Validation Testing at LANL with ENDF/B-VIII.1β4 Files

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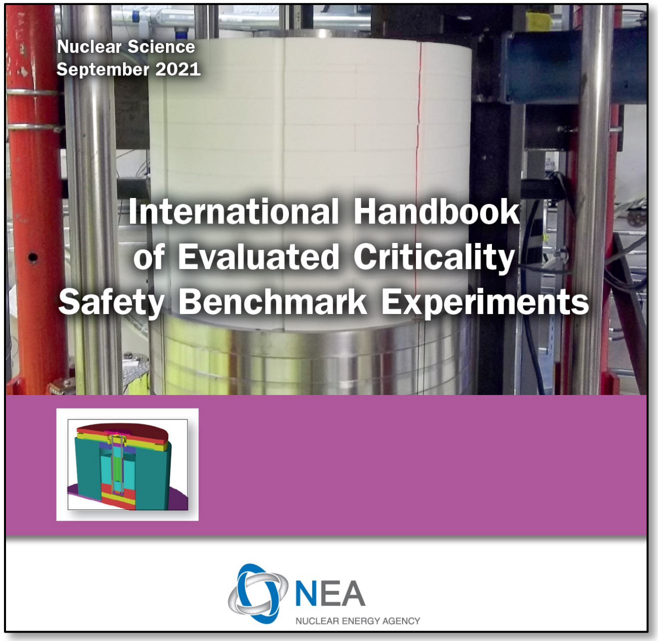
LA-UR-24-28687

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) Pu Benchmark Suites
(6) ^{233}U Benchmark Suites
(7) Reaction Rate Ratios

