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Title: Nuclear Data Evaluations of Medium-mass Nuclei and Actinides

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Nuclear Data Evaluations of Medium-mass Nuclei and Actinides

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Overview

- Evaluation methodology
- Los Alamos modeling tools – CoH and BeoH
- Recent evaluation studies
  - ^{51}V – example of experimental templates
  - ^{233}U – exploring inconsistent data
  - ^{239}Pu – modeling updates
  - Fission product yields
- Summary

Evaluations combine modeling and experimental data to produce mean values and covariances

- Evaluation requires combining experimental data with model calculations or model-free splines to produce quantities of interest.
- Mean values and covariances (uncertainties and correlations) from the evaluation process are turned into evaluated data libraries, such as ENDF/B.
- Both model and experiment have uncertainties and can be wrong, so careful consideration has to be taken when deciding which ingredients to include and how to best combine all available information.
- Evaluated nuclear data is a necessary input for transport codes, such as MCNP, which then provide vital feedback for validation of new evaluation efforts.

The Kalman filter is a typical method to combine these two ingredients

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

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

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

Optimization works well if the parameters remain in the linear region, but assumptions can break down away from there and if the model is complex. Calculations times are relatively short, and covariances are also output.

Experimental inputs deserve careful consideration

- Many measurements are made relative to other, or standard, reaction channels; absolute measurements can then be extracted and reported using the evaluated/accepted cross section value at the time of the measurement; these need to be updated, taking into account current values.
- Experimental uncertainties can be under-reported or missing entirely, which biases evaluated mean values and covariances.
- Full experimental covariances are rarely reported but impact evaluated results.
- A large-scale effort to develop templates of expected experimental covariances has been pursued, based on an effort by the Cross Section Evaluation Working Group (CSEWG).

Templates of expected measurement uncertainties

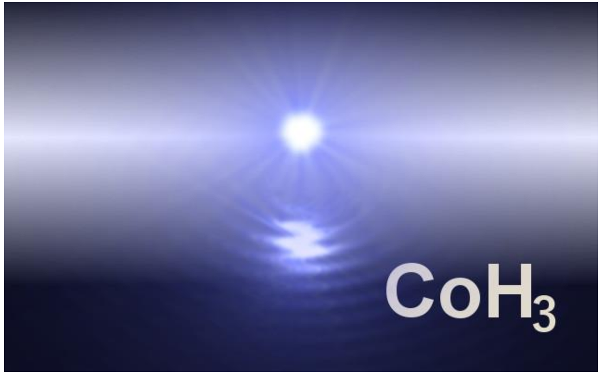
Denise Neudecker[1,*], Amanda M. Lewis[2], Eric F. Matthews[3], Jeffrey Vanhoy[4], Robert C. Haight[1], Donald L. Smith[5], Patrick Talou[1], Stephen Croft[6], Allan D. Carlson[7], Bruce Pierson[8], Anton Wallner[9], Ali Al-Adili[10], Lee Bernstein[3,11], Roberto Capote[12], Matthew Devlin[1], Manfred Drosg[13], Dana L. Duke[1], Sean Finch[14,15], Michal W. Herman[1], Keegan J. Kelly[1], Arjan Koning[12], Amy E. Lovell[1], Paola Marini[16,17], Kristina Montoya[1], Gustavo P.A. Nobre[18], Mark Paris[1], Boris Pritychenko[18], Henrik Sjöstrand[10], Lucas Snyder[19], Vladimir Sobes[20], Andreas Solders[10] and Julien Taieb[16,21]

D. Neudecker, *et al.*, *EPJ Nuclear Sci. Technol.* **9**, 35 (2023) and other articles in that issue

CoH_3: Coupled-Channels Hauser-Feshbach code

❑ Hauser-Feshbach-Moldauer theory for compound nuclear reactions
- 45,000 lines C++ code (~ 140 C++ source files, ~60 headers, ~80 classes)
- maintain by GNU Autotools package

❑ Modules and Models employed
- spherical and deformed optical models
- DWBA for direct inelastic scattering
- Moldauer’s width fluctuation correction with LANL parametrization
- Gilbert-Cameron level density with updated parameters
- pre-equilibrium 2-component exciton model
- Madland-Nix prompt fission neutron spectrum including pre-fission emission
- direct/semidirect capture model
- mean-field models (FRDM and Hartree-Fock BCS)

