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Title: Validation Testing at LANL with ENDF/B-VIII.1 Official Release Files

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Validation Testing at LANL with ENDF/B-VIII.1 Official Release Files

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Materials and Physical Data Group (XCP-5)
Los Alamos National Laboratory

2024 CSEWG Meeting

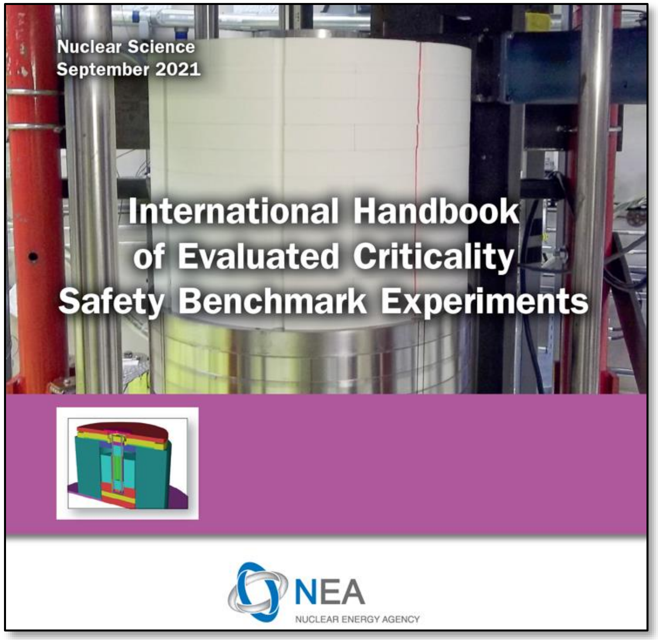
LA-UR-24-XXXXX

Background

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

Validation Tests:

(1) LANL Legacy Benchmark Suite
(2) "Modern" Benchmark Suite
(3) HEU Benchmark Suites
(4) LEU Benchmark Suites
(5) Mixed (U+Pu) Suites
(6) Pu Benchmark Suites
(7) ^{233}U Benchmark Suites
(8) Reaction Rate Ratios
(9) LLNL Pulsed Spheres

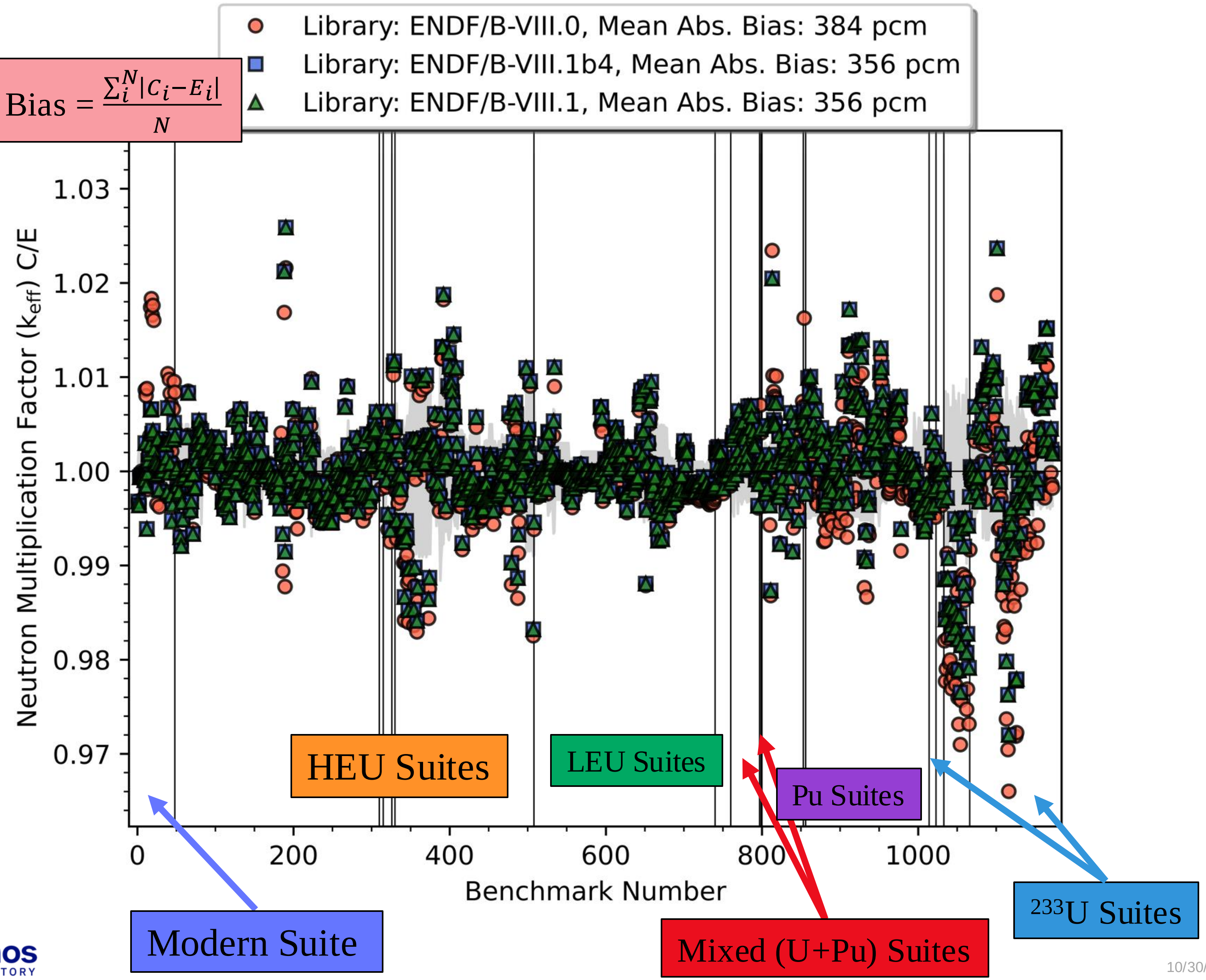


- Benchmark names are taken from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook designations

Organisation for Economic Co-operation and Development (OECD)/Nuclear Energy Agency (NEA), "International Handbook of Evaluated Criticality Safety Benchmark Experiments," NEA/NSC/DOC(95)03 (2021)

