



ENDF report

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f 🔘 in @BrookhavenLab

USNDP Meeting October 1-4, 2024

Outline

- ENDF/B-VIII.1 release status
 - Summary
 - Changes from VIII.0
 - How to get the data
- "Big Paper"
- Other honorary mentions
- ENDF Metrics
- Backup slides in the end with A LOT of details





ENDF/B-VIII.1 release status







ENDF/B-VIII.1 release status

ENDF/B-VIII.1 was released on August 30th, 2024!



ENDF Timeline



* everybody's favorite release

ENDF Timeline



* everybody's favorite release

ENDF Timeline



* everybody's favorite release











The previous release (VIII.0) was great, but...

- Underpredicted depletion at high burnup
- Had deficiencies in leakage benchmarks
- Many other contributions since then







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VIII**.**1

was released <u>Aug 30, 2024</u>!



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- Had deficiencies in leakage benchmarks
- Many other contributions since then







So, what's changed since ENDF/B-VIII.0?



Well,... a lot!





Well,... a lot!

- Summary
- I will avoid going into too many details
- Will have some highlights as backup slides in the end:
 - Neutrons sub library
 - Actinides
 - Structural materials
 - A few other highlights in other sublibraries





What to expect in ENDF/B-VIII.1

Neutrons:

- Actinides:
 - ²³⁹Pu: multi-institution effort, with important updates to fission, nubar, PFNS, capture, URR, RRR, (n,2n)
 - ²³⁵U: resonances, nubar, covariances,
 - ²³⁸U: resonance update to improve performance on depletion benchmarks
 - ^{240,241}Pu: work in concert with changes in ²³⁹Pu and ²³⁸U to recover burnup performance
 - ^{234,236}U: New fast-region evaluations (LANL)
- Stainless steel & other structure materials:
 - 54,56,57 Fe: Corrects leakage deficiency from ENDF/B-VIII.0
 - ^{50,52,53,54}Cr: Thorough re-evaluation, impact in criticality and leakage benchmarks

- ^{206,207,208}**Pb**: complete evaluations (RPI/LANL)
- ^{63,65}Cu: improved performance
- ⁵⁵Mn: Gamma spectra
- 28,29,30 Si: resonance evaluations
- Others:
 - ¹⁹F (INDEN)
 - 6Li, 9Be (LANL)
 - 234,236U (LANL)
 - 140,142Ce (ORNL)
 - 103Rh (RPI/IRSN)
 - ⁸⁶Kr (BNL)
 - 181**Ta** (RPI/ORNL/LANL)
 - Pt isotopes (LANL)
 - Many, many, many more...



What to expect in ENDF/B-VIII.1

<u> TSL:</u>

- 70+ new updated/files
- Polystyrene, zirconium hydride, UC, UN, UO₂, sapphire, lucite, FLiBe, etc...
- Fuel materials with different enrichments
- So many new evaluations that we had to re-think how to identify them.
- Low-temperature extrapolations to light water

Community-wide review and validation

Fission Yields:

- Many fixes
- ...but no changes to the actual yields

Photo-nuclear:

 ~200 updates coming from IAEA CRP

Charged particles:

• A few improvements and fixes



How to get the data?









- Tarballs broadly shared within the community:
 - Are you in the ENDF mailing list?
 - <u>https://lists.bnl.gov/sympa/info/endf</u>
 - Contact me: gnobre@bnl.gov





"How do I access these new nuclear data?"

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 - ENDF section is being re-worked

ENDF/B VII.1



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Status of Big Paper



Big Paper updates

- Got all contributions and corrections in: No "FIXMEs" left!
- Submitted to LANL/LLNL/NNL for <u>final review</u> regarding export control and public utterance
- In meantime, authors are submitting very minor typo/ grammar fixes
- Should submit to Nuclear Data Sheets still this week
- Hoping to make it Open Access



Excluding merge commits. Limited to 6,000 commits.

Commits Avg: 2.03 · Max: 49



ENDF/B-VIII.1: Updated Nuclear Reaction Data Library for Science and Applications

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Some honorary mentions in FY24



Other highlights

- ENDF/B-VIII.1-Beta3 released January 11, 2024
- ENDF/B-VIII.1-Beta4 released June 28, 2024
- Many checks, reviews, tests and validations within the community
- LANL/BNL organized mini-CSEWG in Los Alamos, August 13-15, 2024
 - Lessons learned from ENDF/B-VIII.1
 - Preparation for ENDF/B-IX.0







Historic Fuller Lodge in springtime. Courtesy/Los Alamos Historical Society Archive from https://losalamoshistory.org/fuller-lodge-centerpiece-of-community/