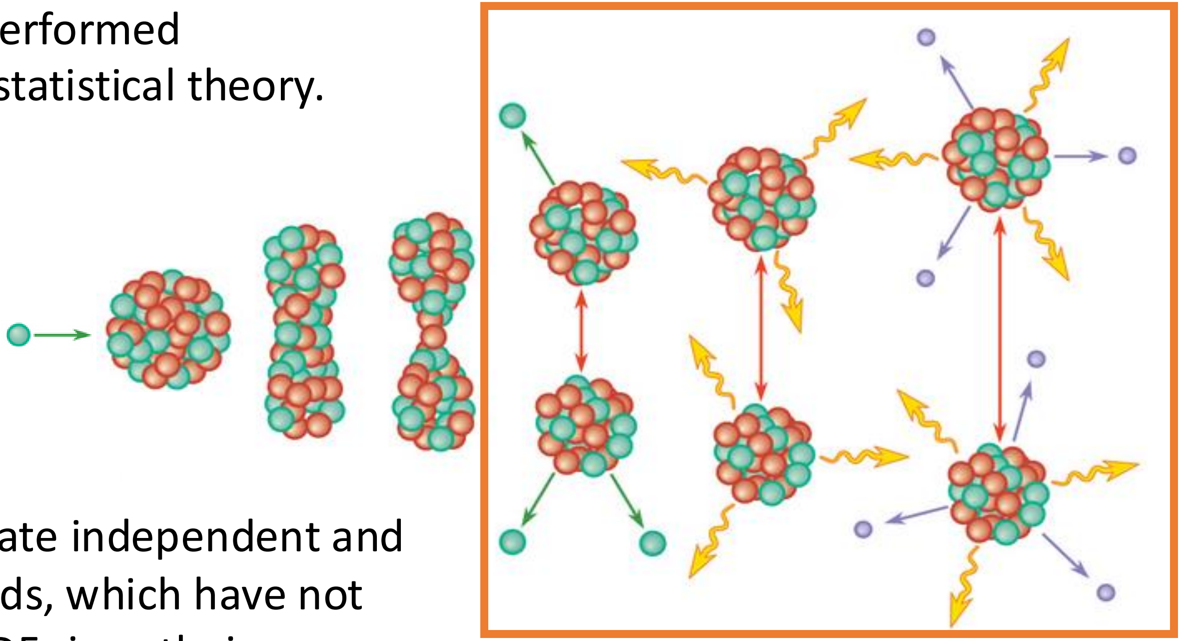


Consistent evaluations in all channels, focusing on fast cross sections

BeoH consistently calculates prompt and delayed fission observables (after scission)

Prompt neutron and γ decay performed through the Hauser-Feshbach statistical theory.

There is currently minimal connection between fission cross sections and other fission observables in both modeling and evaluation.



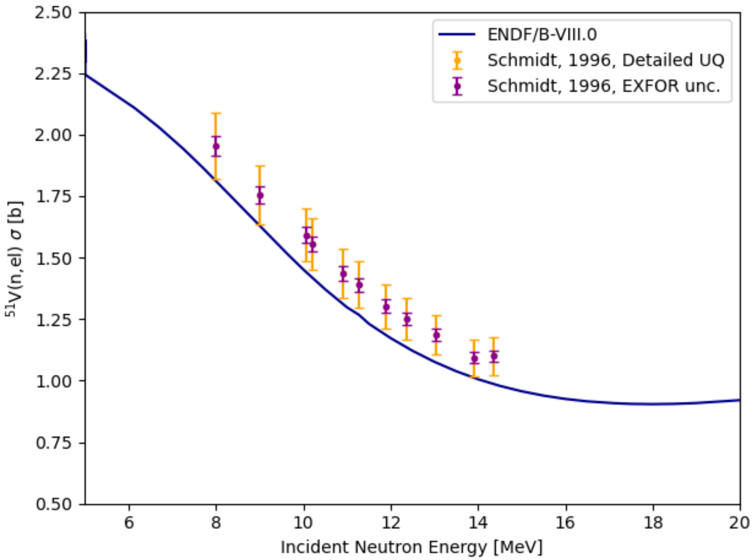
BeoH is being used to re-evaluate independent and cumulative fission product yields, which have not been fully re-evaluated for ENDF since their development by England and Rider (mid ‘90s).

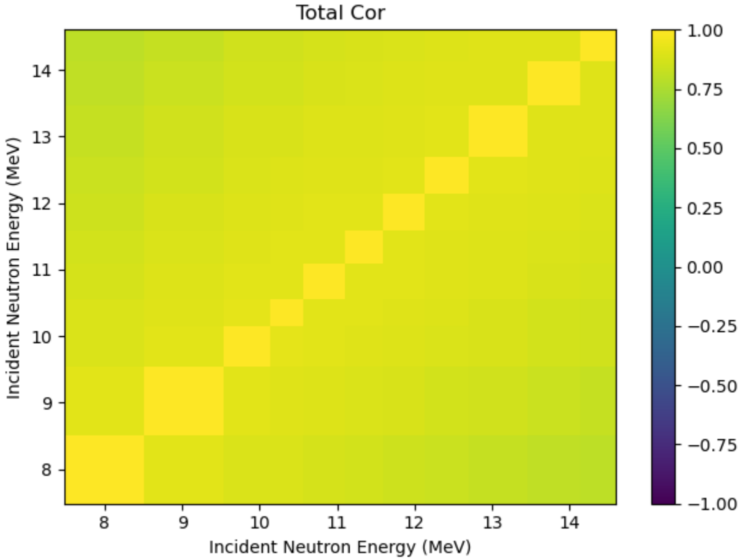
^{51}V

- Example of use of templates of expected experimental uncertainties
- Impact on evaluated covariances

