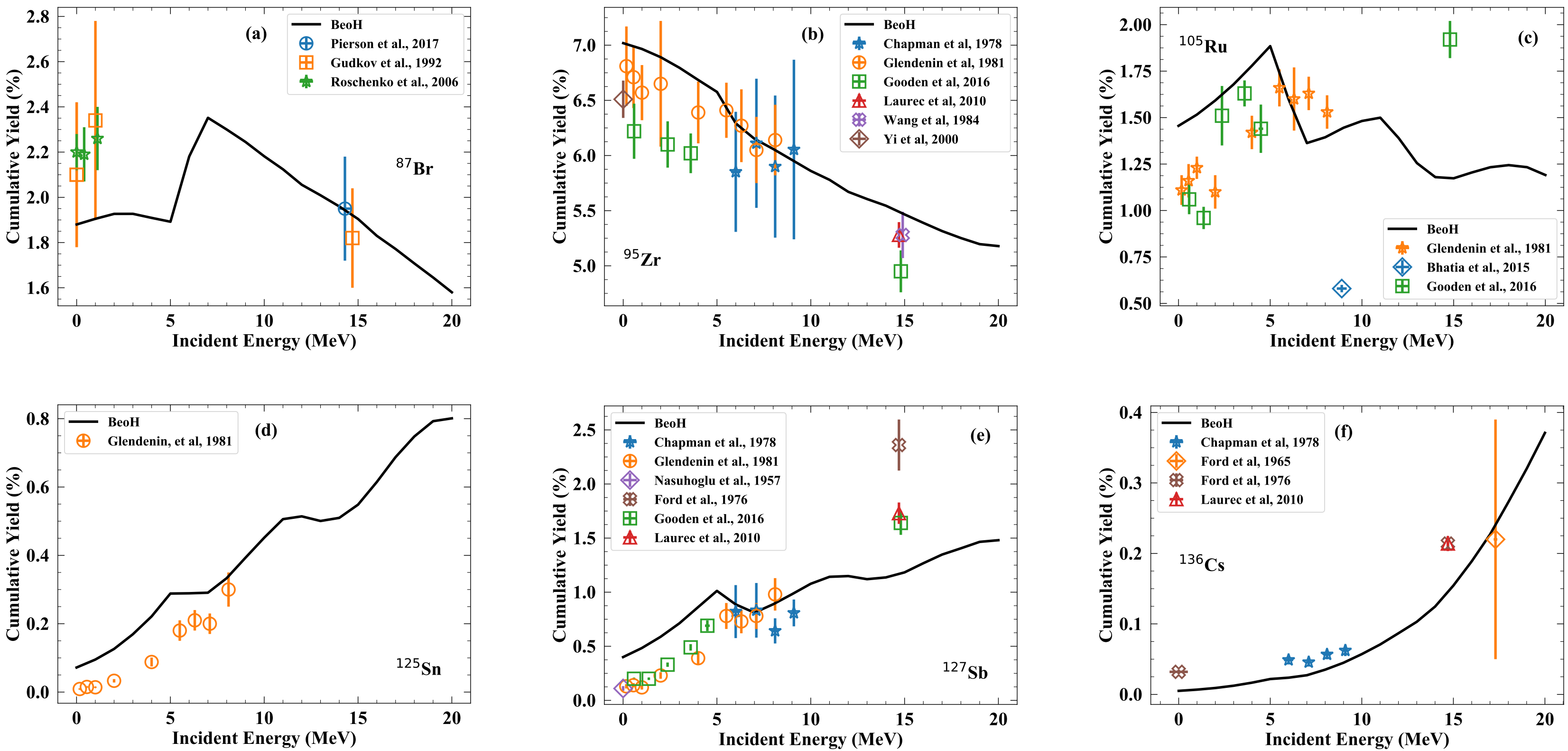
# Cumulative fission product yields already show reasonable agreement without specific optimization

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# 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, submitted to 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

