

# Processing, Verification, and Validation of ENDF/B-VIII.1 Betas at LANL

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# Background

ENDF/B-VIII.1 to be released in the next few months

- LANL to produce application libraries for MCNP users, distributed on [nucleardata.lanl.gov](http://nucleardata.lanl.gov)

In preparation, processing, verification, and validation done for each beta release

- Ensure that NJOY can process any new representations in evaluations
- Identify formatting issues in evaluations
- Identify physics issues in evaluations
- Identify covariance issues earlier than ever!

# NJOY Updates for Processing

*See W. Haeck's NJOY update presentation*

New representations

- MF7/MT451 in thermal scattering laws
- Background R-matrix in Sr-99 evaluation

# Formatting Issues Observed

## Beta1

- Cr-54 MF32 (resonance covariance) section inconsistent with MF2 (resonance parameters)
- Be-9 had incorrect interpolation flag in new capture cross section

## Beta2

- Ta-181 covariance data had bad MT1 value

## Beta3

- O-16 had incorrect NWD value in MT451

All trivial fixes!

# Verification and Validation of LANL Evaluations

As part of this effort, XCP-5 provided support for several T-2 evaluations, including:

- Be-9 (pulsed sphere, quasi-integral, criticality)
- Li-6 (pulsed sphere, Bethe sphere)
- U-236 (reaction rate)

*See M. Paris and I. Stetcu talks*

# Case Study: Be-9 in ENDF/B-VIII.1

Be-reflected Pu sphere  
(PU-MET-FAST-038)

## k-eff Values + Unc.

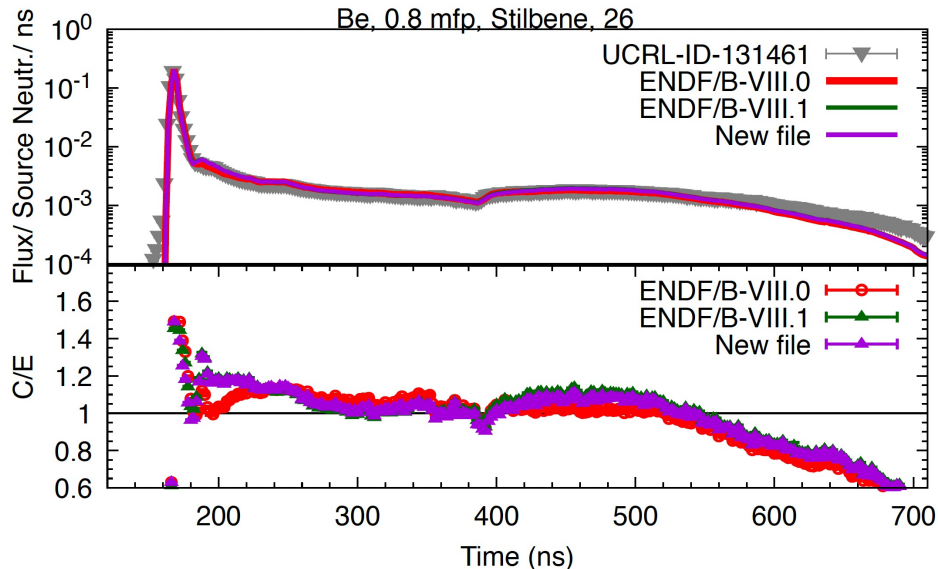
(1) Benchmark:	1.00070	0.00190
(2) ENDF/B-VIII.0:	1.000865	0.00010
(3) ENDF/B-VIII.1b1:	1.001850	0.00010
(4) ENDF/B-VIII.1b1 w/ reverted n2n:	0.998949	0.00010