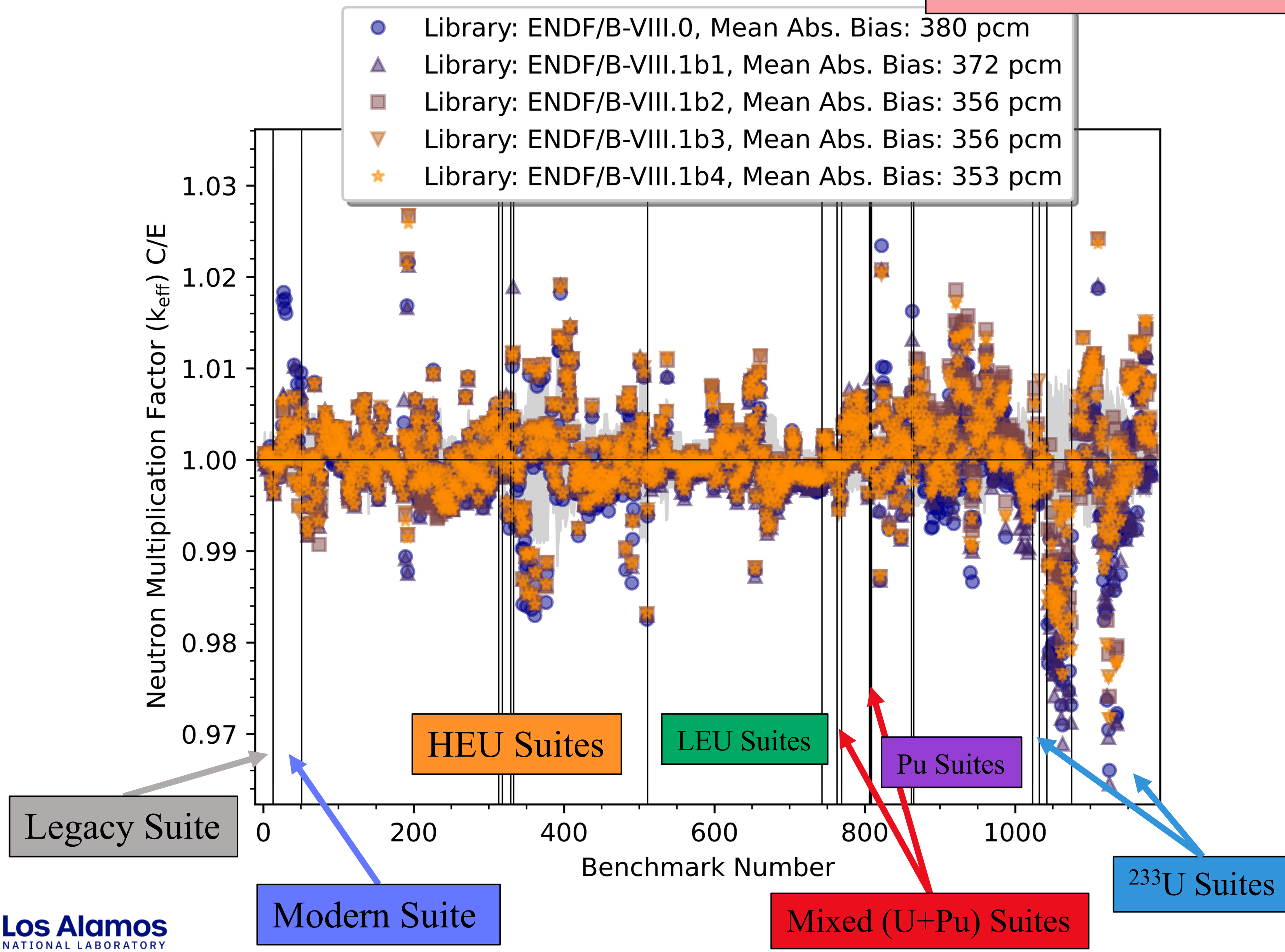


- Benchmark names are taken from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook designations

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)