Data covariance

Model calculation vector

Parameter covariance

Sensitivities

Model predictions and covariance are updated

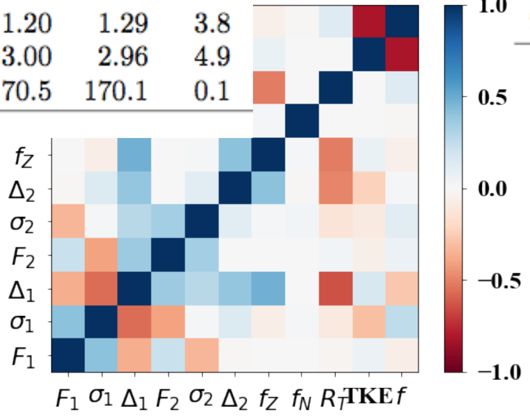
$$\Phi = f(\mathbf{x}_1) \qquad \mathbb{F} = \mathbb{C}\mathbb{P}\mathbb{C}^T$$

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

# Model parameters are updated with uncertainties and correlations

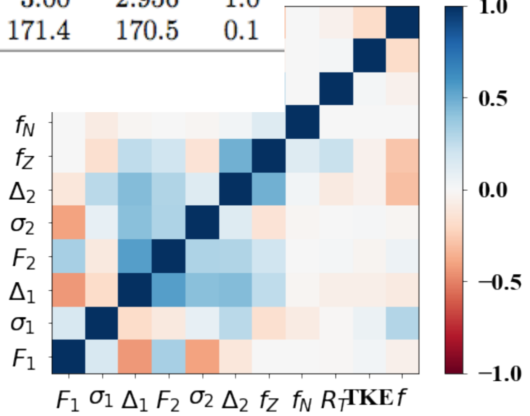
$^{235}$U($n_{th}$,f)

| | pri | post | % change |
|---|---|---|---|
| $F_1$ | 0.793 | 0.824 | 4.3 |
| $\sigma_1$ | 4.83 | 5.05 | 1.4 |
| $\Delta_1$ | 23.0 | 23.1 | 0.5 |
| $F_2$ | 0.205 | 0.197 | 4.7 |
| $\sigma_2$ | 2.73 | 2.92 | 3.1 |
| $\Delta_2$ | 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 |



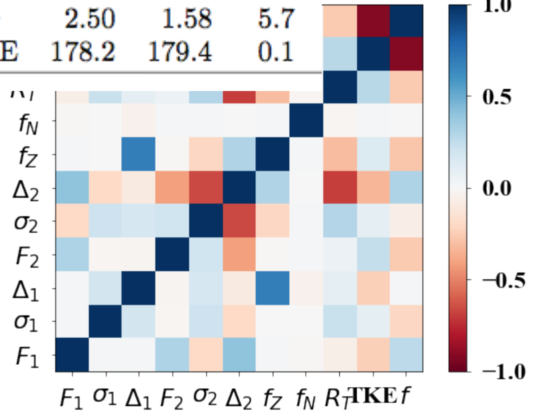

$^{238}$U($n_{1\,MeV}$,f)

| | pri | post | % change |
|---|---|---|---|
| $F_1$ | 0.587 | 0.625 | 3.6 |
| $\sigma_1$ | 5.405 | 5.580 | 1.4 |
| $\Delta_1$ | 22.879 | 23.128 | 0.5 |
| $F_2$ | 0.413 | 0.380 | 4.4 |
| $\sigma_2$ | 3.459 | 3.326 | 2.6 |
| $\Delta_2$ | 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)