**Observation:** new Be-9 evaluation  
“too hot” in beta1

**Possible path:** adjust (n,2n) reaction  
to lower reactivity

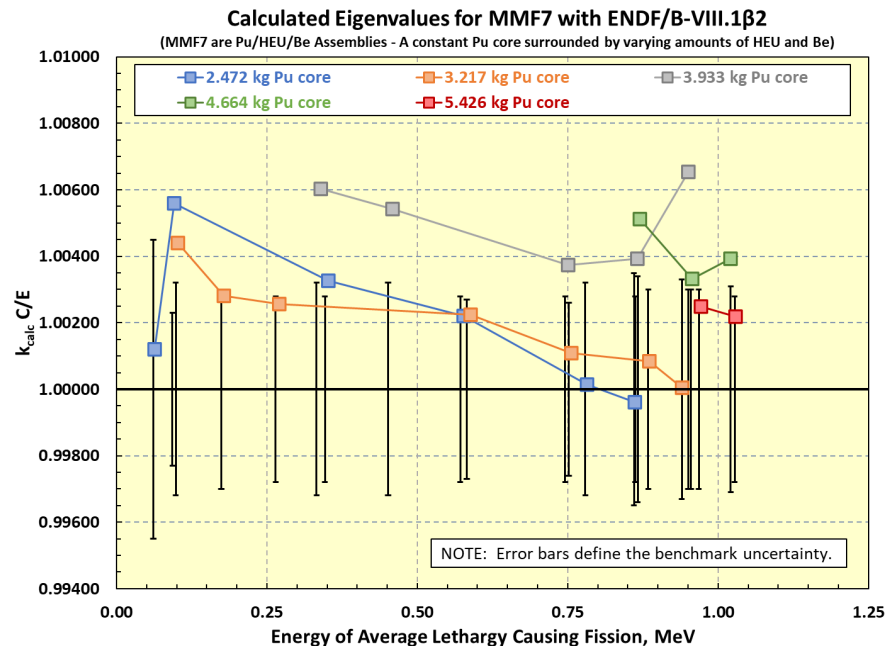
- Not included in R-matrix fit
- High enough uncertainty and sensitivity

# Be-9 (continued)

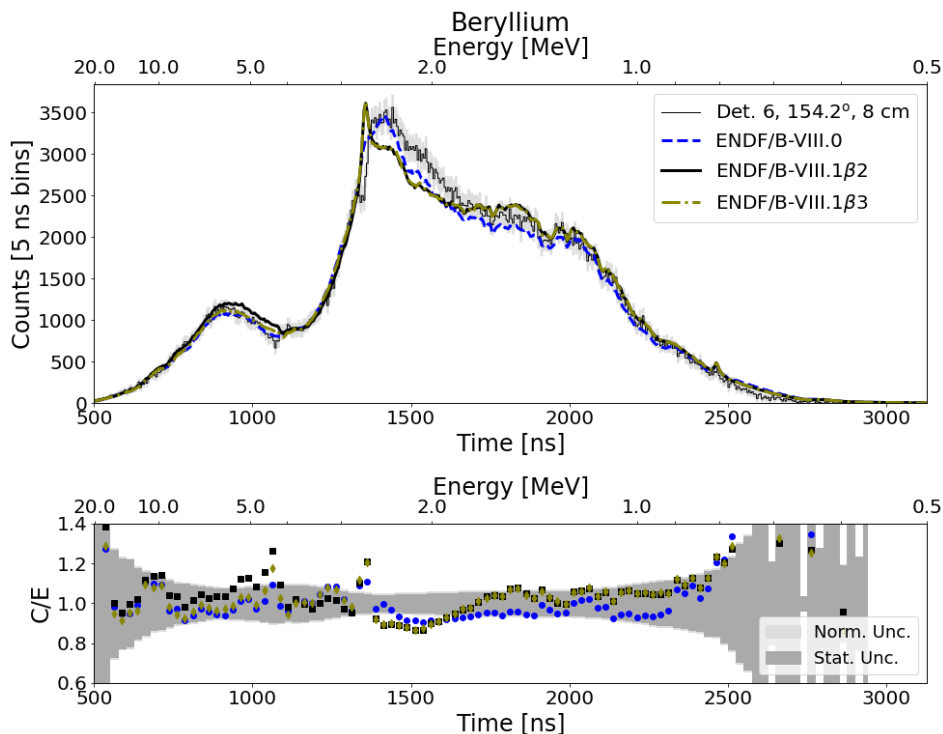


Markedly worse performance near peak  
in 8.1 candidates

More (n,2n) sensitivity for more thermal benchmarks (!)