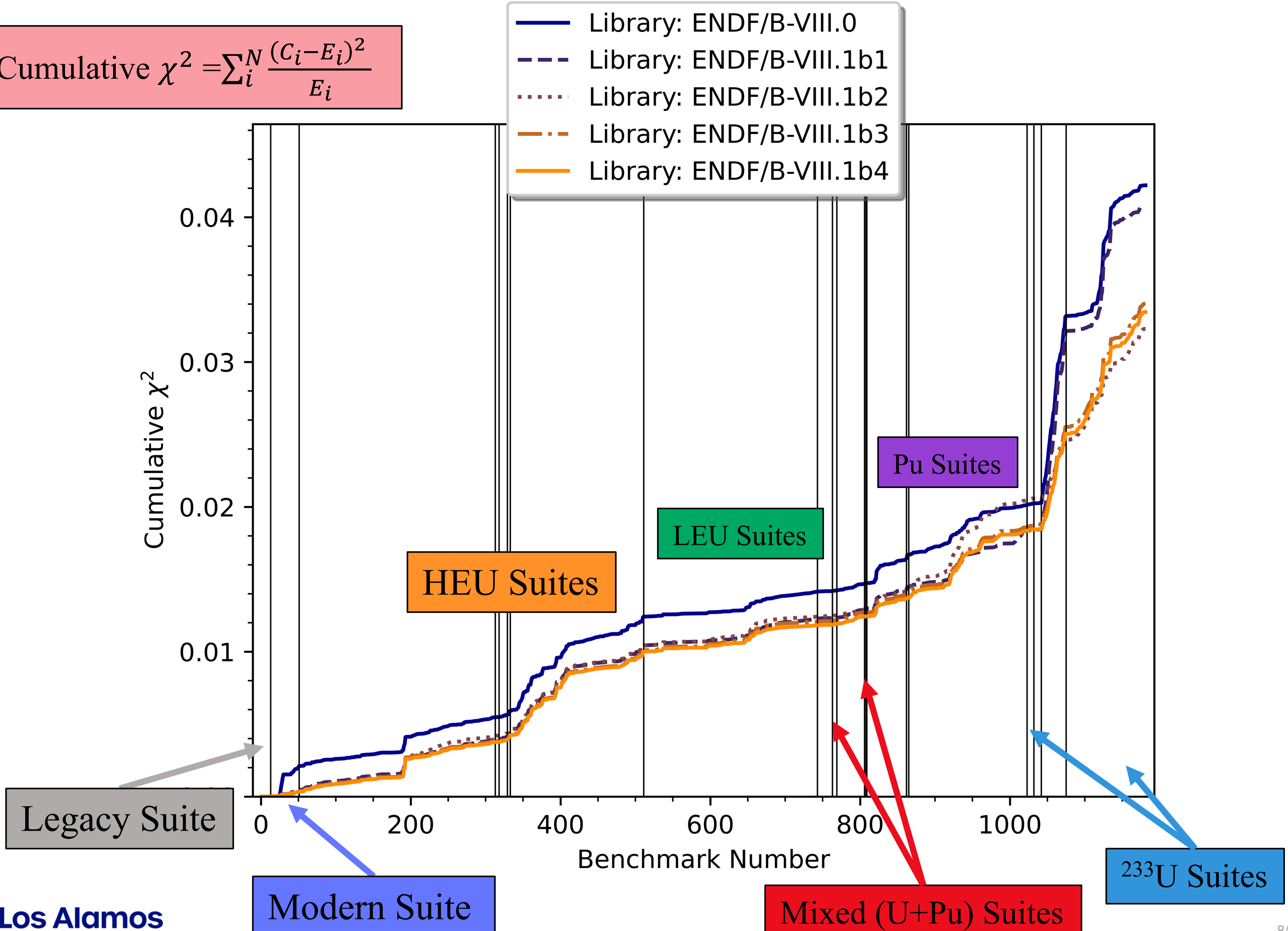
Everything, Everywhere, All at Once

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

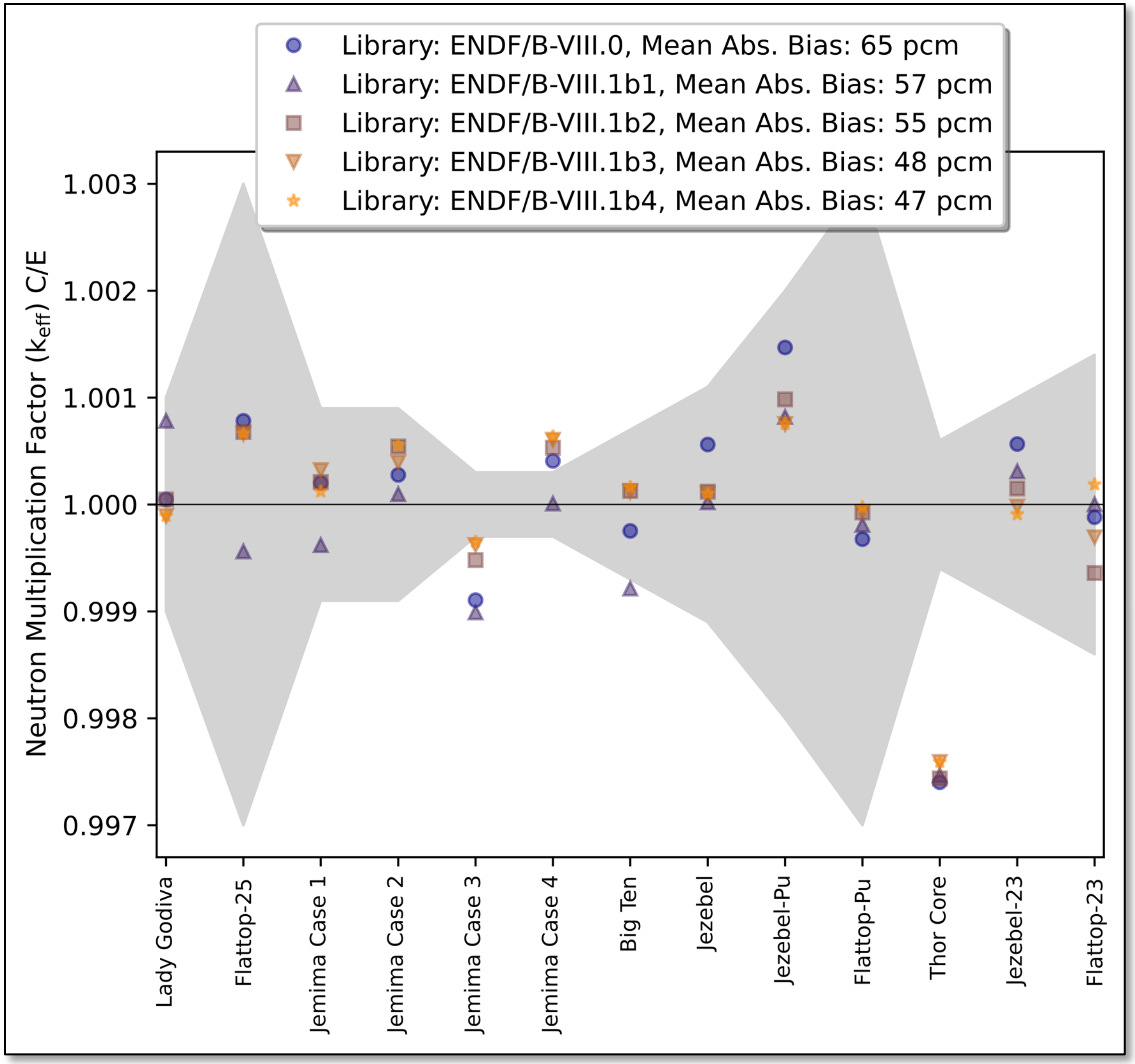