ENDF metrics for FY24



ENDF evaluation metrics

• This is a **challenge**

- Not all evaluation contributions
 are created equal
- <u>All</u> linear combinations of "size" and "impact" of contribution are possible
- There is some degree of intrinsic arbitrariness
- Looked at all repository commits in FY24, separated by lab and "weighed" the contributions



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Conclusion

- ENDF/B-VIII.1 has been released!!
 - Hooray!
 - Big thanks to the whole community who contributed in all steps of this huge effort!
- Big Paper:
 - Submitted for final export control review
 - Should submit to NDS soon
- (Somewhat subjective) metrics: High productivity in ENDF-world



Acknowledgements

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Vational Laboratory

Backup slides



Actinides



Fuel-isotope example: Substantial change to ²³⁹Pu via (inter)national contributions.

Updates:

Maxwellian (T=1.42 MeV)

PNS / 0.7

0.8

0.6 0.1

1.06

1.04

1.02

0.98

BLOOKI

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10 20

prompt nubar

gy (MeV)

- New prompt neutron multiplicities (ORNL, INDEN, LANL)
- New cross sections in the RRR (ORNL).
- New cross sections in the fast (INDEN, LANL).
- New PFNS from thermal-30 MeV (INDEN, LANL).

²³⁹Pu(n_{1.5 MeV},f)

Outgoing Neutron Energy (MeV)

LANL eval. (D. Neudecker) Including

IL/ LLNL Chi-Nu and CEA PFNS data.

Los Alamos

Despite substantial changes, good performance maintained in simulating critical assemblies.

10

Section (mb) 0000 0000

7000 Tota

6000

5000L

Cross 8000





Work by INDEN, LANL, LLNL. ORNL.

ENDE/B-VIII 0



8/12/24

14



For Whisper users: New covariances provided among them for ²³⁹Pu, ²³⁴⁻²³⁶U, Ce, Pb, Ta, etc.!



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For Whisper users: CSEWG tested covariances for VIII.1 more stringently but work remains.

Testing included:

- See if covariance could be processed via LANL's NJOY and ORNL's AMPX processing codes (i.e., formats are correct),
- Mathematical properties (positive semidefinite, -1 <= cor <= +1, covariance constraints,
- Are uncertainties within reasonable limits given standards and templates of expected measurement uncertainties (see:)?
- Forward-propagating uncertainties through integral testing uncertainties.

<u>To-Do:</u>

- We still miss covariances for several isotopes and energy ranges,
- Discussion on uncertainties in RRR.
- Updates to newest standards.



<u>Fissile</u> material		PU				
Spectrum		FAST	INTER	MIXED	THERM	
Number of Benchmarks		152	4	9	624	
Experimental Uncertainty (pcm)		334	710	587	426	
Total (<u>pcm</u>)	ENDF/B-VIII.1b4	931	551	536	645	
	ENDF/B-VIII.0	921	1403	1055	1099	
	ENDF/B-VII.1	436	565	459	625	
Cross- <u>sections</u> (with correlations)	ENDF/B-VIII.1b4	841	360	224	106	
	ENDF/B-VIII.0	857	1368	983	998	
	ENDF/B-VII.1	409	546	356	500	
P1-elastic	ENDF/B-VIII.1b4	66	-	-	-	
	ENDF/B-VIII.0	66	-	-	-	
	ENDF/B-VII.1	-	-	-	-	
	ENDF/B-VIII.1b4	390	389	479	632	
nubar	ENDF/B-VIII.0	300	271	275	308	
	ENDF/B-VII.1	76	88	114	168	
PFNS	ENDF/B-VIII.1b4	27	25	53	59	
	ENDF/B-VIII.0	117	106	265	297	
	ENDF/B-VII.1	118	106	265	297	

Table from Oscar Cabellos/ UPM.

²³⁹Pu

- Community-wide collaboration to provide unique recommended file
- Updates to
 - fission
 - nubar
 - PFNS
 - capture
 - URR
 - RRR
 - (n,2n)

Brookhaven

National Laboratory

- Other fast-region reactions
- Covariance evaluations were submitted for final release
- Key ingredient to improve burn-up performance



FIG. 7. Experimental and evaluated 239 Pu PFNS for $E_{inc}=1.5$ (top) and 14 MeV (bottom).

235**U**

- Updates to
 - Resonance evaluation below 20 eV
 - Updated Unresolved Resonance Range (URR): detailed shape of the fission cross section follows better the measured data in the URR and above.
 - Fission cross section
 - nubar: LANL evaluation (above 200keV) and additional changes from 40eV up to 500eV
 - PFNS (above thermal): Chi-Nu based evaluation
 - Covariance data: Spurious cross-reaction covariance elements between the resonance and the fast energy ranges were removed because they gave rise to negative eigenvalues. Cross-covariances between nubar and fission cross section were removed for the same reason.