# Be-9 (continued)



RPI quasi-integral data helped identify error in total cross section and in (n,2n) representation

Thanks to Y. Danon and A. Daskalakis!

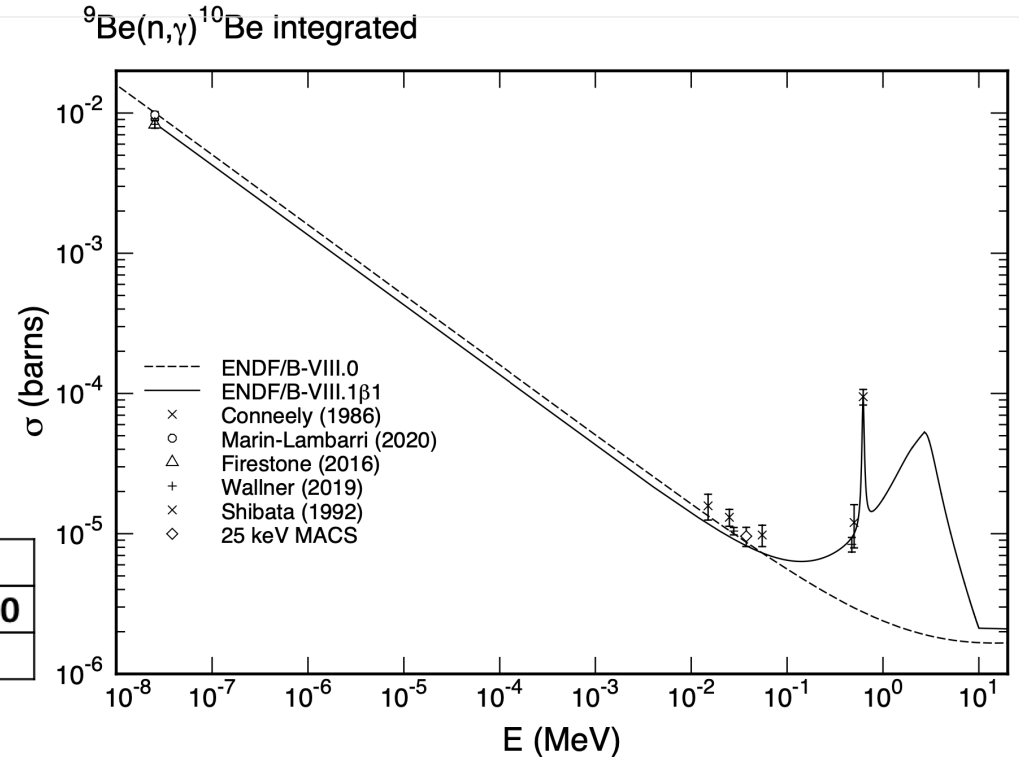
Conclusion: revert to ENDF/B-VIII.0 for now



# Be-9 Capture

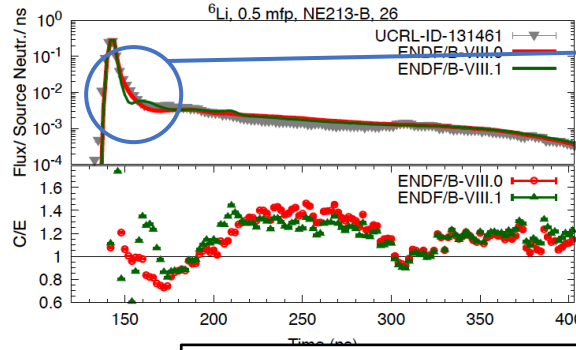
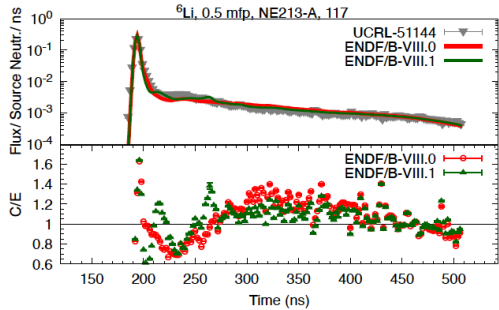
- NCERC measurement suggested capture cross section too small at fast energies
- Recent Wallner data suggested resonance structure
- Iterative approach to new cross section, accepted into VIII.1