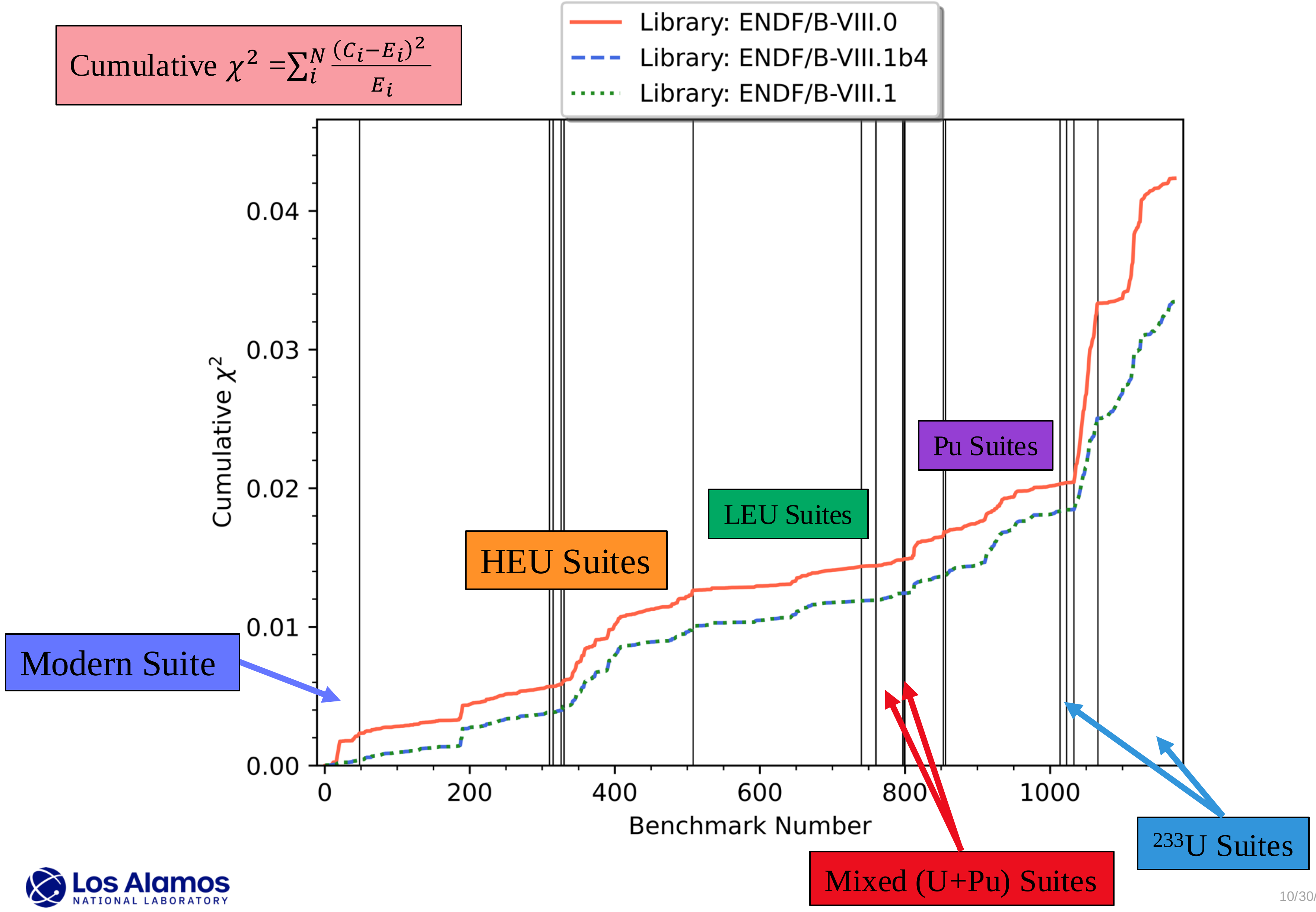
Everything, Everywhere, All at Once

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

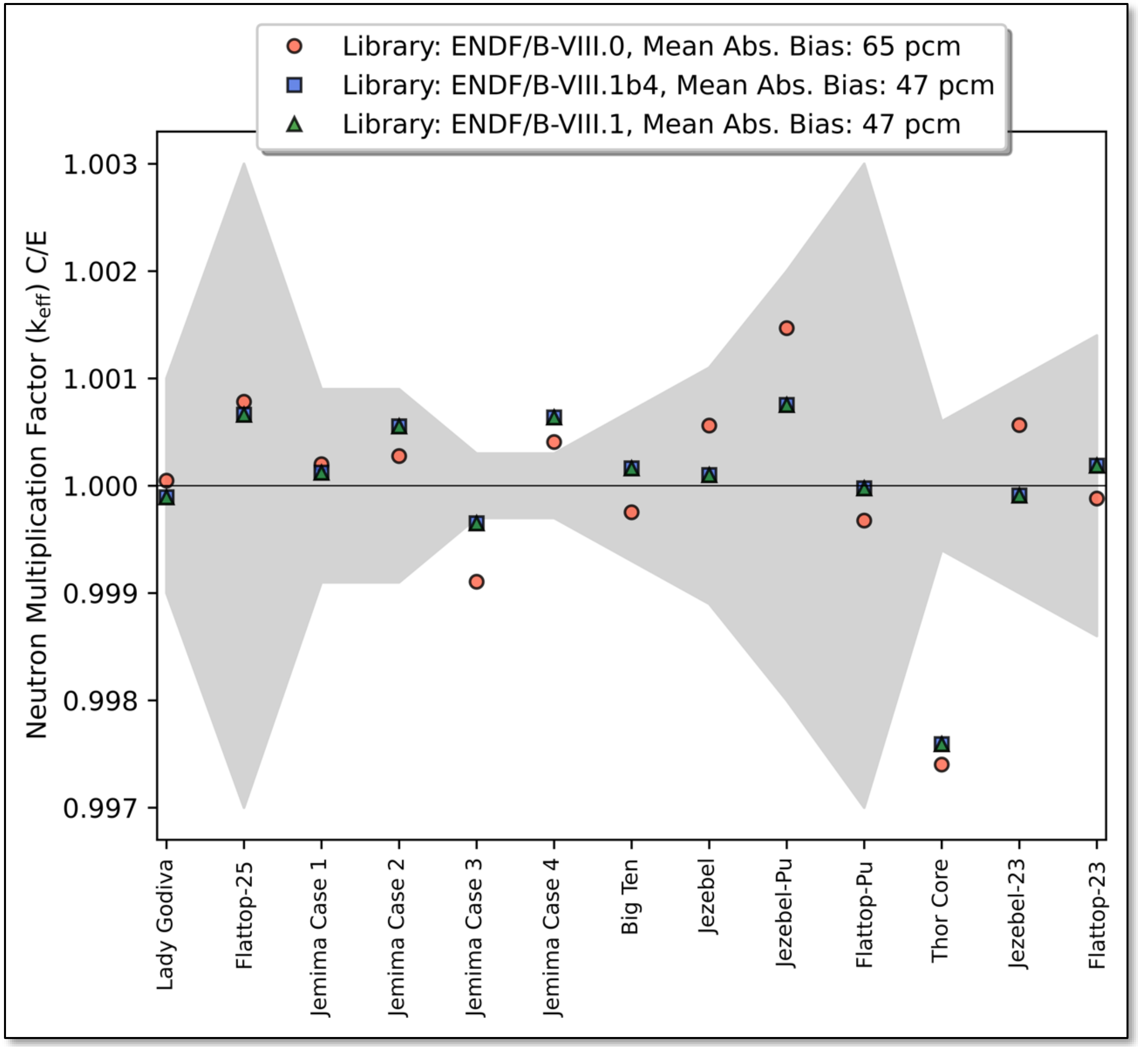


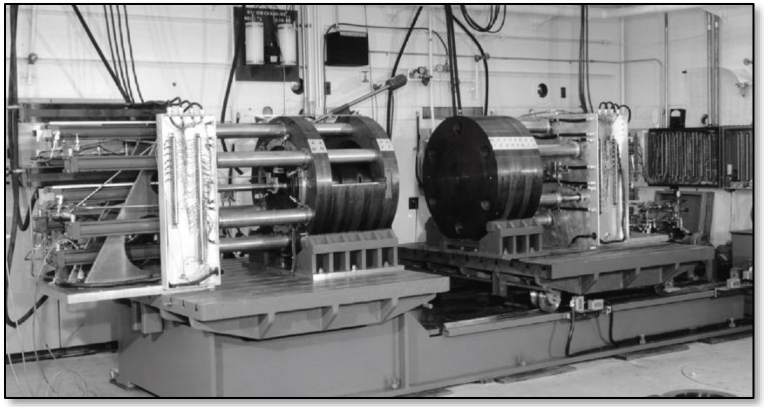
Everything, Everywhere, All at Once

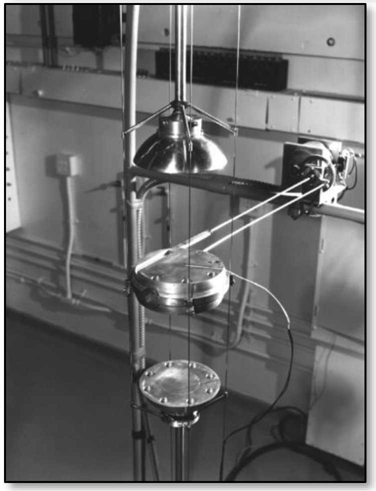
Cumulative $\chi^2 = \sum_i^N \frac{(C_i - E_i)^2}{E_i}$

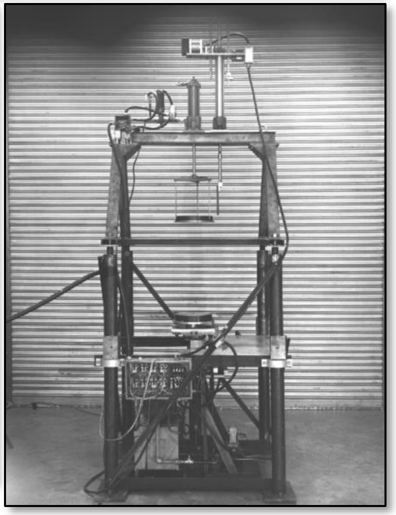


Legacy Benchmark Suite









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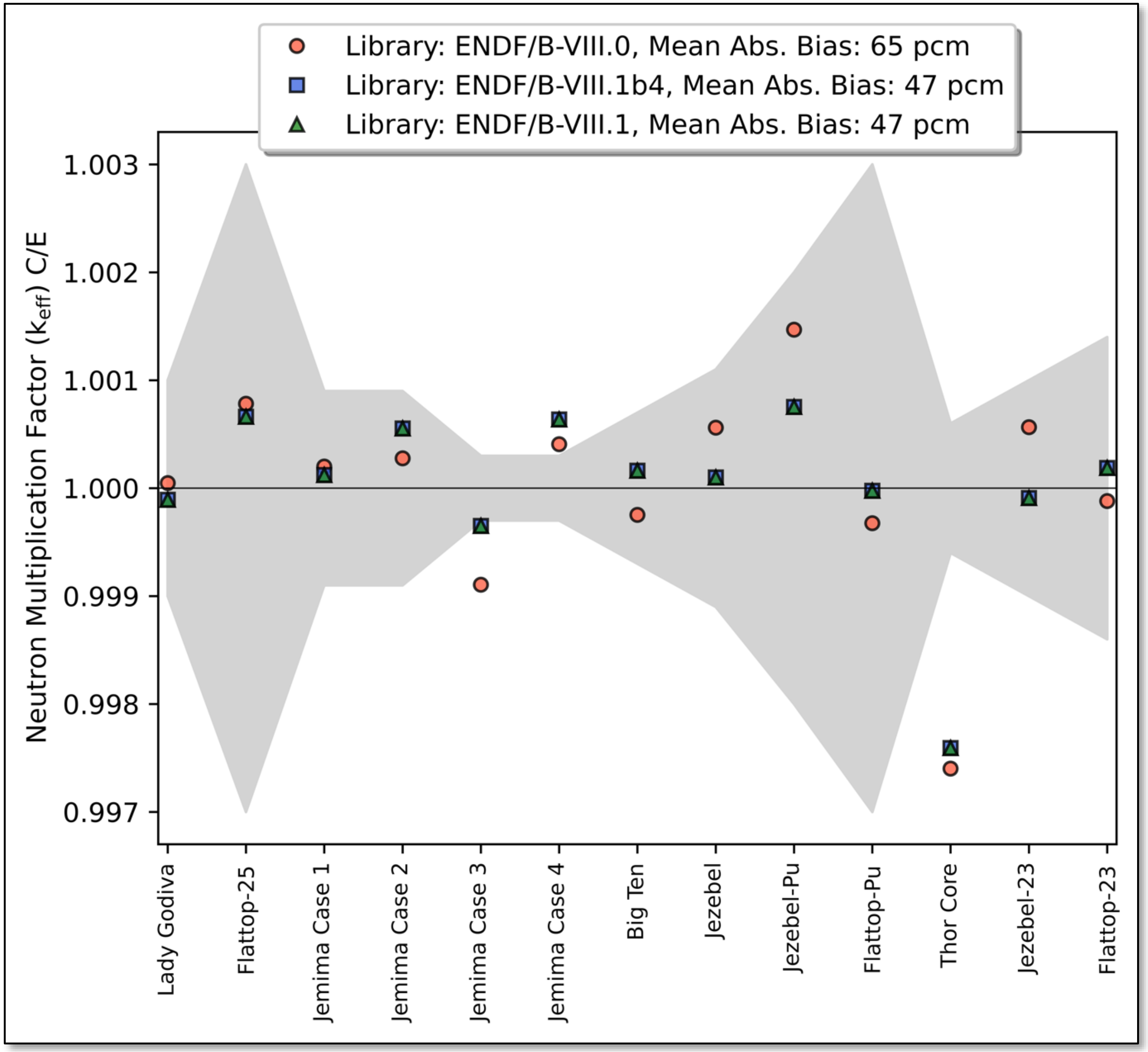
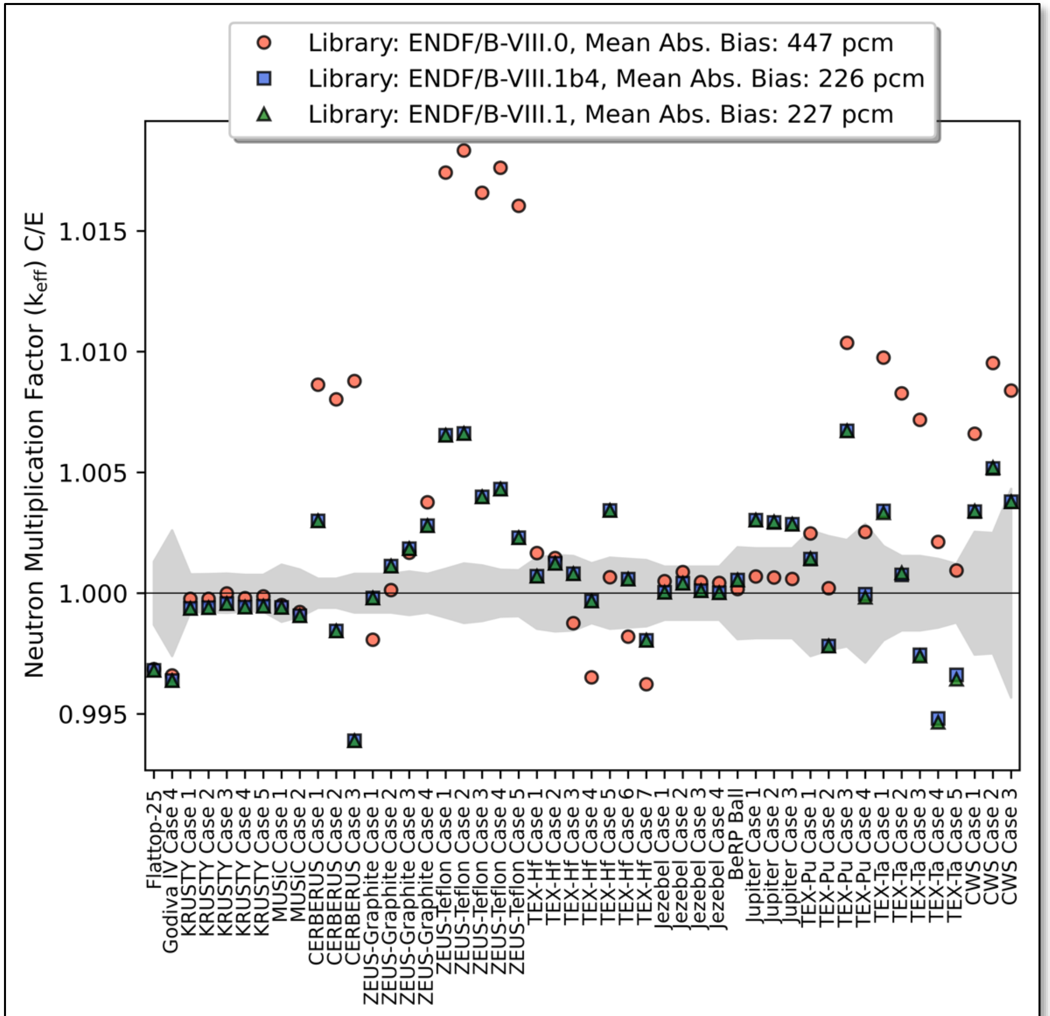
"National Criticality Experiments Research Center (NCERC): The First 10 Years of Operation," *Nuclear Science and Engineering* **195** Supplement 1 (2021)