FIG. 60. $n+^{235}U$ fission and capture neutron yield data calculated for three nuclear data libraries are compared with the RPI measured data [177] below 0.5 eV.



238**U**

- Updates to
 - RRR: evaluation taken from JENDL-5 above 100eV, and from VIII.0 below 100eV. Also, increased capture from 100 eV up to 20keV
 - nubar: LANL-INDEN collaboration. Adopted JENDL-5 evaluation from 1 up to 5 MeV, new LANL evaluation above 5 MeV
 - Important component in the burn-up issue



240,241**Pu**

- A compromise: better for depletion (not perfect) but worse for PST benchmarks
- Recommended ^{239,240,241}Pu files combined with recommended ²³⁸U solve the burnup problem.
- Updates to
 - Resolved Resonance Region (RRR): CEA evaluations



234,236**U**

- Model calculation using CoH3 with Souhkoviskii 2005 potential
- Fission: below 500 keV (234U) keep ENDF/B-VIII.0; above that: new fit to include Tovesson 2014 data for 234U
- Calculation: fission transmission adjusted so that the calculation reproduces the fission data. Point-by-point fit to determine an energy-dependent adjustment
- Capture: calculation-based evaluation that reproduces very well the latest measurement by DANCE below 100 keV (234U) and other existing data (236U). The gamma-gamma width is consistent with the resonance analysis.
- All the other channels have been taken from CoH3 calculations
- LSSF flag set to 1 for MT=1,18,102. Background cross section in the replaced by full
- cross section in the URR.
 - PFNS taken from JENDL-4
 - PFG properties taken from BeOH calculations



233**U**

- Updates to
 - PFNS: Use of the IAEA U-233 PFNS for thermal neutrons with average energy Eav=2.030 MeV (ENDF/B-VIII.0 value ~2.074 MeV). Talou et al PFNS evaluation (IAEA PFNS CRP) is used in the fast region.
- Adjustment of thermal cross sections to agree with TNC from IAEA Standards 2017.
- Introduction of energy dependence for nubar below 30eV from Reed et al data.
- Introduction of energy dependence for nubar from 500eV up to 300keV from Gwin et al data measured relative to Cf-252(sf).
- Resonance parameters were completely refitted (M. Pigni) adding new experimental data (Berthomieux, Calviani, Tarrio, Leal-Cidoncha). Capture resonance yields renormalized to be close to Weston data.
- Criticality was improved compared to ENDF/B-VIII.0 (see solution benchmarks as a function of FEPIT, Mosteller U-233 benchmarks, and UCT (LWBR) benchmarks).



Structural materials

Cr, Fe, Pb, Cu, Ta...



Summary of Cr evaluations

Isotope and reactions updated:

- *^{50,53}Cr: thermal and up to 10 keV; all reactions in fast region.
- *^{52,54}Cr: all reactions in fast region.
- *Reconstructed isotopic angular distributions in resonance region.

Motivation and deficiencies in ENDF/B-VIII.0:

- * Chromium is an important alloy in stainless steel. After VIII.0 evaluation of iron, it is essential to better constrain Cr files.
- *^{50,53}Cr: Cluster of capture resonances in the region 1-10 keV drive criticality in Cr-sensitive benchmarks. ENDF/B-VIII.0 followed data with inaccurate correction determination in this region (e.g., MS)

What new data/theory motivated the new evaluation/update:

- *Appropriate normalization of Guber ⁵³Cr(n,g) data (ORNL) in the 1-10 keV region
- *Neutron and gamma ⁵²Cr inelastic data from Mihailescu (GEEL)
- *New soft-rotor dispersive optical potential for ^{50,52,54}Cr, interpolated as rigid rotor for ⁵³Cr

What validation testing has been be done

- *Chromium-sensitive benchmarks identified, in particular KBR-15 (HEU-COMP-INTER-005 k_∞) and ZPR-6/10 (PU-MET-INTER-002) with strong sensitivity to Cr – both are big outliers (11% and 2% in k, respectively)
- *Oktavian-Cr 14 MeV leakage: Not in SINBAD, new model developed in JSI
- *New evaluation greatly improves reactivity prediction and performs well for the 14 MeV benchmark





Used $^{\mbox{Nat}}\mbox{Cr}$ transmission data to constrain the normalization of isotopic capture data

- Model calculations extended to 65 MeV (for fusion applications).
- Model- extrapolation to unstable 51Cr.