	C/E		
Position	New Eval	1st Eval	ENDF-8.0
Center	0.919	41.23	0.134

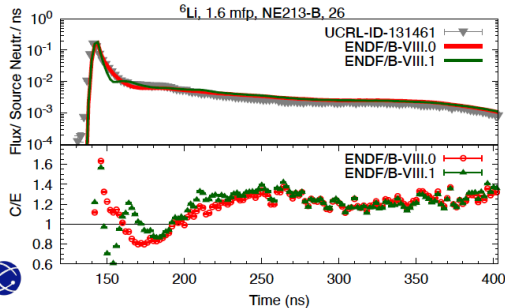


# Case Study: Li-6 in ENDF/B-VIII.1

## $^6\text{Li}$ : Distinct changes are observed.



Observed “extra bump” in pulsed sphere spectra.



We discussed whether change by change of spectral reaction from the system.  
MF = {3,4} MT=5

- Pulsed spheres show surprising new shape
- Li-6 has new representation (MF4/5 to MF6)
- Evaluators suggest kinematic flag could be explanation

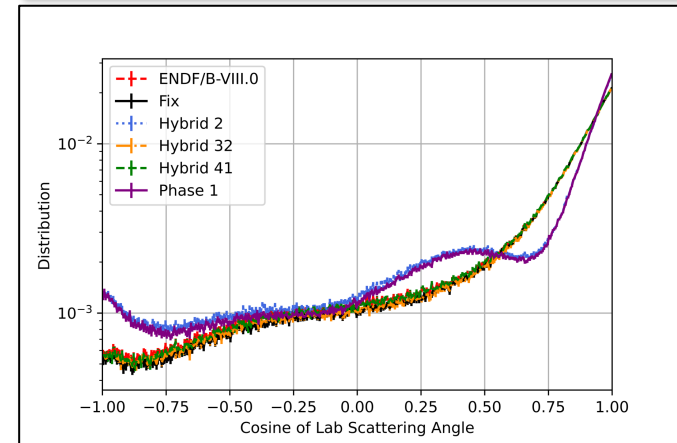
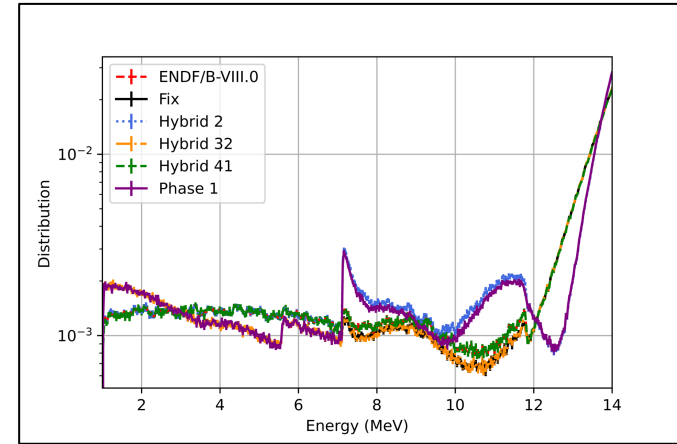
From D. Neudecker, mini-CSEWG