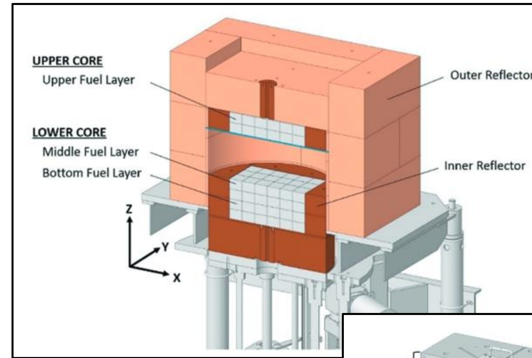
Legacy Benchmark Suite

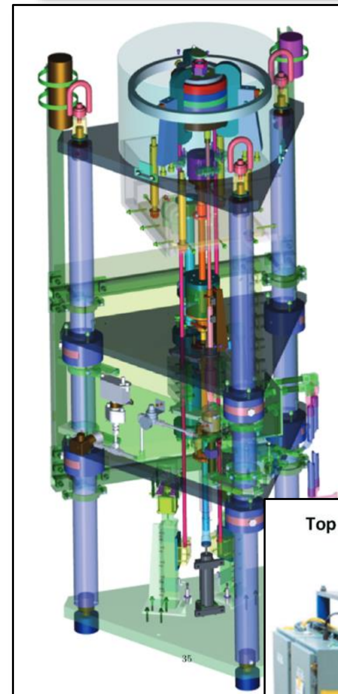


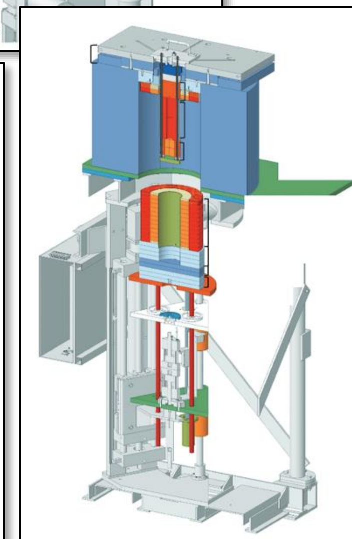
- This suite provides an overview of accuracy for fast/intermediate cross sections of ^{235,238}U, ^{239}Pu as well as ^{233}U and ^{232}Th
- Good agreement between simulated and experimental criticality for HEU/Pu "bare" systems (i.e., Lady Godiva and Jezebel)
- Flattop-23 bias not necessarily bad… ^{233}U and ^{238}U changes are shown to improve prediction capability
- Significant effort put into ^{239}Pu evaluation – adjustment of mean values such that Jezebel (Rev. 5) C/E ≈ 1

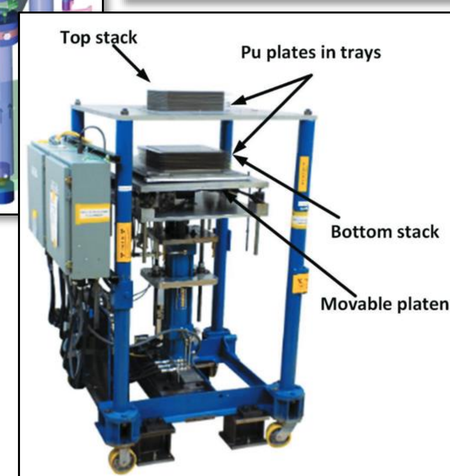
Modern Benchmark Suite







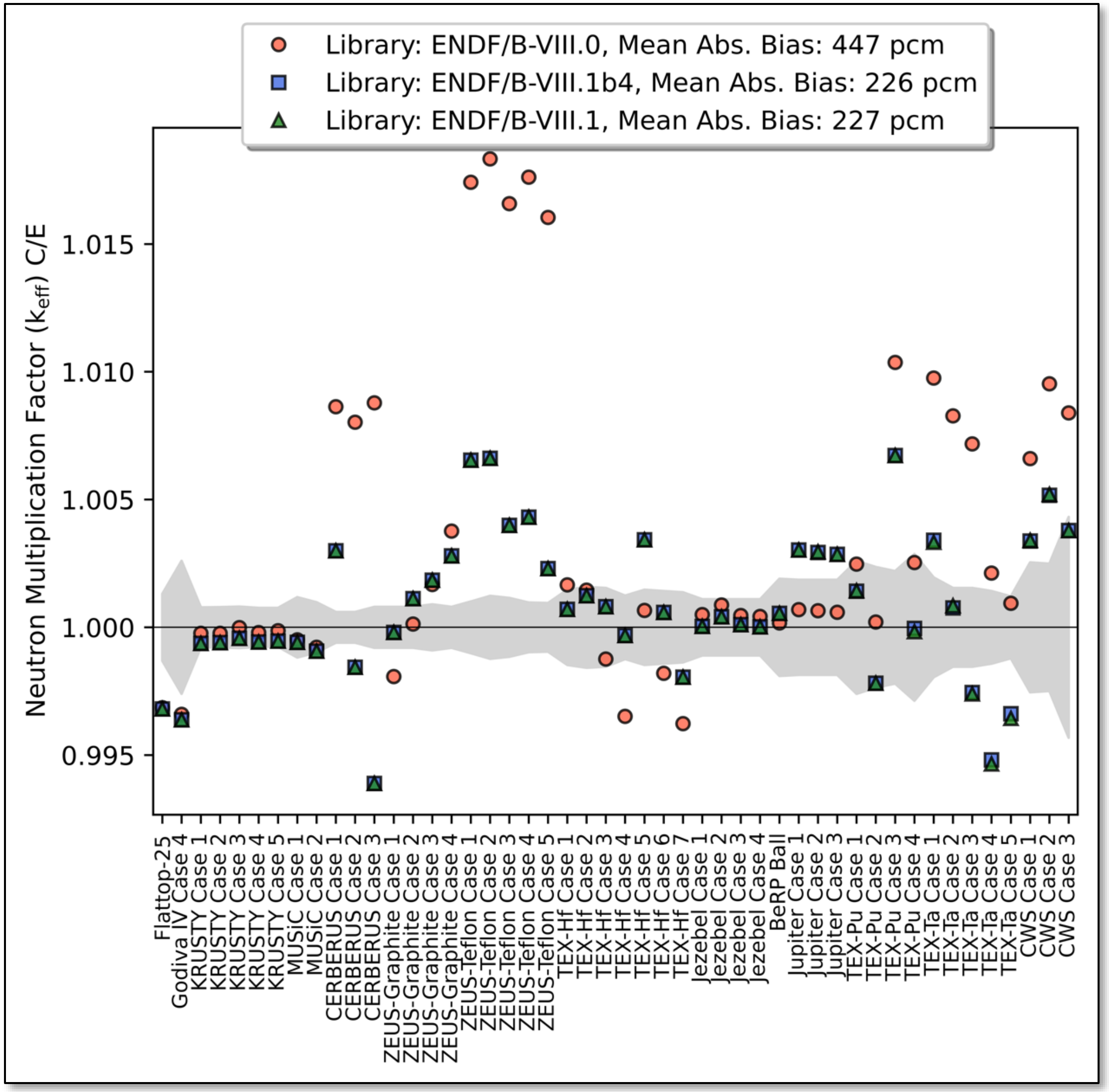




Kilowatt Reactor Using Stirling Technology (KRUSTY), Thermal/Epithermal eXperiments (TEX)
Measurement of Uranium Subcritical and Critical (MUSiC), Chlorine Worth Study (CWS)
ZEUS-Teflon, Critical Unresolved Region Integral Experiment (CURIE)

"National Criticality Experiments Research Center (NCERC): The First 10 Years of Operation," *Nuclear Science and Engineering* **195** Supplement 1 (2021)

Modern Benchmark Suite



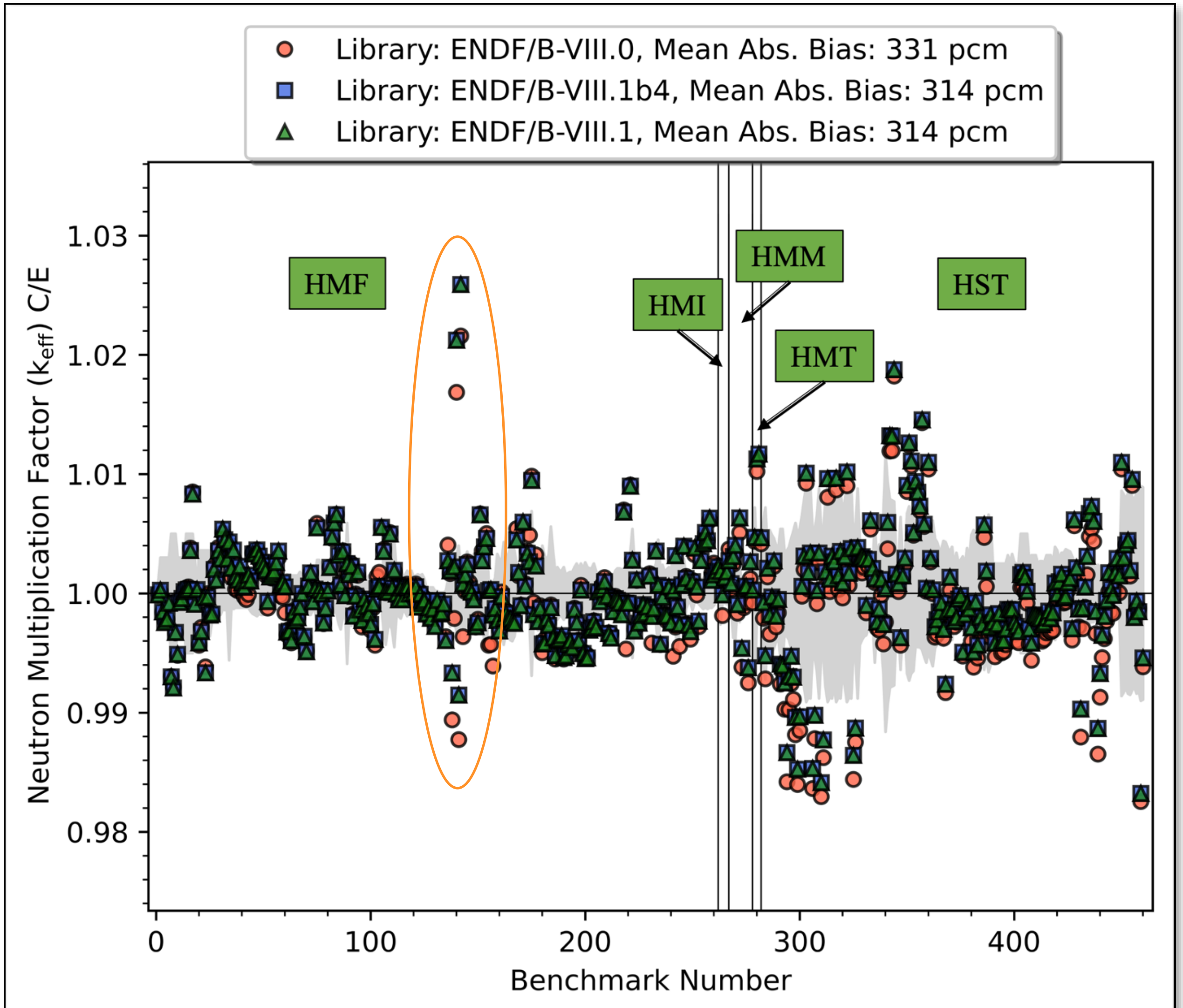
- *NEW* well-characterized experiments <u>recently accepted</u> into ICSBEP Handbook
- This suite provides an overview of accuracy for modern thermal/intermediate/fast cross sections of fuel/moderator/reflector materials
- Significant reduction in bias using ENDF/B-VIII.1 b/c of multiple evaluation updates:

1. ^{239}Pu (Jezebel, TEX)
2. ^{181}Ta in fast energy region (TEX-Ta)
3. ^{19}F (ZEUS-Teflon, CURIE)
   (Teflon formula = C_2F_4)

- Future file investigations:

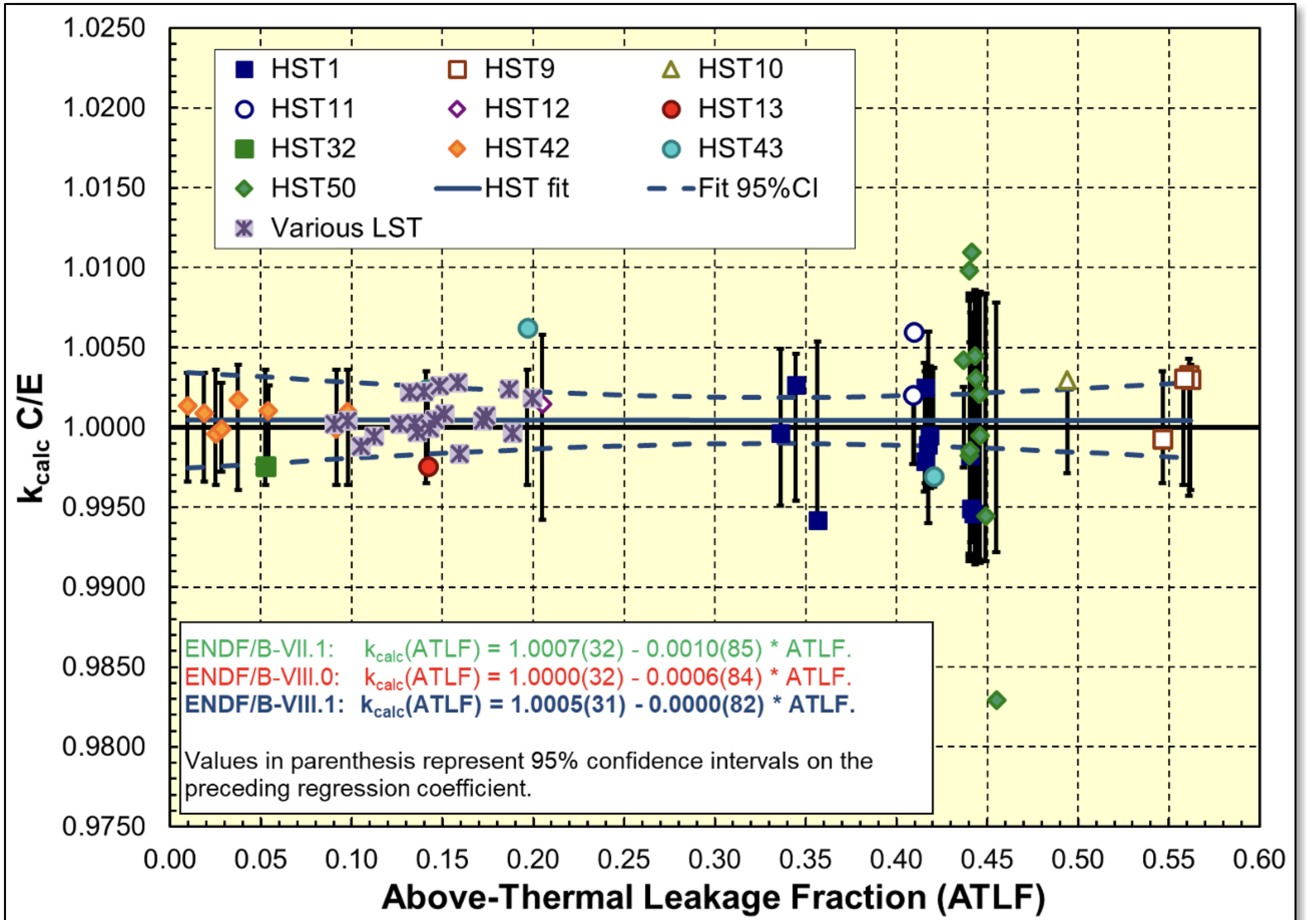
1. ^{9}Be (KRUSTY, BeRP Ball)
2. Pb (Jupiter) – discussions w/ IAEA
3. Ta in thermal energy region/h-poly TSL File/S(α, β) (TEX-Ta)

HEU Benchmark Suites



- Changes in ^{235,238}U don't produce significant changes in HEU metal benchmarks simulated results
- The standout benchmark in HMF suite around benchmark number 140 is HMF-57, HEU reflected by lead – increase in k_{eff} from new Pb file is both good (HMF-57 Cases 1&4) and bad (HMF-57 Cases 3&5)
- Noticeable increase in k_{eff} in HST suite (e.g., benchmark numbers 300-340 show a clear increase in k_{eff} from E8.0 to E8.1 for uranyl-nitrate/fluoride solutions)

HEU Benchmark Suites



- Correlation of k_{eff} as a function of ATLF for a select suite of thermal benchmarks has provided a test of thermal ^{235}U nuclear data for decades
- LST benchmarks are not included in regression fit, but are used to support conclusion of no bias in C/E as a function of enrichment
- E8.1 intercept higher than E8.0, but results remain consistent between E8.0 and E8.1 – slope is now zero, which is excellent progress

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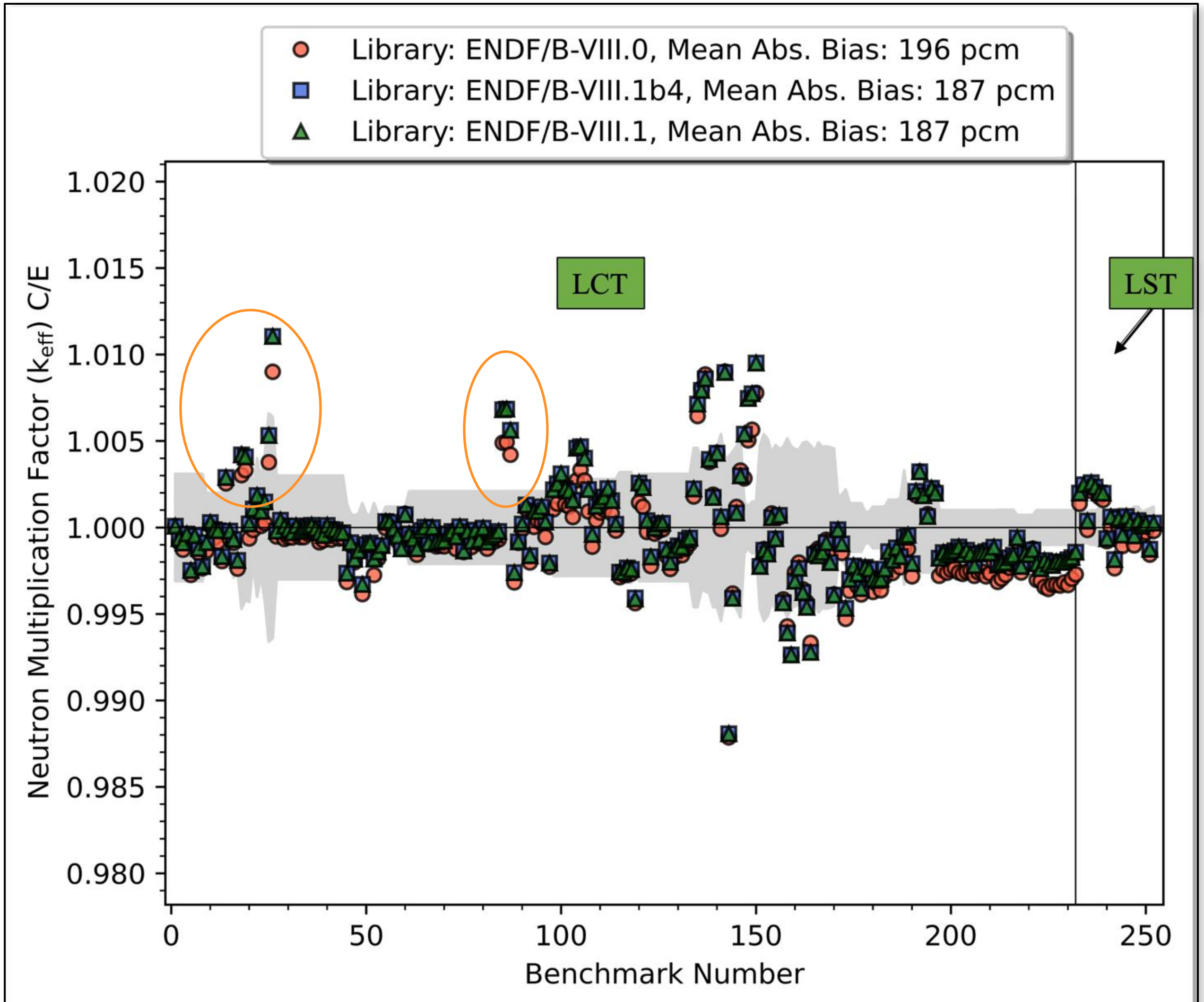
LEU Benchmark Suites



- Changes in ^{235,238}U don't produce significant changes in LEU benchmarks simulated results – there is a slight increase in reactivity
- Reactor lattice category ("LCT", LEU-COMP-THERM) shows excellent overall performance
- LCT benchmark numbers 10-30 with higher C/E values include LCT-5, LEU in water containing dissolved Gd
- LCT benchmark numbers 80-90 with higher C/E values include LCT-10, water-moderated LEU reflected by Pb

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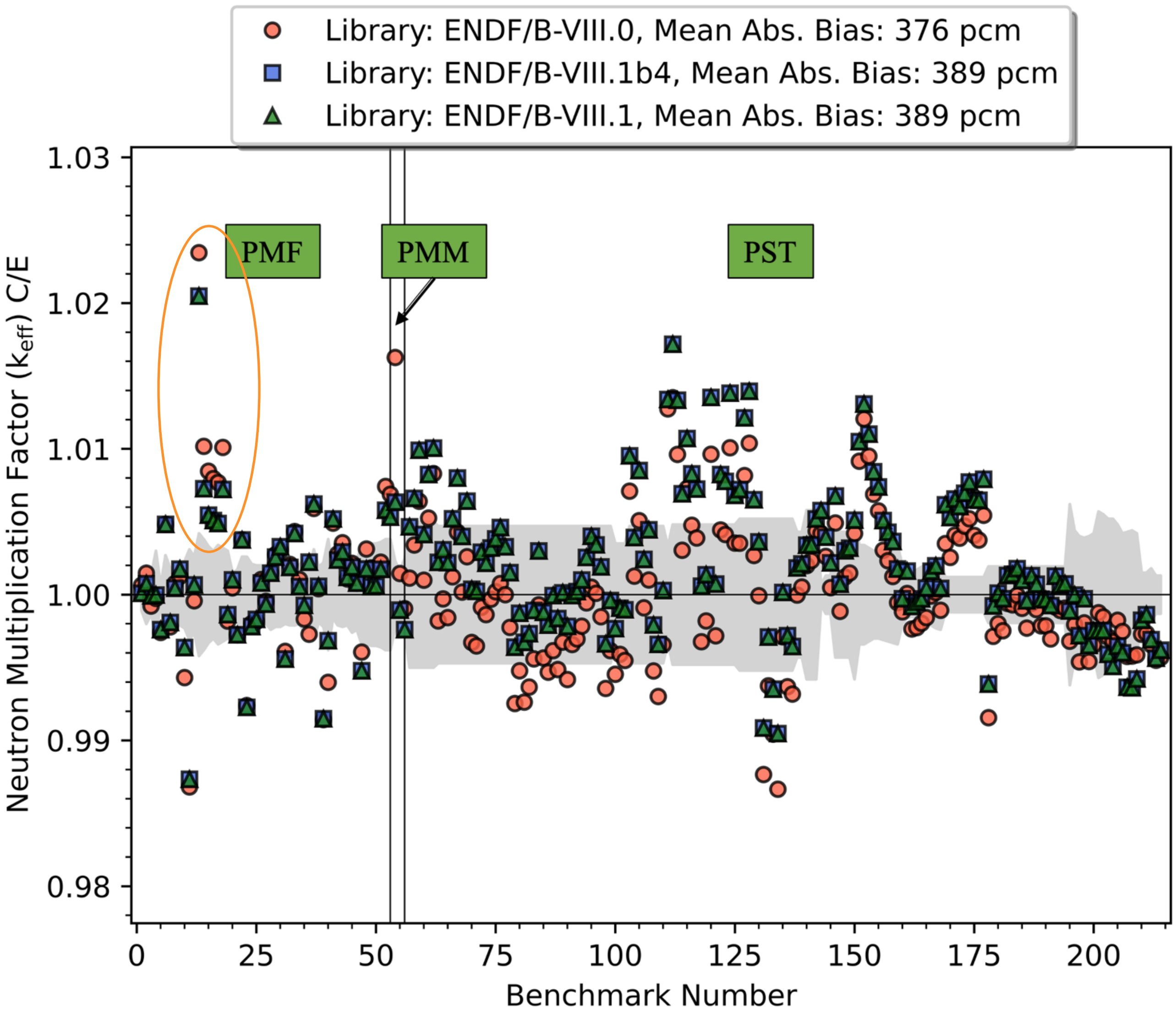
Pu Benchmark Suites