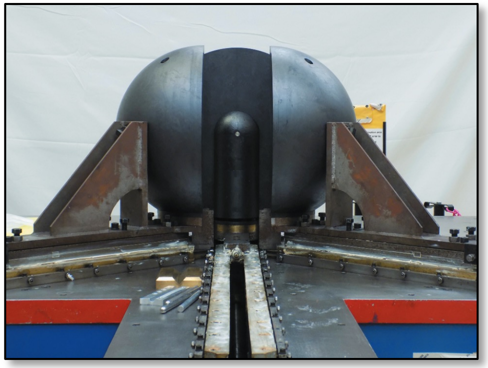
Everything, Everywhere, All at Once

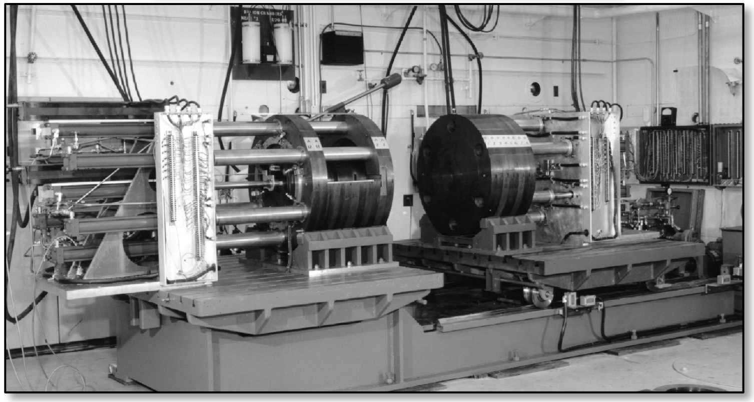
Cumulative $\chi^2 = \sum_i^N \frac{(C_i - E_i)^2}{E_i}$