## Li-6 (continued)

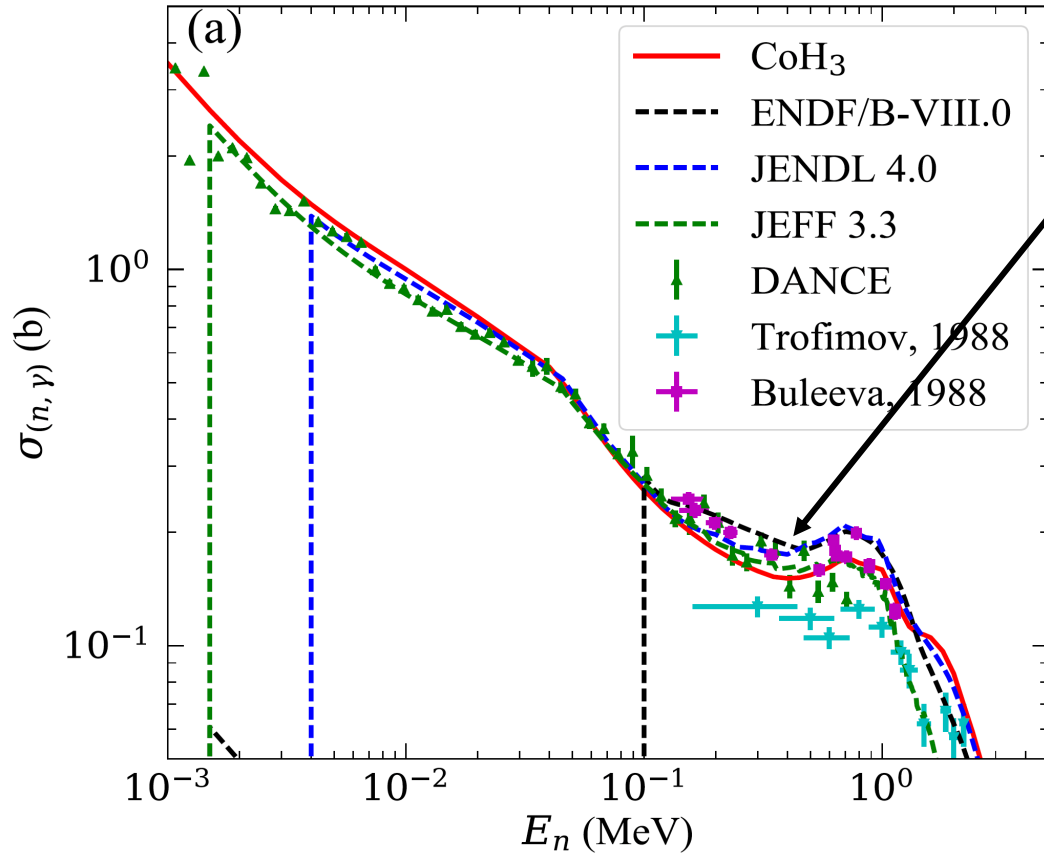
### “Broomstick problem”

- Use MCNP to output energy/angle distributions from 14.1 MeV neutrons, difficult to compare in ENDF file
- Substitute representations from E8.0 into E8.1 file (hybrid MT)

Conclusion: extrapolation of elastic scattering distributions was to blame!

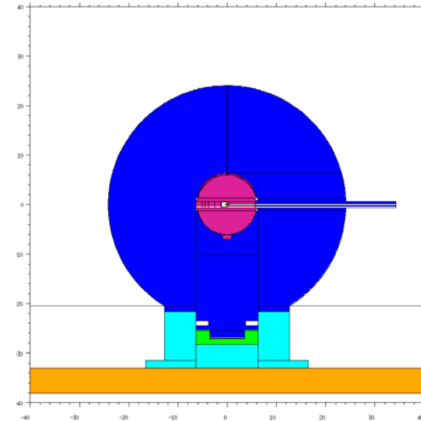


# Case Study: U-236 in ENDF/B-VIII.1



- New evaluation performed with CoH3
- Capture cross section fitted much lower than in ENDF/B-VIII.0

Validation question: are differential or integral (RR) data more important when discrepant?



# Library Generation

## Full beta libraries generated for each release

- ACE libraries for fast neutron data, TSLs
- JSON format for covariance files

## Types of testing

- Files readable in MCNP
- ACETk, checkACE
- CovVal
- Validation suites (ICSBEP, pulsed spheres, Bethe spheres, etc)