^{51}V cross sections do not have covariances in ENDF/B-VIII.0

- Templates of expected experimental uncertainties were used to develop experimental covariances for the total and elastic cross section data
- Uncertainties are increased and correlations across energy are strong

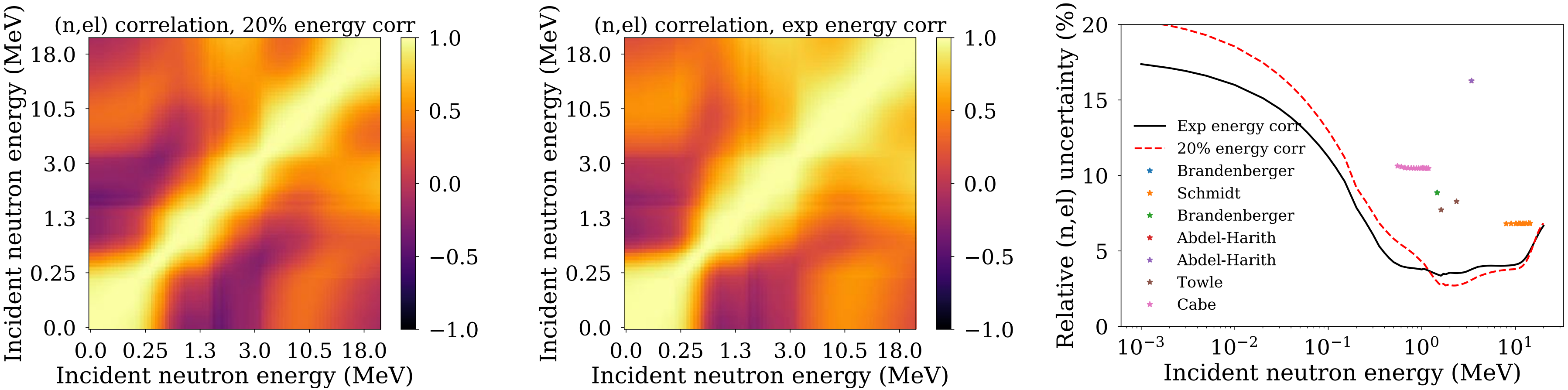




Work with D. Neudecker and A. Khatiwada (XCP-5); figures from A. Khatiwada

Experimental covariances impact evaluated covariances

- Our standard procedure has been to assume 20% correlation between incident energies (much weaker than the experimental correlations)
- Uncertainties and correlations change when templates are used to construct the experimental covariances



^{51}V next steps

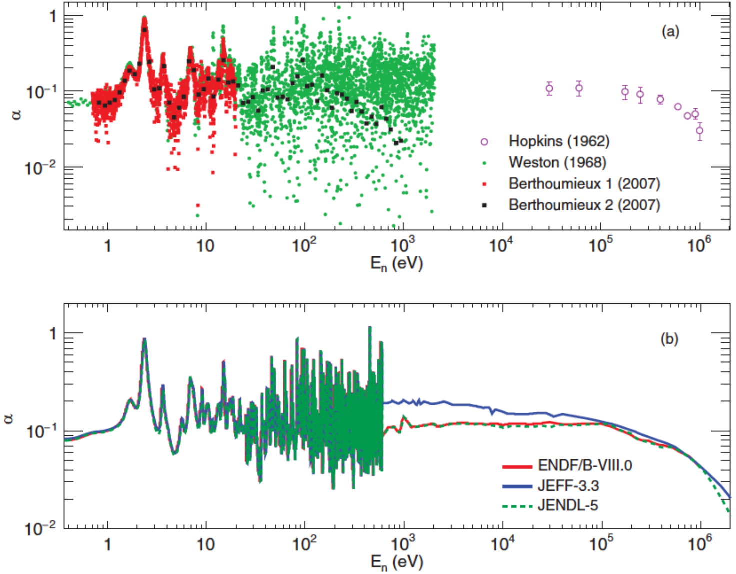
- A crit exists with different configurations of varying thickness for ^{51}V (HMF025)
- XCP-5 Nuclear Data Team has the MCNP input decks for these simulations
- These calculations will allow us to understand how the different evaluated covariances impact the modeled crits (means and uncertainties), compared to our “standard” procedure of an assumed, flat correlation