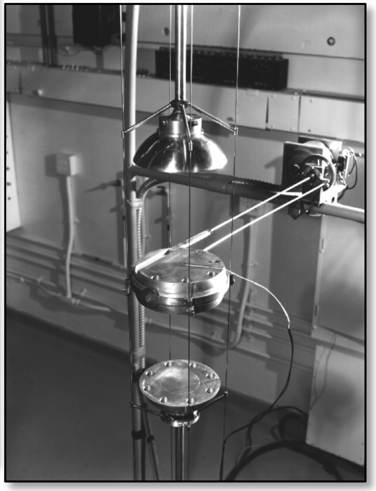


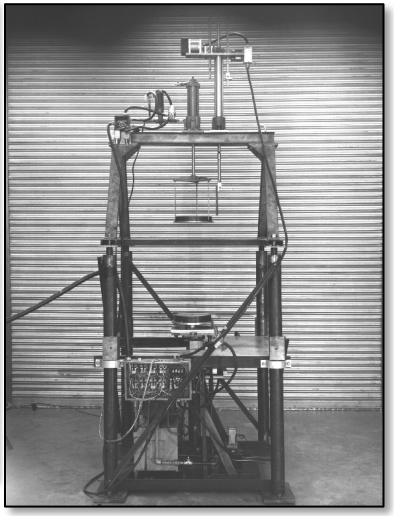
Legacy Benchmark Suite





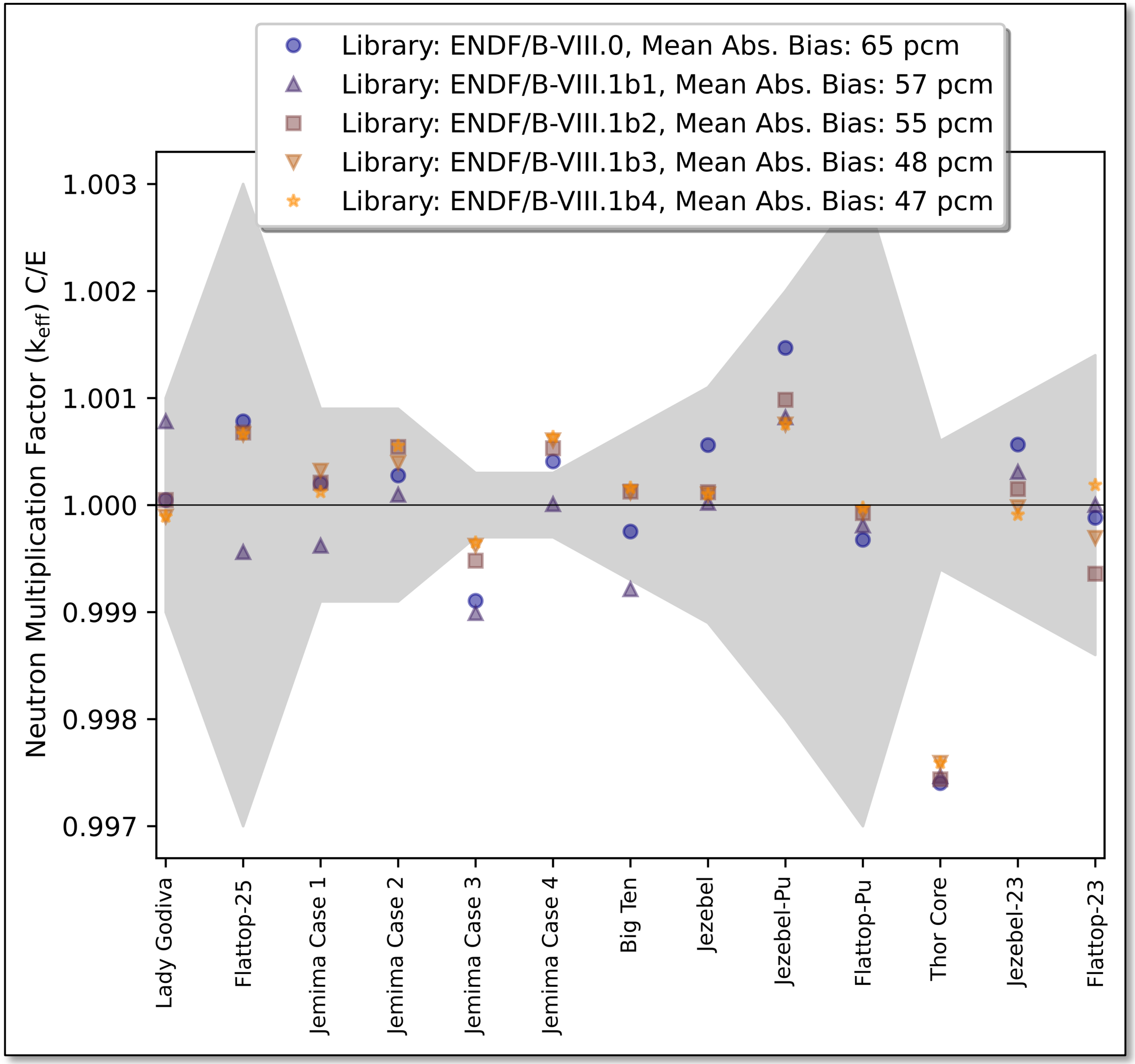