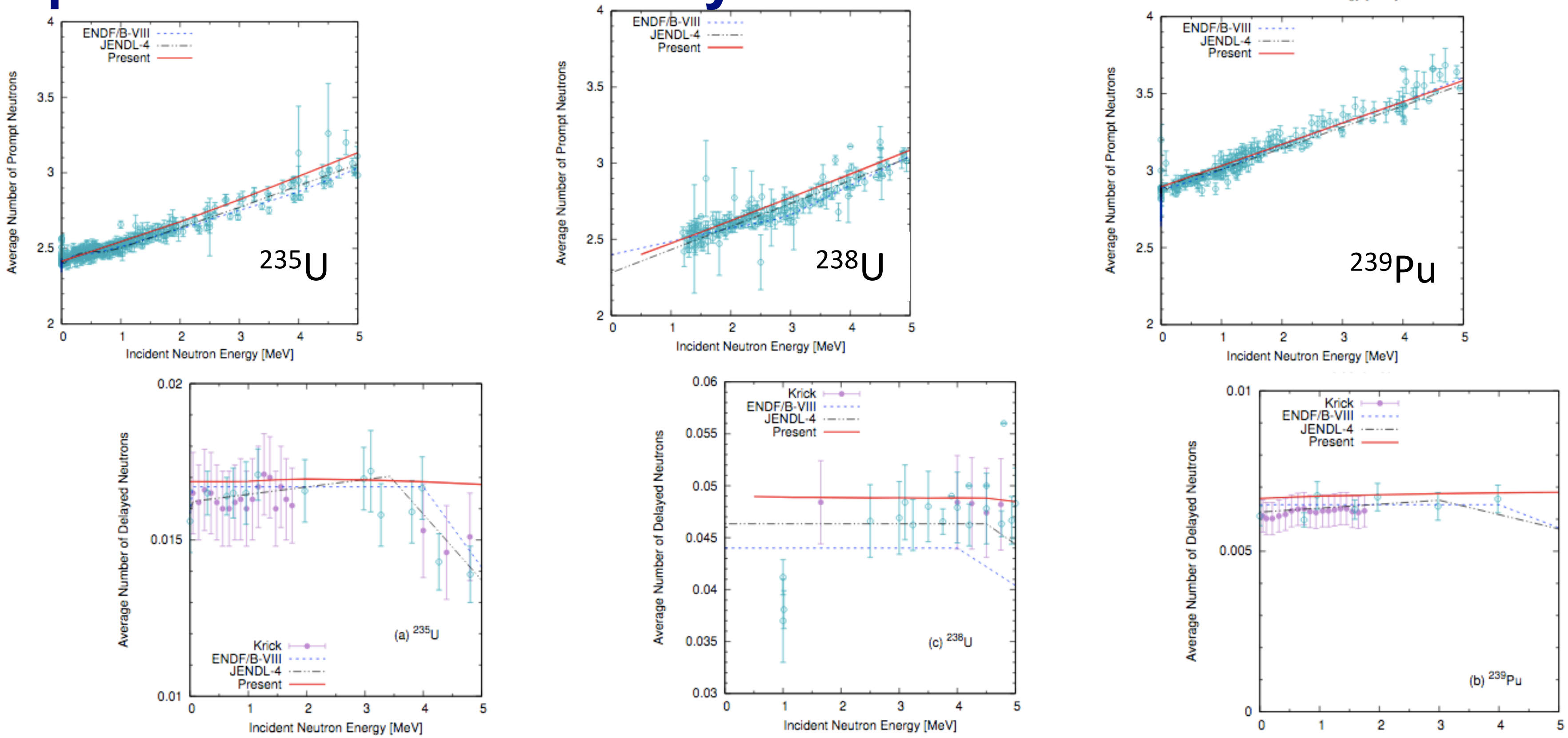
| | pri | post | % change |
|---|---|---|---|
| $F_1$ | 0.234 | 0.248 | 4.1 |
| $\sigma_1$ | 3.51 | 3.26 | 5.2 |
| $\Delta_1$ | 14.9 | 14.1 | 1.8 |
| $F_2$ | 0.765 | 0.718 | 4.6 |
| $\sigma_2$ | 6.06 | 6.58 | 0.5 |
| $\Delta_2$ | 20.8 | 20.1 | 0.5 |
| $f_{Z0}$ | 1.00 | 2.58 | 4.4 |
| $f_{N0}$ | 1.00 | 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 |