- PMF benchmark numbers 10-20 with higher C/E values include PMF-16, water-moderated Pu – not much documentation and extrapolated to critical for some cases
- Changes in plutonium metal intermediate/fast (PMI/F) systems are favorable due to ^{239}Pu file update
- PST benchmark simulated results are slightly concerning – E8.0 "success story" of reducing PST bias
- E8.1 PST bias difference on order of hundreds of pcm
- PST benchmark numbers 195-210 include PST-34, Pu nitrate with Gd in water, which have a different k_{eff} trend than what is shown for most PST benchmarks

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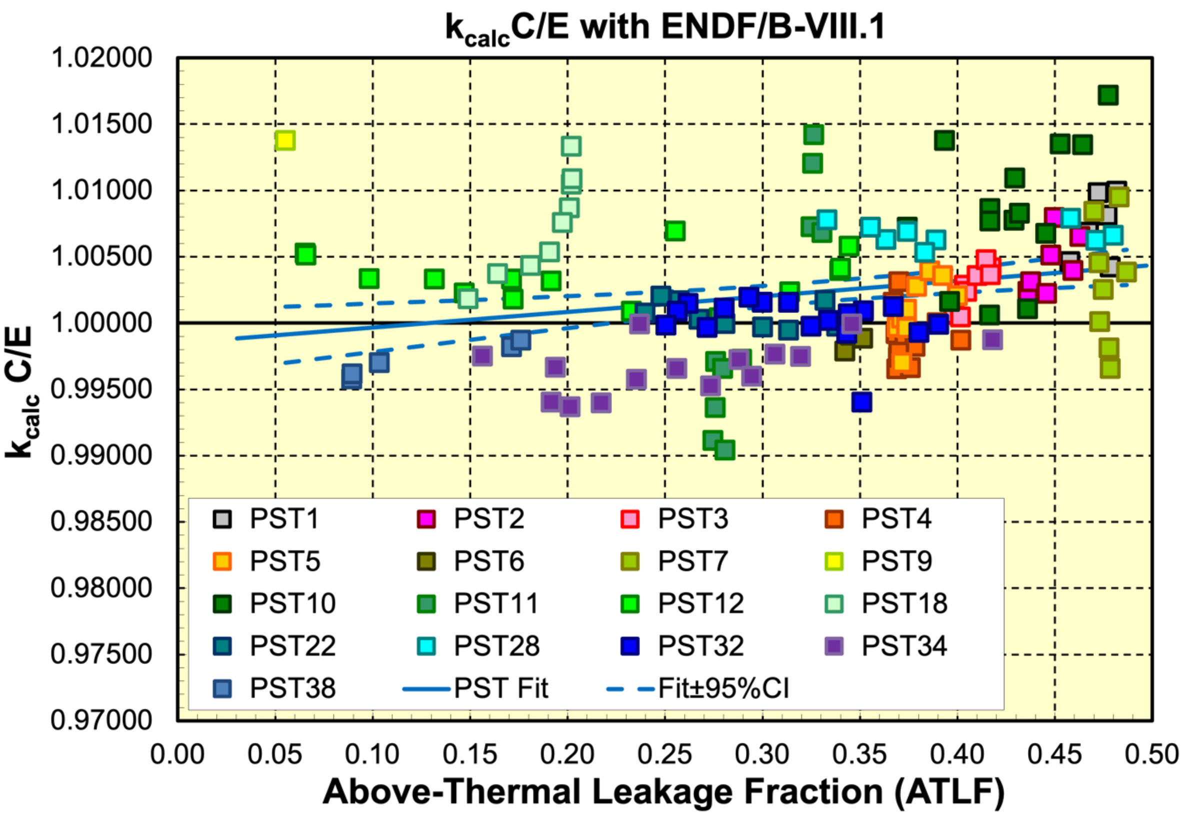
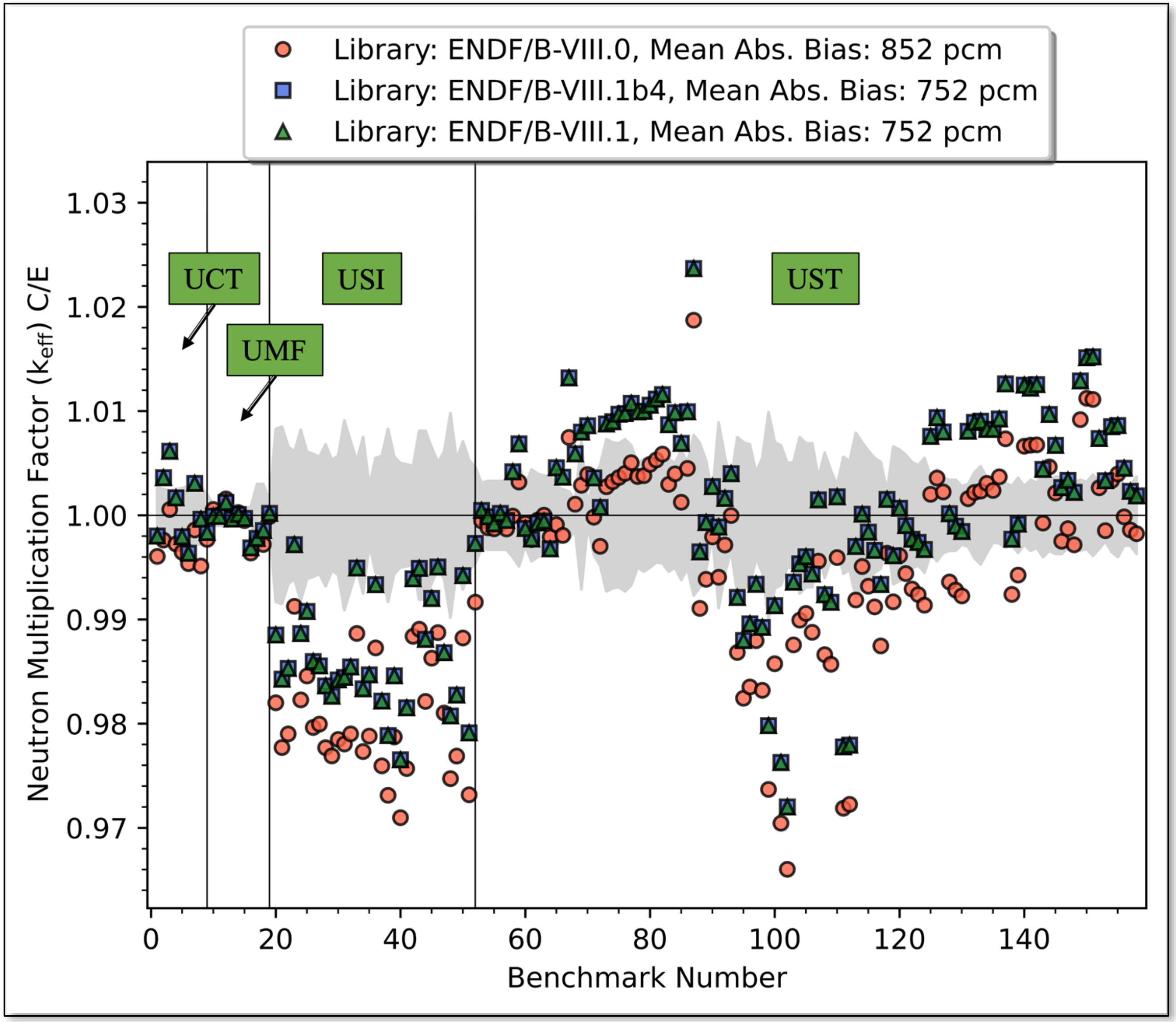
Pu Benchmark Suites



- Increase in criticality for PU-SOL-THERM (PST) benchmarks breaks nearly flat trend observed for E8.0
- The success of E8.0 ^{239}Pu evaluation to reduce magnitude of trend line as a function of ATLF should be revisited – consider ^{239}Pu thermal PFNS and neutron multiplicity
- Challenge: changes in ^{239}Pu satisfy depletion metrics and reactivity temperature coefficients

^{233}U Benchmark Suites



- Overall, there is a significant reduction in mean absolute bias for ^{233}U benchmarks simulated results from changes in the ^{233}U file; however, C/E values are still very far from unity…