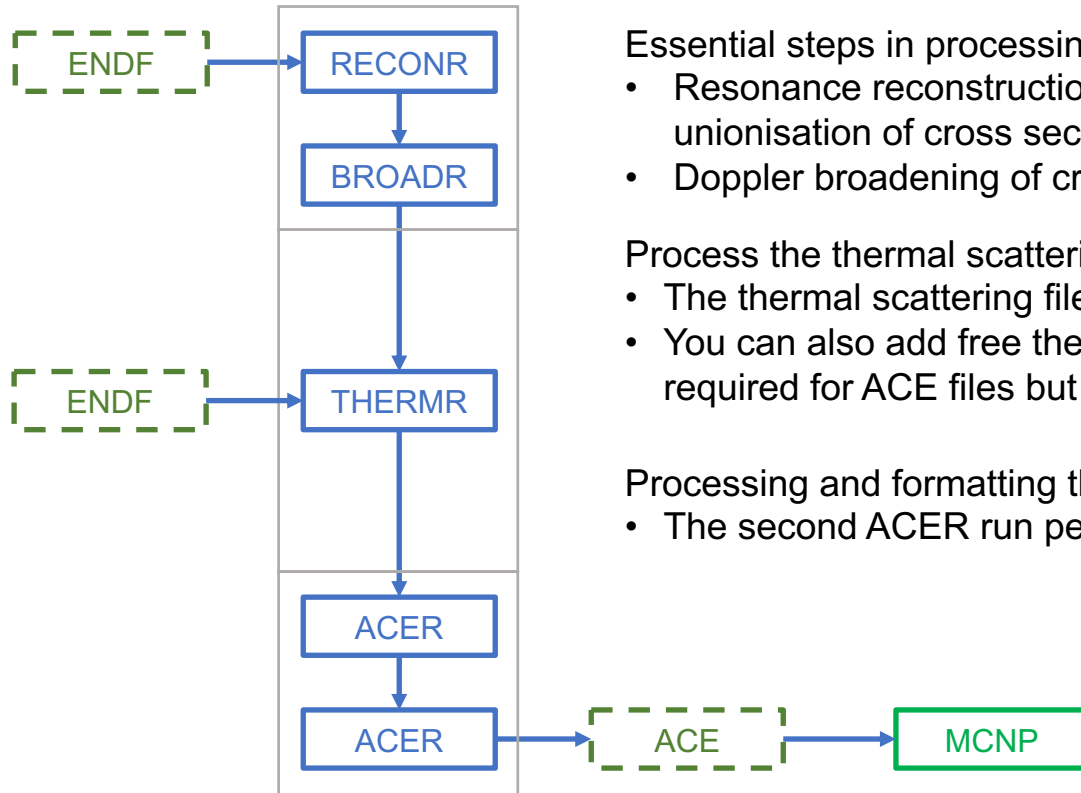
 LA-UR-23-23450

1. **Release of ENDF/B-VIII.1beta1-Based ACE Data Files**

Gibson, Nathan Andrew  ; Haeck, Wim  ; Kleedtke, Noah Andrew  ; Neudecker, Denise  ; Parsons, Donald Kent  ; et al.

LA-UR-23-23450 ; 2023-04-19

# Processing thermal scattering data for MCNP



Essential steps in processing data for the free nuclide

- Resonance reconstruction, linearisation and unionisation of cross section data
- Doppler broadening of cross section data

Process the thermal scattering data

- The thermal scattering file is used here
- You can also add free thermal gas treatment (not required for ACE files but deterministic codes do need it)

Processing and formatting the data into an ACE file

- The second ACER run performs several tests

TSL processing still requires manual intervention in many cases

- Beta3 processed much more smoothly than Beta2
- LANL tools/procedures improving to ensure files are processed correctly

# Some Validation Results

- ENDF-6 formatted files were processed into A Compact ENDF (ACE) files using NJOY2016.71 (<https://github.com/njoy/NJOY2016>)

## Validation Tests:

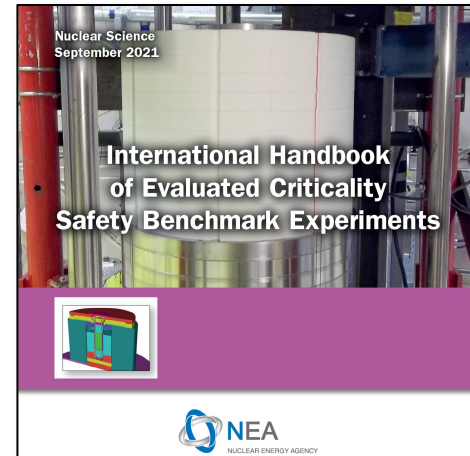
- (1) Bethe Spheres
- (2) LANL Legacy Benchmark Suite
- (3) “Modern” Benchmark Suite
- (4) HEU Benchmark Suite
- (5) LEU Benchmark Suite
- (6) Mixed (U+Pu) Benchmark Suite
- (7) Pu Benchmark Suite
- (8)  $^{233}\text{U}$  Benchmark Suite