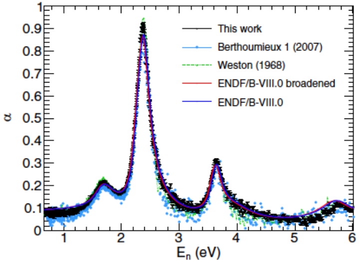
^{233}U

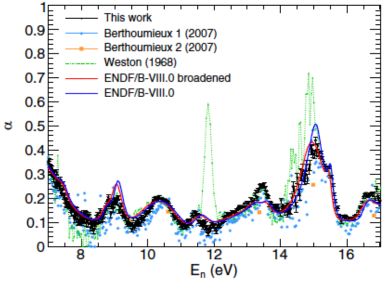
- New measurements (capture to fission ratio) were recently performed at LANSCE prompting a study of the fast energy region

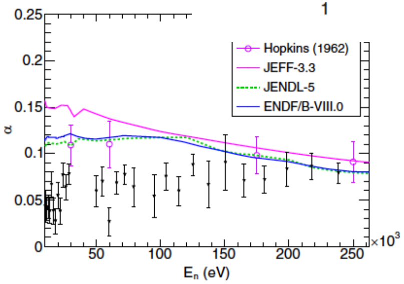
^{233}U capture measurements and evaluations

- RRR: good agreement between the evaluations
- URR (2-30 eV): agreement between ENDF/B-VIII.0 and JEFF-3.3, discrepancies with JENDL-5
- Fast region: only one data set which cannot be reproduced in statistical model using Γ_γ width extracted from resonance analysis
- Recent LANSCE measurement for ^{233}U(n,γ) (NCSP-funded) using DANCE+NEUANCE, good agreement with existing data below the fast energy region



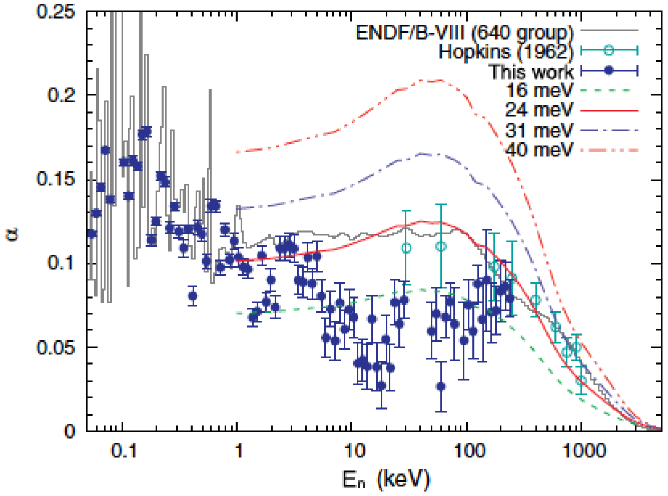


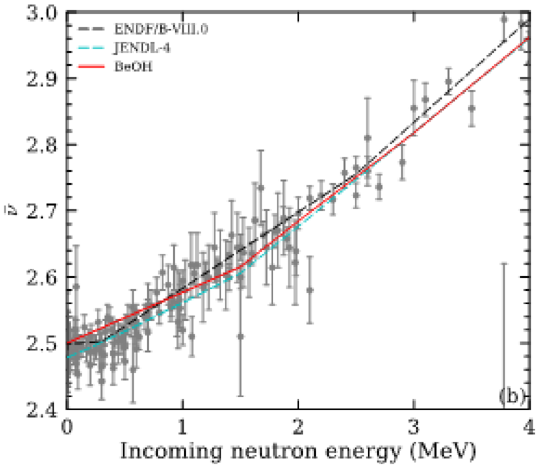




Leal-Cidoncha *et al., PRC* **108**, 014608 (2023)

^{233}U capture cross section and neutron multiplicity





The capture cross section is challenging to model consistently with the data but has an impact on criticality benchmarks

Neutron multiplicity can be calculated with BeoH, where a slightly different shape compared to evaluations is seen

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^{233}U criticality benchmarks with updated (n,γ) and nubar

Benchmark	ENDF/B-VIII.0	Test evaluation	Experiment
U233-COMP-THERM-001-002	0.99893	1.01250	0.99802
U233-MET-FAST-001-001	1.00056	1.00329	1.0004698
U233-MET-FAST-005-001	0.99765	0.99671	0.99765
U233-SOL-INTER-001-001	0.98197	0.99647	0.98183
U233-SOL-INTER-001-033	0.99169	1.00757	0.99167
U233-SOL-THERM-001-001	0.99922	1.00714	0.999419