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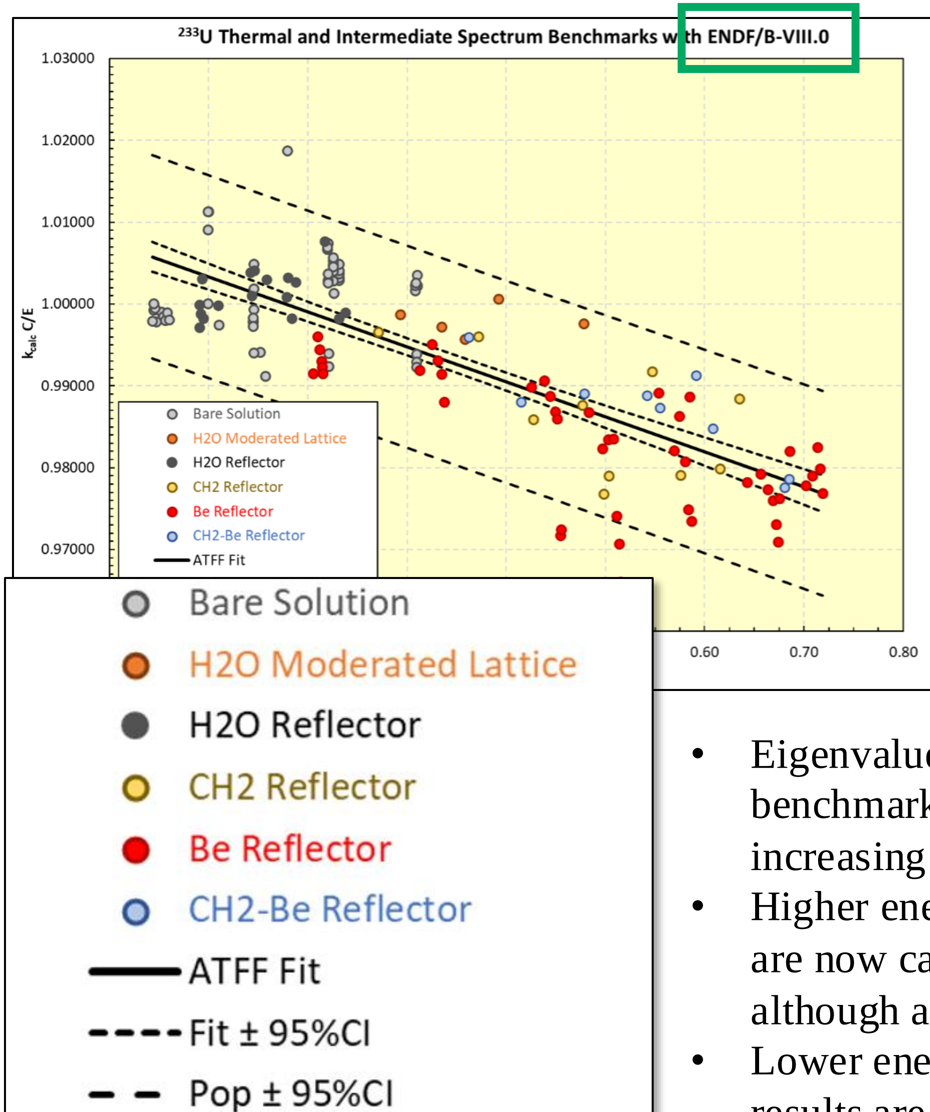
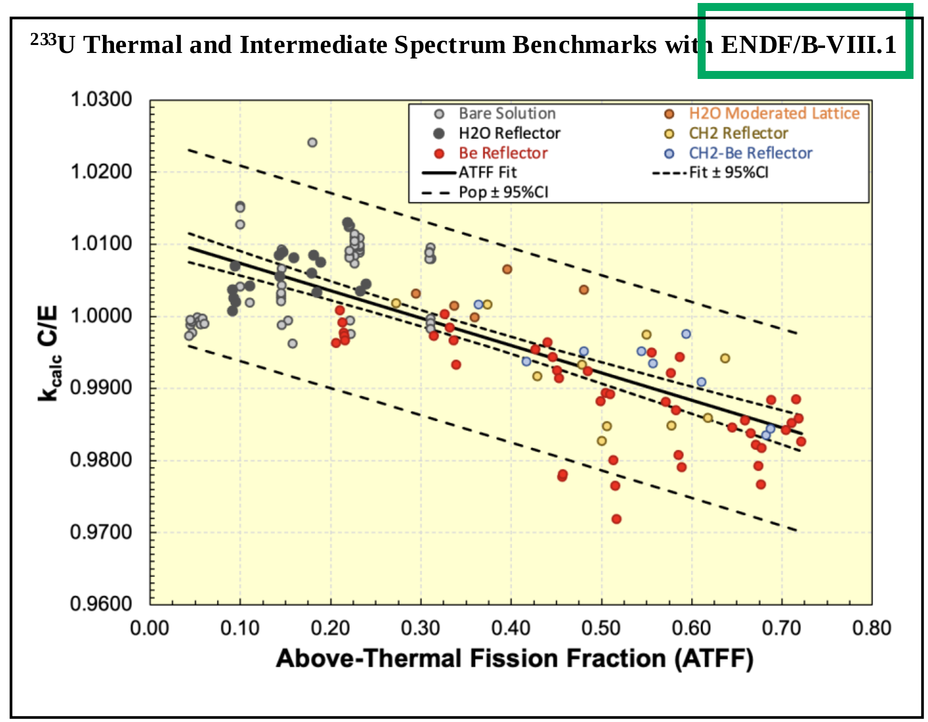
^{233}U Benchmark Suites





- Eigenvalue calculations for thermal and intermediate energy benchmarks have exhibited a strong, negative trend with increasing energy for decades – results for E8.1 follow this trend
- Higher energy: the Be and combined Be-CH_2 reflected systems are now calculated about 1000 pcm higher – good result although average results are still low
- Lower energy (i.e., ATFF from ~0.1 to 0.3): the near unity E8.0 results are now too large, with an apparent positive trend in calculated eigenvalue – LWBR lattice results are also worse than those obtained with E8.0

Reaction Rate Ratios

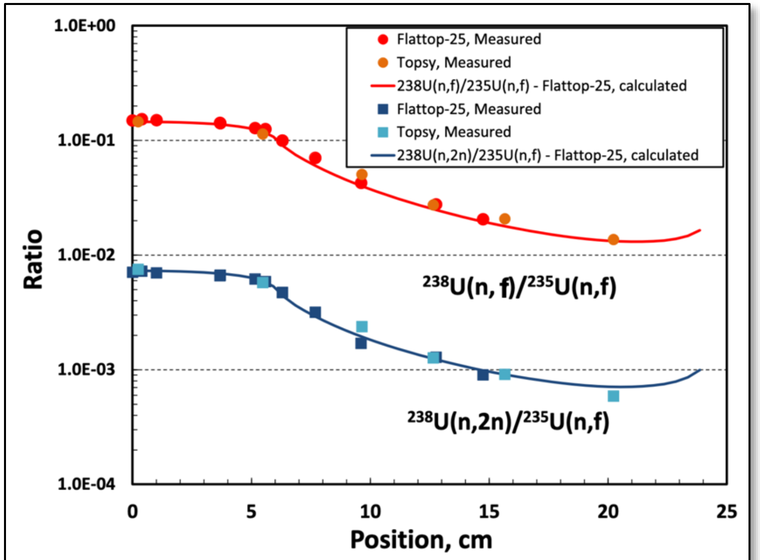
Experiment, Ratio	Measured Value	Calculated Value ENDF/B-VIII.0	Calculated Value ENDF/B-VIII.1
Lady Godiva, $\frac{^{233}U(n,f)}{^{235}U(n,f)}$	1.59(3)	1.58	1.58
Lady Godiva, $\frac{^{237}Np(n,f)}{^{235}U(n,f)}$	0.8516(120)	0.8311	0.8307
Lady Godiva, $\frac{^{238}U(n,f)}{^{235}U(n,f)}$	0.1643(18)	0.1582	0.1580
Lady Godiva, $\frac{^{239}Pu(n,f)}{^{235}U(n,f)}$	1.4152(140)	1.3844	1.3832
Big Ten, $\frac{^{238}U(n,f)}{^{235}U(n,f)}$	0.0375(9)	0.0357	0.0359
Big Ten, $\frac{^{239}Pu(n,f)}{^{235}U(n,f)}$	1.198(28)	1.170	1.169
Jezebel, $\frac{^{233}U(n,f)}{^{235}U(n,f)}$	1.578(27)	1.566	1.566
Jezebel, $\frac{^{237}Np(n,f)}{^{235}U(n,f)}$	0.9835(14)	0.9768	0.9710
Jezebel, $\frac{^{238}U(n,f)}{^{235}U(n,f)}$	0.2133(23)	0.2119	0.2106
Jezebel, $\frac{^{239}Pu(n,f)}{^{235}U(n,f)}$	1.4609(130)	1.4273	1.4242
Jezebel, $\frac{^{239}Pu(n,2n)}{^{239}Pu(n,f)}$	None	0.0023	0.0022
Jezebel, $\frac{^{239}Pu(n,\gamma)}{^{239}Pu(n,f)}$	None	0.0345	0.0359
Jezebel-23, $\frac{^{237}Np(n,f)}{^{235}U(n,f)}$	0.997(15)	0.984	0.984
Jezebel-23, $\frac{^{238}U(n,f)}{^{235}U(n,f)}$	0.2131(26)	0.2116	0.2110
Flattop-Pu, $\frac{^{237}Np(n,f)}{^{235}U(n,f)}$	0.8561(120)	0.8569	0.8511
Flattop-Pu, $\frac{^{238}U(n,f)}{^{235}U(n,f)}$	0.1799(20)	0.1793	0.1779
Flattop-Pu, $\frac{^{239}Pu(n,2n)}{^{239}Pu(n,f)}$	None	0.0020	0.0019
Flattop-Pu, $\frac{^{239}Pu(n,\gamma)}{^{239}Pu(n,f)}$	None	0.0458	0.0468
Flattop-23, $\frac{^{237}Np(n,f)}{^{235}U(n,f)}$	0.910(13)	0.900	0.899
Flattop-23, $\frac{^{238}U(n,f)}{^{235}U(n,f)}$	0.1916(21)	0.1882	0.1870
Flattop-25, $\frac{^{233}U(n,f)}{^{235}U(n,f)}$	1.608(30)	1.578	1.578
Flattop-25, $\frac{^{237}Np(n,f)}{^{235}U(n,f)}$	0.7804(100)	0.7716	0.7710
Flattop-25, $\frac{^{238}U(n,f)}{^{235}U(n,f)}$	0.1492(16)	0.1445	0.1443
Flattop-25, $\frac{^{239}Pu(n,f)}{^{235}U(n,f)}$	1.3847(120)	1.3615	1.3602

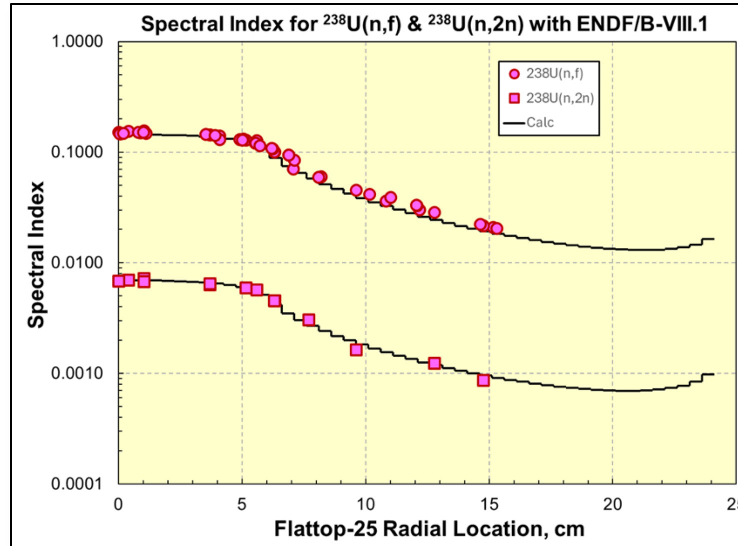
- No significant changes in the reaction rate ratios calculated values from E8.0 to E8.1
- Small decrease in $^{239}Pu(n,f)/^{235}U(n,f)$ and $^{238}U(n,f)/^{235}U(n,f)$ from E8.0 to E8.1