Benchmark names from International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook designations

## Validation Metrics:

Tritium Production

$$k_{\text{eff}} \\ \downarrow$$



# Validation Overview

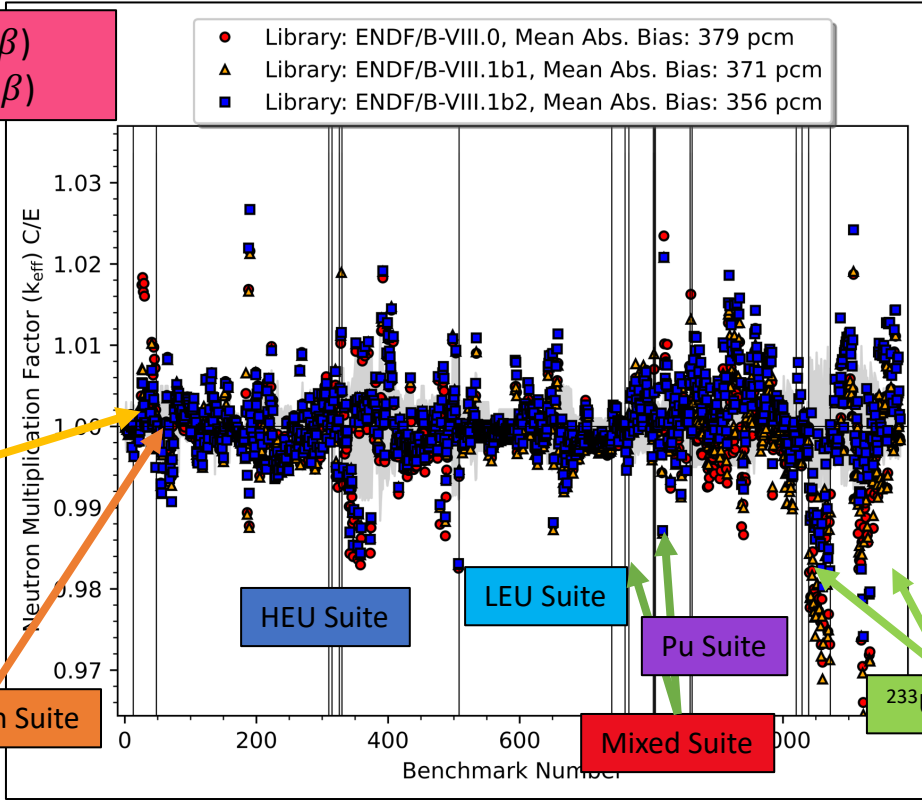
$$\text{Mean Absolute Bias} = \frac{\sum_i^N |C_i - E_i|}{N}$$

1b1 →  $\beta 1$  Files + 8.0  $S(\alpha, \beta)$   
1b2 →  $\beta 2$  Files +  $\beta 2$   $S(\alpha, \beta)$

- Library: ENDF/B-VIII.0, Mean Abs. Bias: 379 pcm
- ▲ Library: ENDF/B-VIII.1b1, Mean Abs. Bias: 371 pcm
- Library: ENDF/B-VIII.1b2, Mean Abs. Bias: 356 pcm