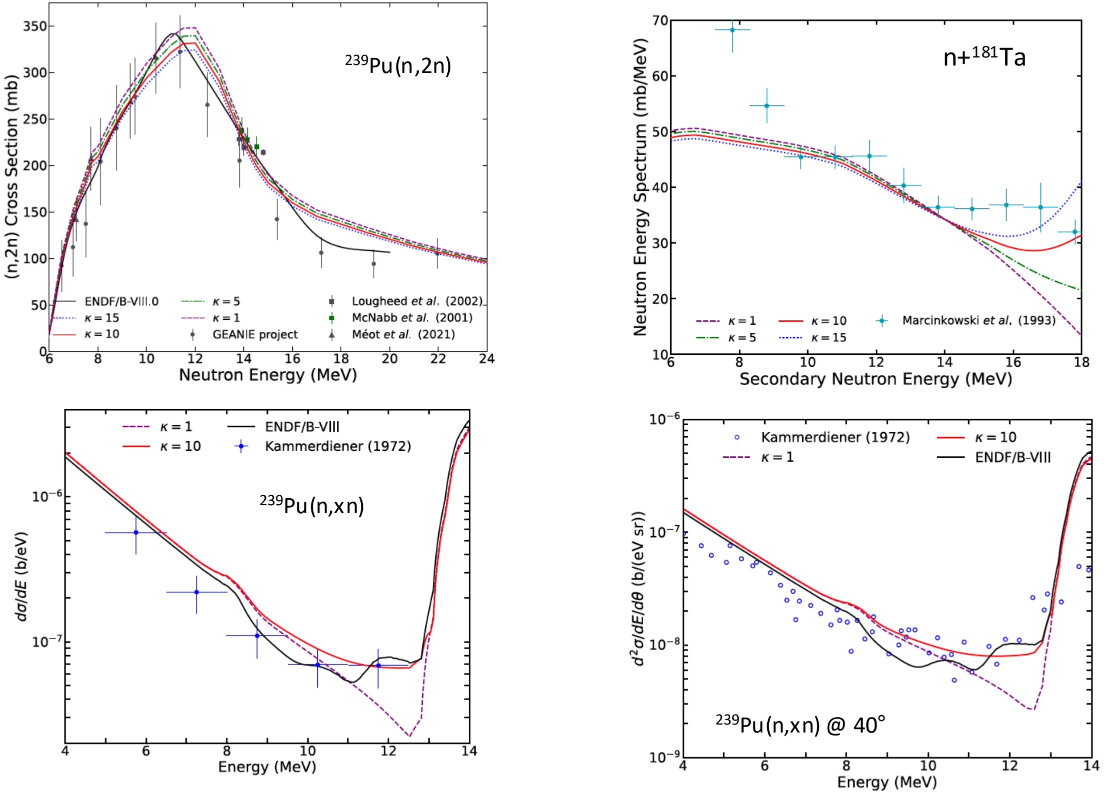
- No tweaks based on criticality benchmarks
- Only capture and nubar changed

Future plans: NCSP-funded re-evaluation of minor-U nubars and ^{233}U cross sections; evaluating these quantities at the same time allows us to better understand changes in benchmark performance

^{239}Pu

- ^{239}Pu evaluations have been a significant focus over the past several years, including cross sections, prompt fission neutron spectrum (D. Neudecker), and neutron multiplicity (with D. Neudecker)
- Modeling updates allow us to perform more consistent evaluations across reaction channels and use new capabilities for first-time evaluations

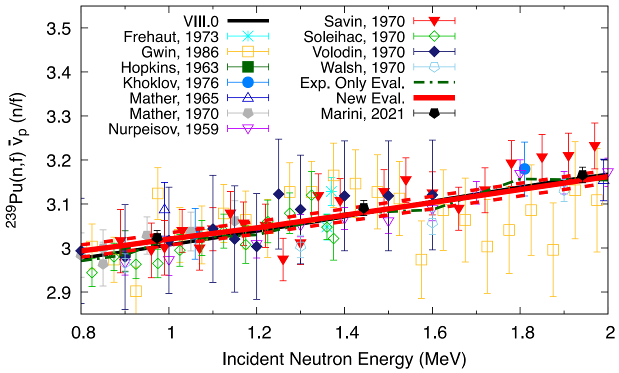
Collective enhancement was introduced into CoH