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

$$\mathbb{F} = \mathbb{CPC}^T$$

# Prompt and delayed neutron multiplicities are reproduced simultaneously

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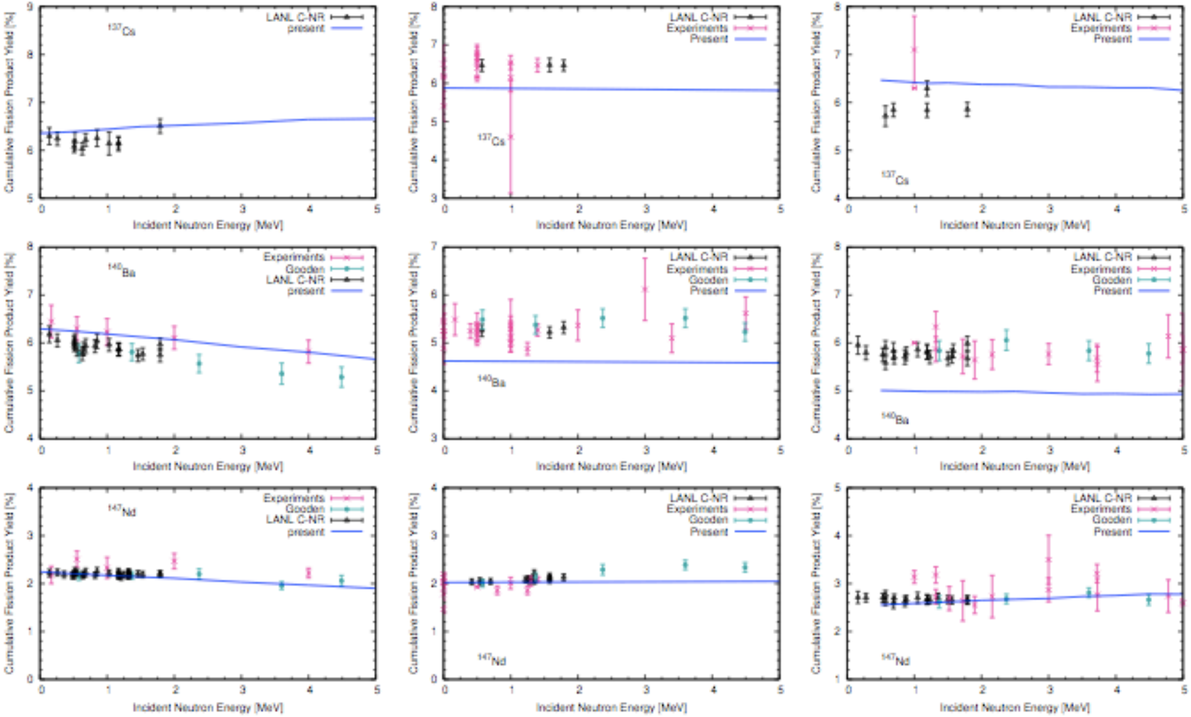
# A variety of cumulative fission product yields can also be reproduced

$^{235}$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, submitted to JNST, LA-UR-21-20820

# Summary

- The Hauser-Feshbach fission fragment decay code, BeoH has been updated to include multi-chance fission; the decay of excited fission fragments via neutrons and $\gamma$ rays is followed consistently through prompt and delayed emission.
- Many neutron, $\gamma$-ray, and fission fragment yield observables can be reproduced simultaneously.
- A Kalman filter has been implemented to adjust parameters describing the fission fragment initial conditions to prompt and delayed average neutron multiplicity and certain cumulative fission product yields with low reported uncertainty in the England and Rider evaluation, for first-chance fission (up to 5 MeV).
- This parametrization serves as a good starting point for further optimization to a wider variety of cumulative fission product yields, including experimental data. This optimization is ongoing and will be extended beyond 5 MeV incident energy.
- $^{235}U$, $^{238}U$, 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 in collaboration with SPIDER.