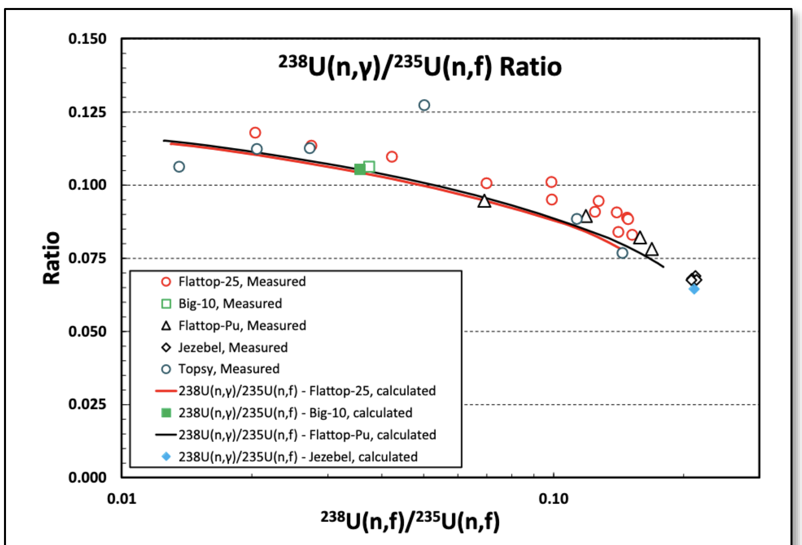
Reaction Rate Ratios

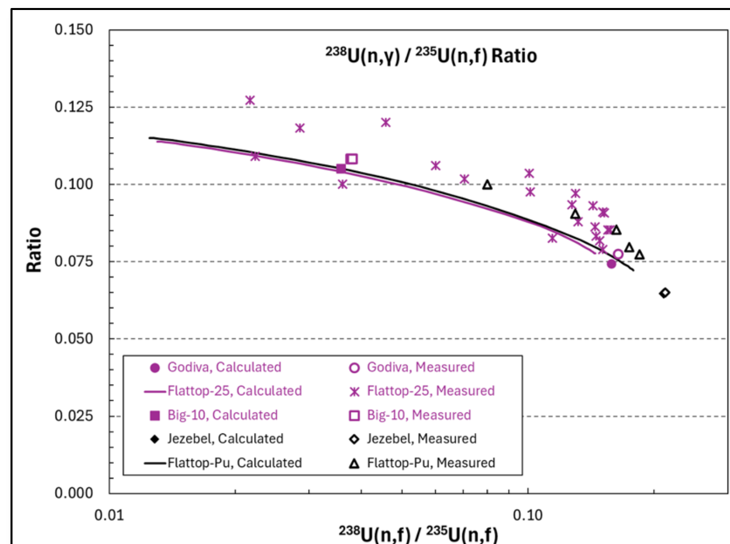
ENDF/B-VIII.0

ENDF/B-VIII.1



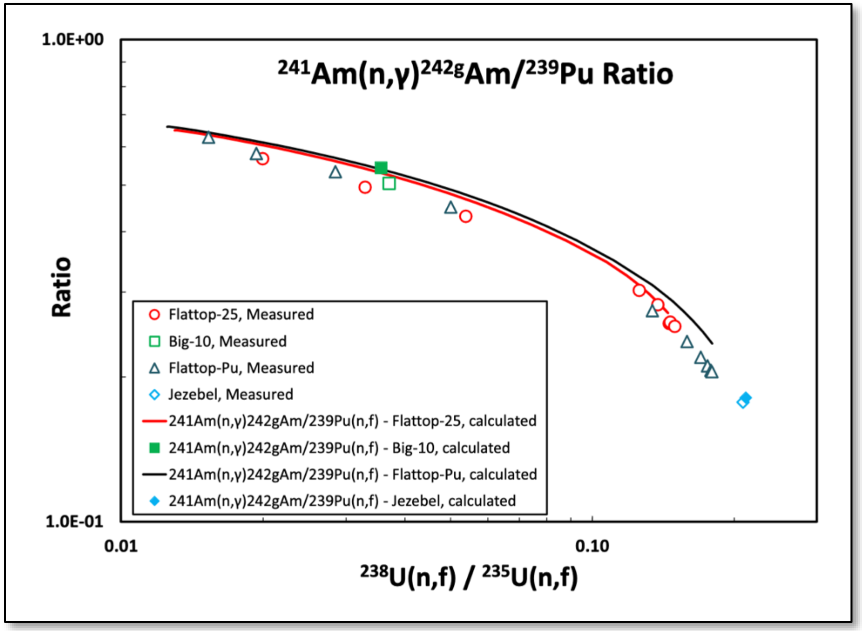




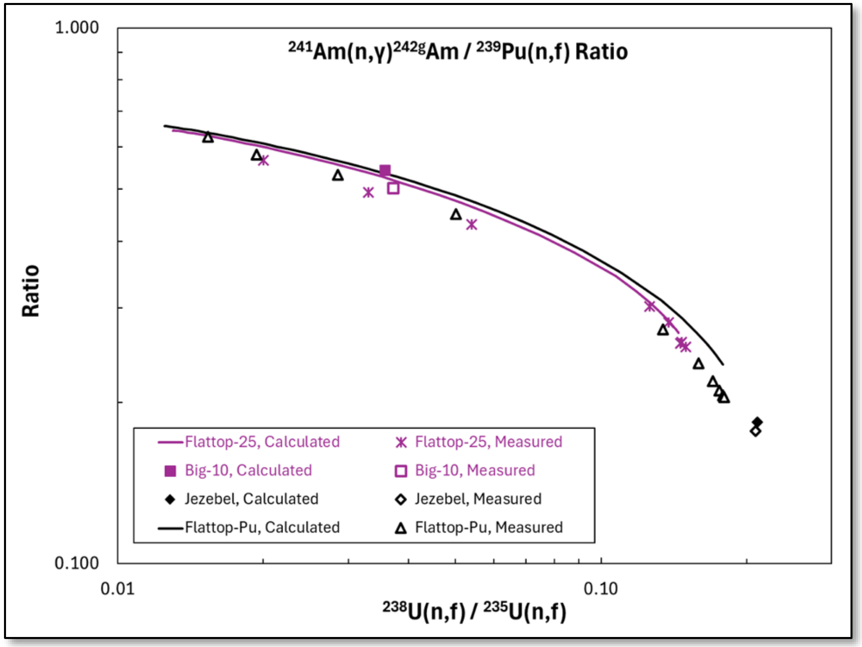


Reaction Rate Ratios

ENDF/B-VIII.0



ENDF/B-VIII.1



- Reaction rate ratio values changed from E8.0 to E8.1 by amounts less than experimental uncertainty – there has been effort by A. Lee (LANL, C-NR) to reanalyze reaction rate ratio experimental values
- Reaction rate ratio experiment data was collected from the following sources:

(1) A. Lee, "Compendium of LANL Historical Critical Assembly Experiments: 1953-1976 A Radiochemistry Reassessment," Los Alamos Technical Report LA-UR-23-32767

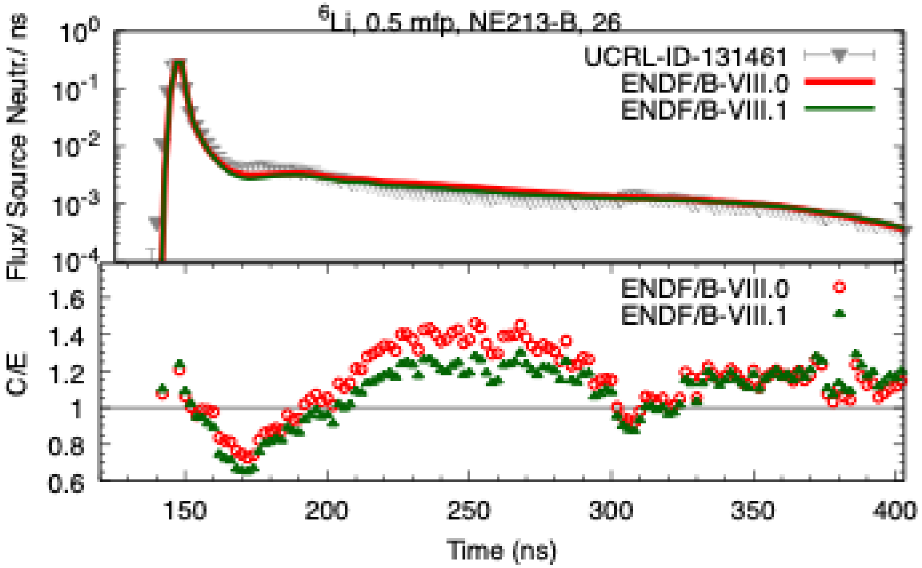
(2) D. A. Brown et al., "ENDF/B-VIII.0: The 8th Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data," *Nuclear Data Sheets* 148 (2018)

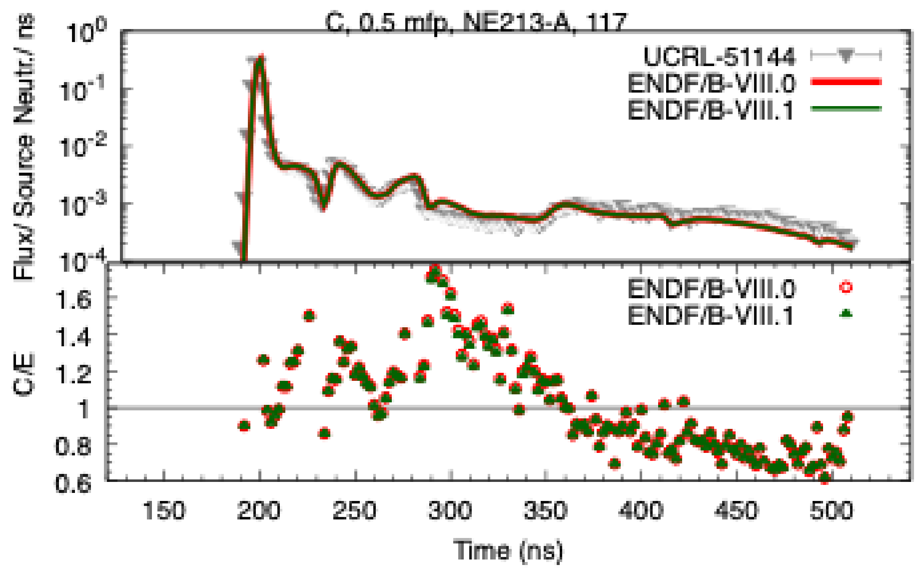
(3) P. G. Young et al., "Evaluation of Neutron Reactions for ENDF/B-VII: $^{232-241}$U and ^{239}Pu," *Nuclear Data Sheets* 108 (2007)

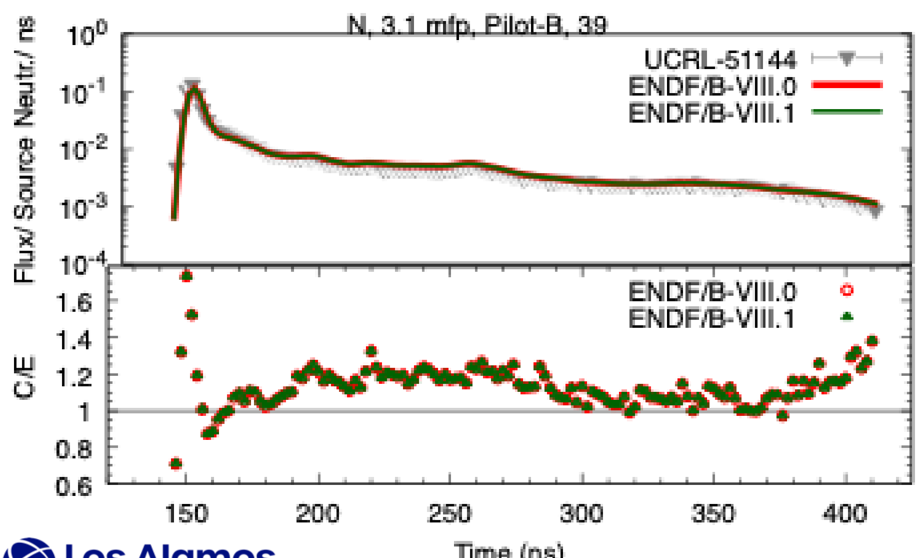
A few LLNL Pulsed Spheres simulations indicate some nuclear data could be further improved for IX.0.