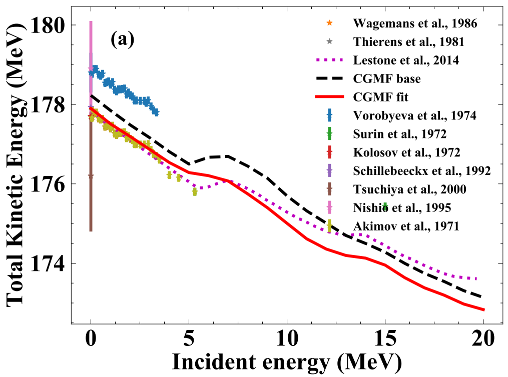


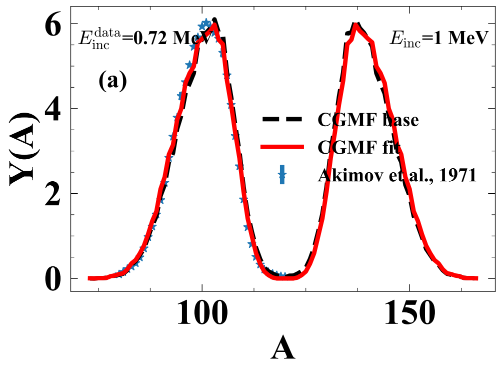
Sensitivity to the enhancement is seen in the (n,2n) and (n,xn) reaction channels leading to better agreement with experimental data

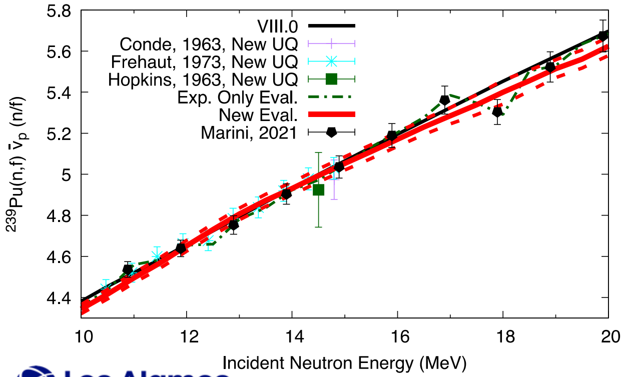
Mumpower et al, PRC **107**, 034606 (2023)

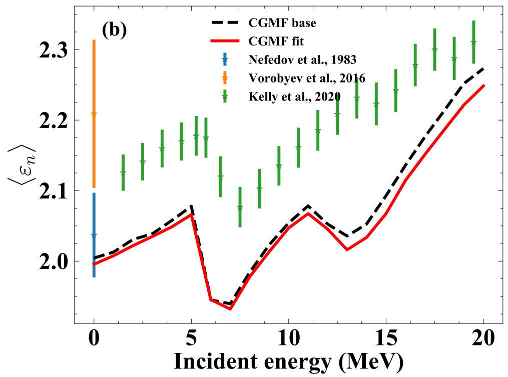
Model codes were used to evaluate neutron multiplicity for the first time











Fission modeling (with CGMF) keeps consistency with prompt observables and fission fragment initial conditions; neutron energies are a historical challenge

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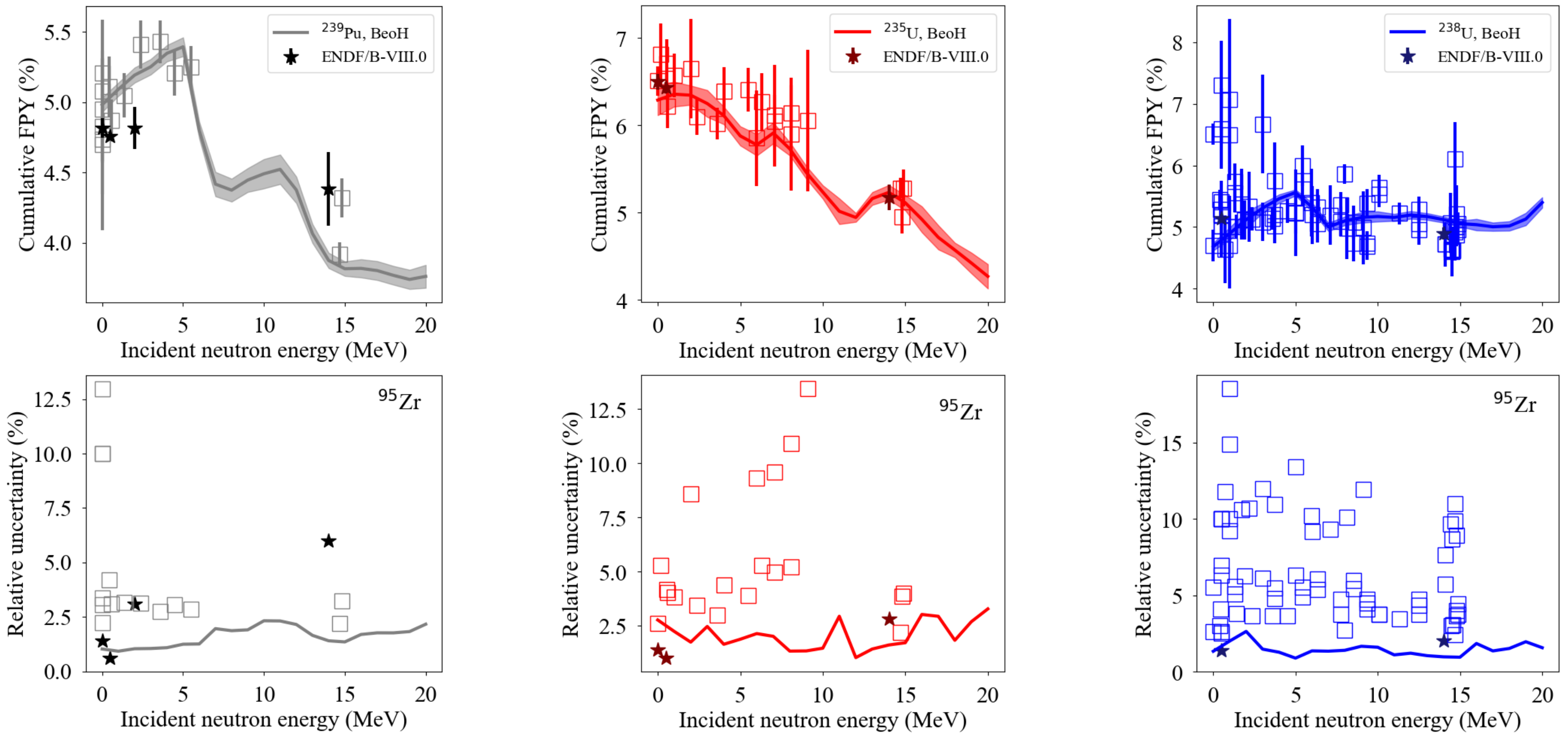
D. Neudecker, *et al., Front. Phys.* **10**, 1056324 (2022)