Summary of Cr evaluations

Isotope and reactions updated:

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Summary of Fe evaluations

- Complete evaluations for all Fe isotopes had been done for VIII.0
- However,...
 - Inelastic was too high
 - 30% underestimation of the fast neutron transmission through thick iron shells
- New evaluations:
 - New resolved resonances for ^{54,57}Fe
 - Adopted IRDFF reactions for ⁵⁴Fe
 - For ⁵⁶Fe:
 - adopted mostly VIII.0 resonances, with one important change in the capture width of the 27.7 keV resonance
 - Some typos in the original evaluation were corrected (one resonance energy was changed from 767.240 keV to 766.724 keV and the spurious resonance at 59.5 keV was deleted).



Figure 1. Comparison of the ^{nat}Fe measured elastic cross sections below 7 MeV vs ENDF/B-VIII.0, JEFF-3.1.1, and current INDEN evaluation.



Figure 9. Comparison of the updated ${}^{57}Fe$ total cross sections (green line) with the data by Pandey (blue circles) and the original ENDF/B-VIII.0 averaged cross sections (red line).



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FIG. 41. Criticality differences to the experimental benchmark values C/E of selected stainless steel ICSBEP benchmarks. Experimental benchmark values are compared to JEFF-3.3, ENDF/B-VII.1, ENDF/B-VIII.0 and the new INDEN evaluation of iron isotopes adopted for the ENDF/B-VIII.1 library (INDEN r61).



FIG. 43. Measured neutron leakage of the 252 Cf(sf) neutron source measured at 1 m distance from a 50.2x50.2x50.4 cm³ stainless steel block [139]. Experimental benchmark values C/E-1 are compared with transport calculations using JEFF-3.3, JENDL-4.0, ENDF/B-VIII.0 and the new ENDF/B-VIII.1 library that adopted the INDEN Fe and Cr evaluations.







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Lead evaluations

- Complete new evaluations for 206,207,208Pb
- Good performance in pulsed spheres
- May have uncovered issues with some criticality benchmarks: Further work may be needed!





63,65**Cu**

 Updated resonances and fast regions and angular distributions.





Performance improved dramatically in copper-sensitive benchmarks



Performance improved dramatically in copper-sensitive benchmarks



Performance improved dramatically in copper-sensitive benchmarks



Other sublibraries



TSL

- Many, many updates and new contributions
- So much so, we had to create new way to uniquely identify materials
- Moderators, Fuels, Special Purpose

V.

THERMAL NEUTRON SCATTERING					
SUDLIDRARI					
A. Moderators					
1. Light water (H_2O)					
2. Beryllium (Be-metal)					
3. Beryllium-Metal with Distinct Effects					
$(\mathrm{Be+S}_d)$					
4. Beryllium Oxide (BeO)					
5. Calcium Hydride (CaH_2)					
6. FLiBe Molten Salt					

	7.	Nuclear/Reactor Graphite (20%)	92	
8. Crystalline Graphite with Distinct				
		${ m Effects}\;({ m graph}{+}{ m S}_d)$	93	
	9.	Anhydrous Hydrogen Fluoride (HF)	94	
	10.	Heavy Paraffinic Oil	95	
	11.	Silicon Carbide (SiC)	95	
	12.	Silicon Dioxide (SiO ₂ , α Phase)	97	
	13.	Polystyrene $((C_8H_8)_n)$	98	
	14.	Lucite $((C_5O_2H_8)_n)$	99	
	15.	Zirconium Carbide (ZrC)	101	
	16 .	Beryllium Carbide (Be_2C)	102	
	17.	Zirconium Hydride $(ZrH_x \text{ and } ZrH_2)$	103	
	18.	Yttrium Hydride (YH_2)	105	
	19.	Lithium-7 Hydride (^{7}LiH) and		
		Deuteride (^{7}LiD)	106	
Β.	Fue	els	108	
	1.	Plutonium Dioxide (PuO_2)	108	
	2.	Uranium Carbide (UC)	109	
	3.	Uranium Metal (U-metal)	111	
	4.	Uranium Nitride (UN)	112	
	5.	Uranium Dioxide (UO_2))	113	
	6 .	Uranium Hydride (UH_3)	114	
С.	C. Special Purpose			
	1.	Liquid hydrogen and deuterium (l-H ₂ ,		
		$l-D_2$)	115	
	2.	Sapphire Single-Crystal Neutron Filter		
		(Al_2O_3)	116	
	3.	Magnesium Oxide Neutron Filter		
		(MgO)	117	
	4.	Magnesium Fluoride Neutron Filter		
		(MgF_2)	117	
	5.	Beryllium Fluoride Neutron Filter		
		(BeF_2)	118	



neutron-induced fission yields

The only change relative to the previous release for the neutron-induced fission yields sublibrary is for 241Pu. An important bug introduced in ENDF/B-VI.2 was fixed by A. Mattera. The list of changed files is:

• nfy-094_Pu_241.endf