Legacy Suite

Modern Suite



HEU Suite

LEU Suite

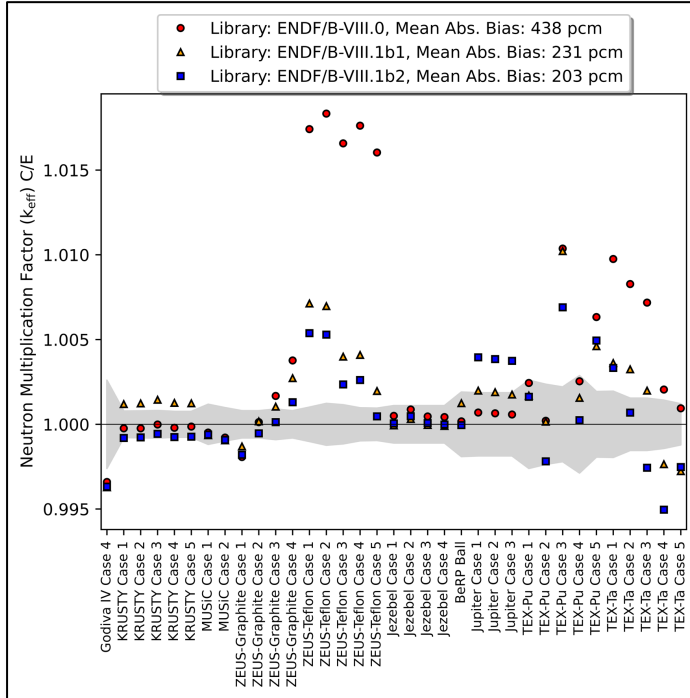
Pu Suite

Mixed Suite

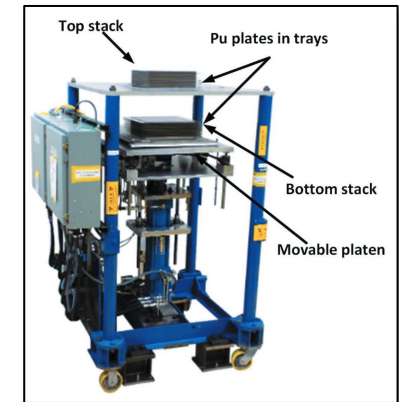
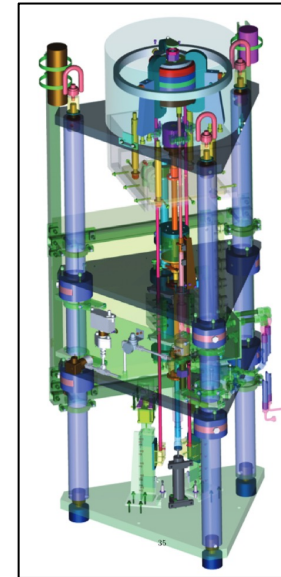
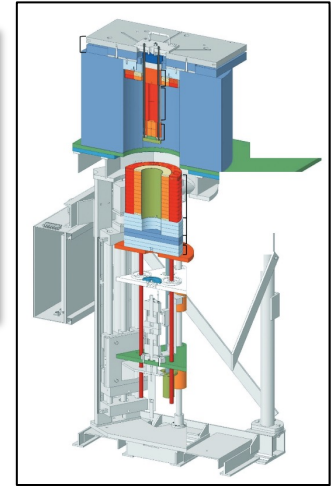
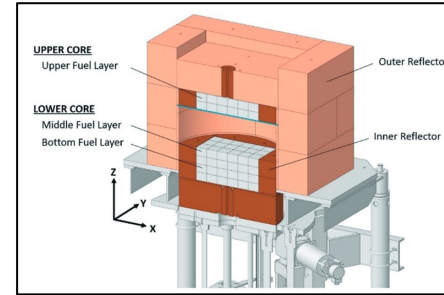
<sup>233</sup>U Suite



# Modern Benchmark Suite



Kilowatt Reactor Using Stirling Technology (KRUSTY)  
 Thermal/Epithermal eXperiments (TEX)  
 Measurement of Uranium Subcritical and Critical (MUSIC)  
 ZEUS-Teflon, Critical Unresolved Region Integral Experiment (CURIE)



# Covariances

- Processed with NJOY/ERRORR to internal-use JSON format
- Mathematical checks and physical bounds checks used
- Numerous issues identified and evaluators contacted

Testing at this level is unprecedented pre-release in ENDF!  
We have a ways to go, but this is a great start to ensuring  
covariances are treated appropriately.

# Summary

## Processing, verification, and validation of ENDF/B-VIII.1 betas

- ACE files created, release process tested
- Simple formatting issues caught and fixed
- Pulsed Spheres and related high-uncertainty experiments used to benefit LANL evaluations
- Validation work both ensures processing is working and that library is performing well
- Covariance issues identified, evaluators contacted

This was a team effort! Entire XCP-5 nuclear data team involved, leveraging other appropriate funding sources to supplement NCSP funding and interests.