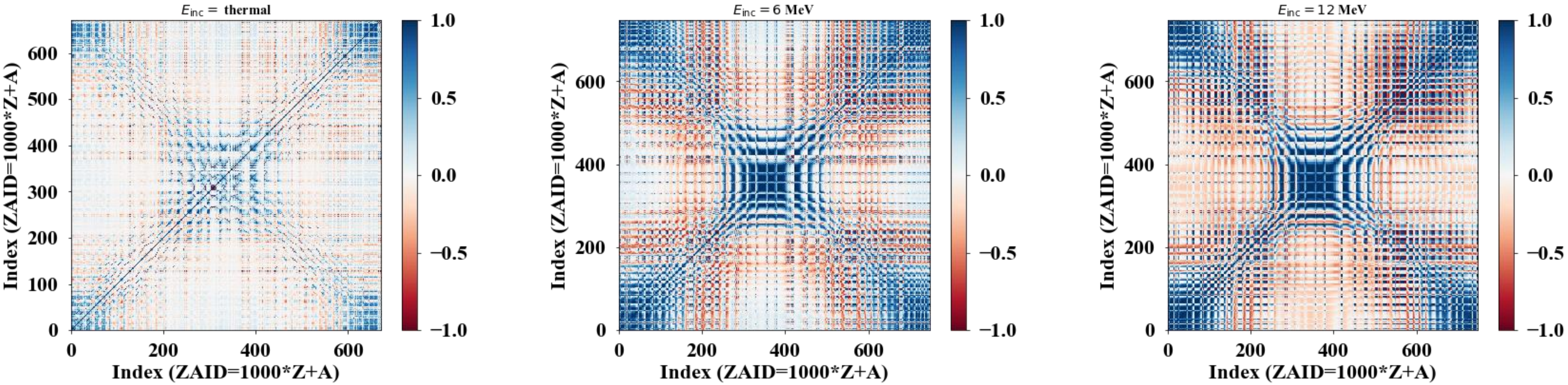
Fission product yields

- New modeling capabilities and experimental data measurements all for a full re-evaluation of independent and cumulative fission product yields
- Covariances are being developed for the first time
- Validation can be performed using historic R-values