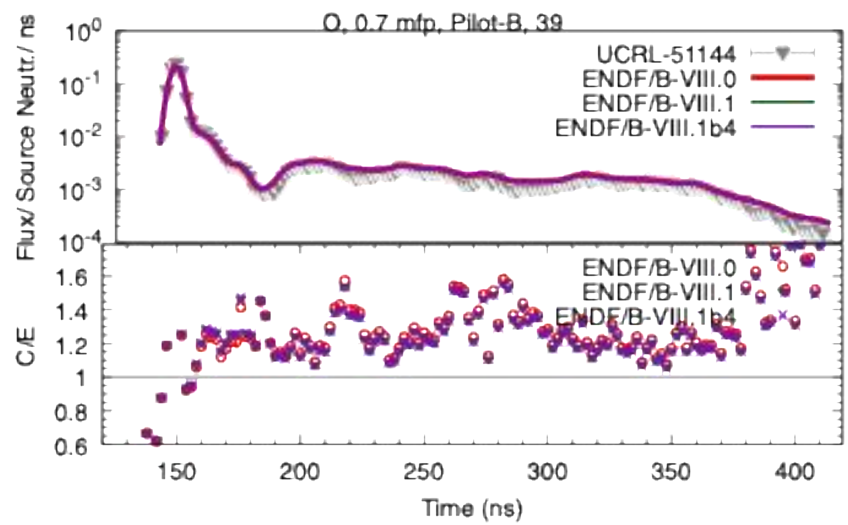
- Light elements: ^{6}Li, C, ^{14}N, ^{16}O
- Structural material element: ^{27}Al, Fe, Mg, Ti, Pb
- Actinides: ^{238}U, Pu

Light elements: ^{6}Li, C, ^{14}N, ^{16}O spheres seem biased, explore angular distribution and inelastic levels.

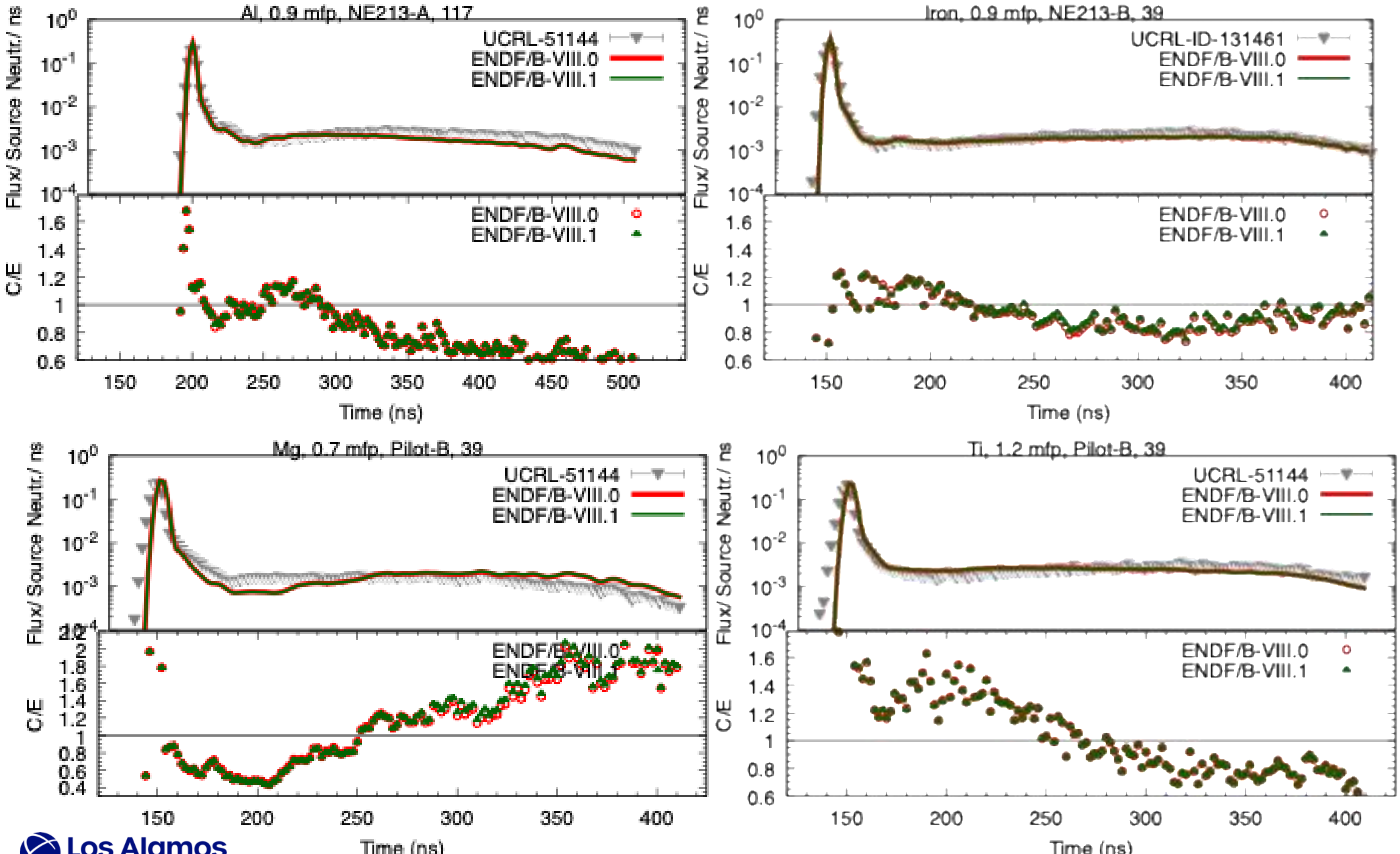








Structural material nuclear data: ^{27}Al, Fe, Mg, Ti, continuum becomes more important with higher Z.



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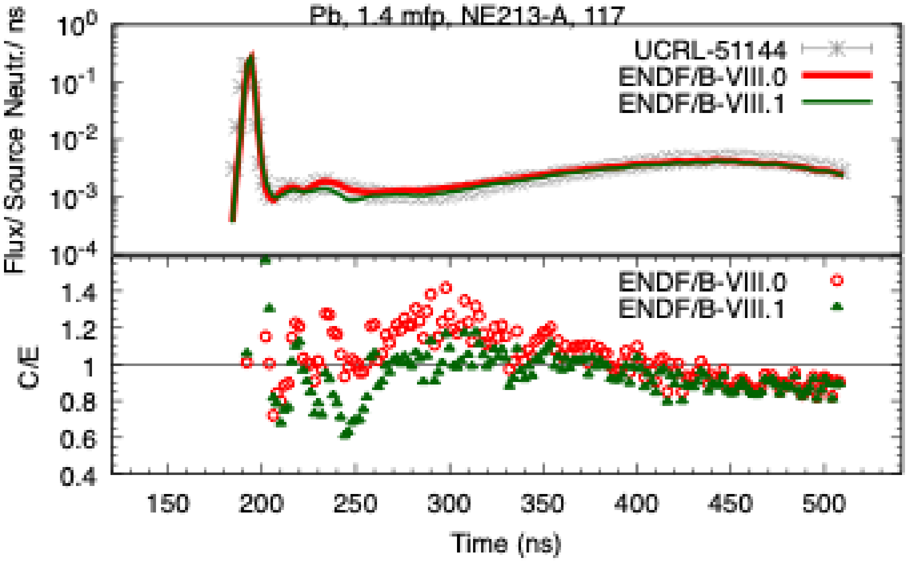
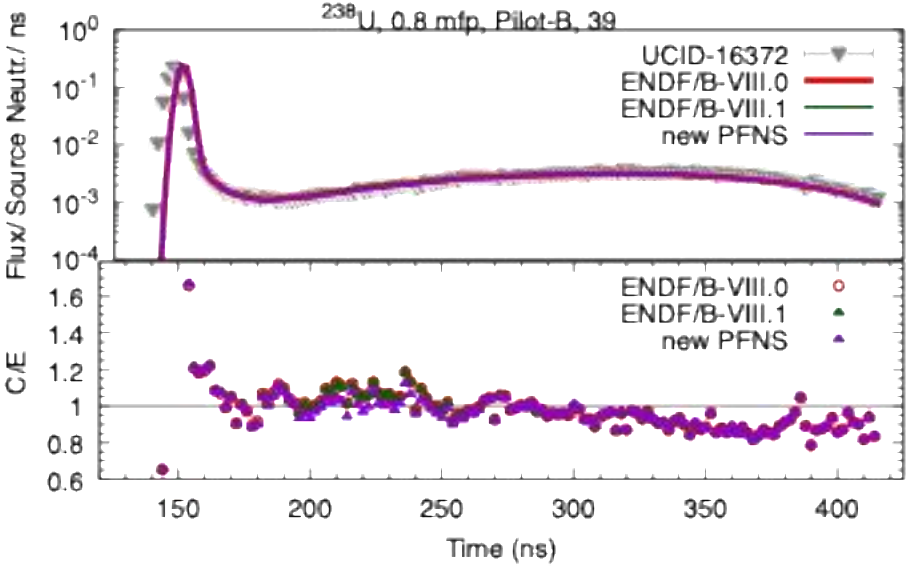
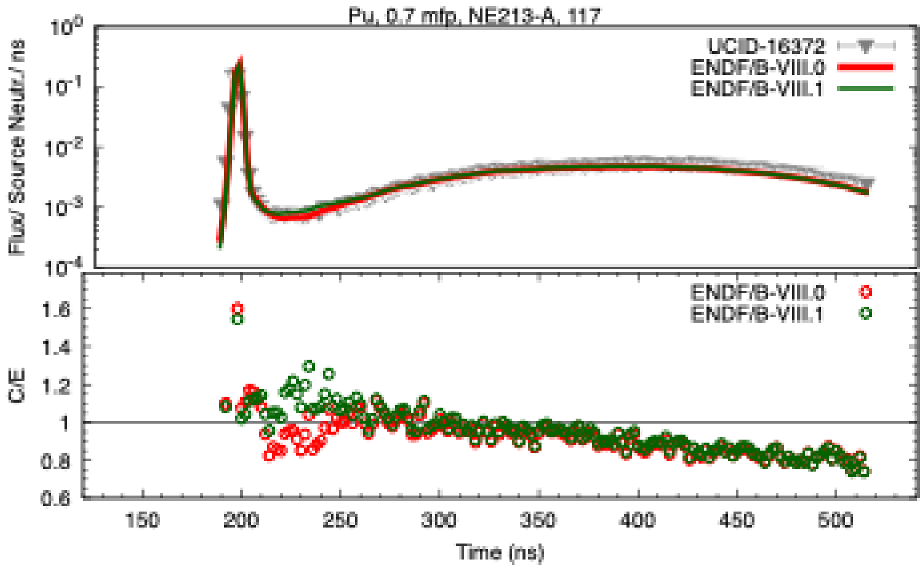
A bit more work Pb is needed; new ^{238}U PFNS might improve LPS, inelastic ^{239}Pu improvements needed.







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Conclusions

- ENDF/B-VIII.1β4 release results ≡ ENDF/B-VIII.1 official release results
- ENDF/B-VIII.1 is in great shape – many important advances made, especially for major actinides
- Future investigation: ^{9}Be (BeRP Ball and KRUSTY), Pb (future work for specific isotopes discussed with IAEA), Gd (benchmarks with Gd do not follow general calculated k_{eff} trend), ^{239}Pu changes relative to PU-SOL-THERM benchmark calculations, ^{233}U changes relative to U233-SOL-THERM benchmark calculations
- ENDF/B-IX → emphasize tuning nuclear data to modern benchmarks
- **What other validation metrics, benchmarks, or methods should be investigated for ENDF/B-IX nuclear data files?**

Acknowledgments

Research reported in this publication was supported by the U.S. Department of Energy Advanced Simulation and Computing (ASC) program at Los Alamos National Laboratory. The authors would like to thank members of the LANL Nuclear Data Team for their help in processing and verifying ENDF/B-VIII.1 nuclear data files.

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Questions?

Contact the Los Alamos National Laboratory
Nuclear Data Team by email at nucldata@lanl.gov