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



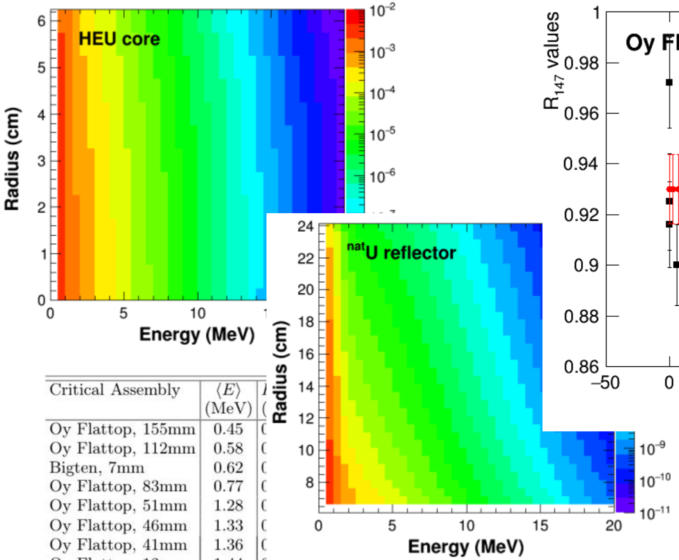
Correlations matrices are being developed at discrete energies from thermal to 20 MeV



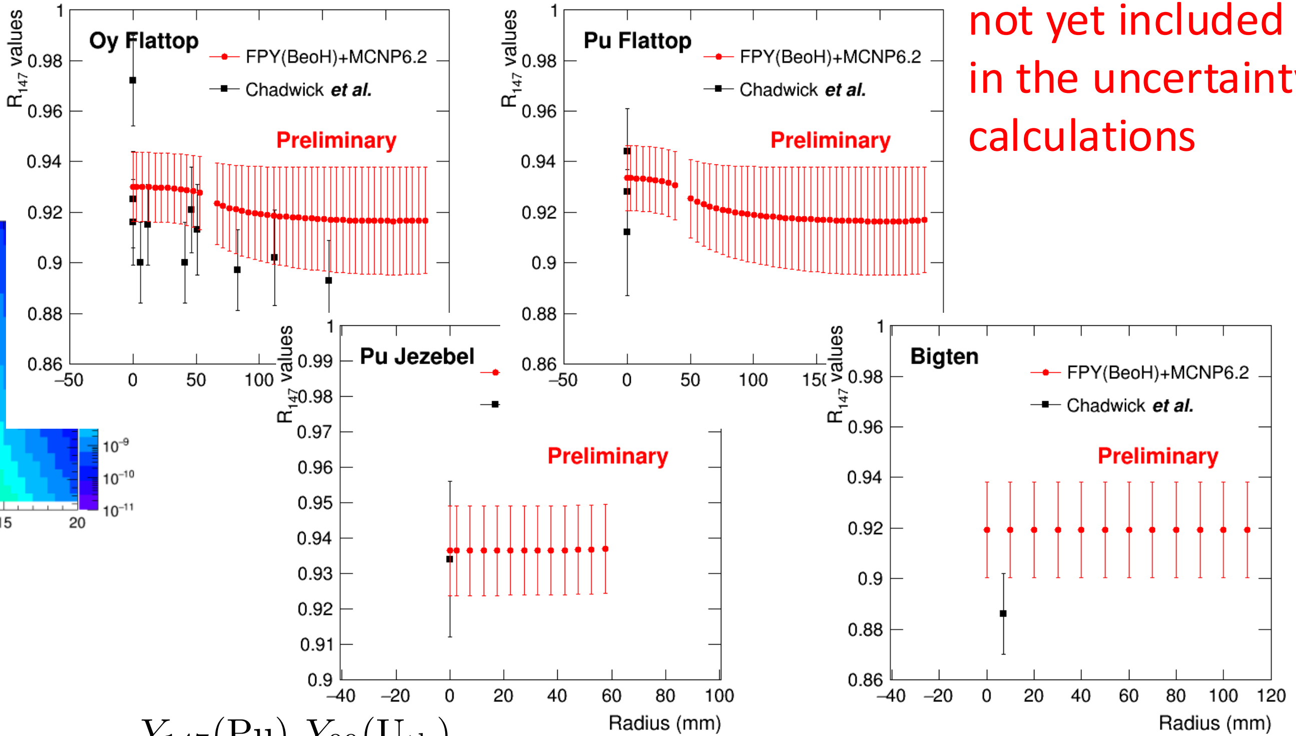
Example for ^{239}Pu cumulative FPYs at specific incident neutron energies. Correlations between FPYs change with incident energy, taking into account multi-chance fission. Cross-energy correlations can be given as well. Currently, no ENDF format for FPY correlations (being developed in house).

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

Correlations are not yet included in the uncertainty calculations



Critical Assembly	⟨E⟩ (MeV)		
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%



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

Calculations and figures by G. Rusev (LANL)
M.B. Chadwick, et al., NDS 111, 2923 (2010)

Summary and conclusions

- Evaluations require a thoughtful combination of experimental data and model calculations to produce the best possible values of quantities of interest.
- Significant work is being done at Los Alamos, in T-2 and with collaboration of many other groups, to improve evaluation inputs, models, and methodology.
- Simulating benchmarks with MCNP provides a critical validation step in the evaluation process.