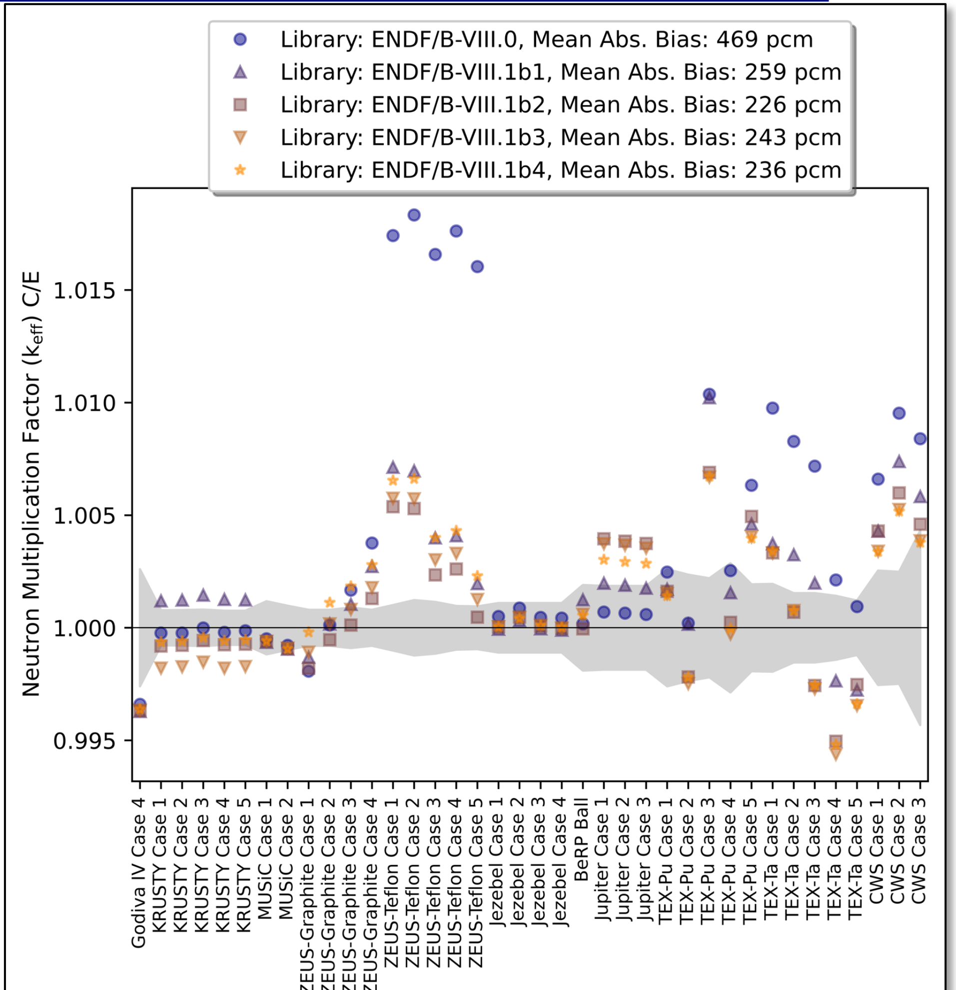
"National Criticality Experiments Research Center (NCERC): The First 10 Years of Operation," *Nuclear Science and Engineering* **195** Supplement 1 (2021)

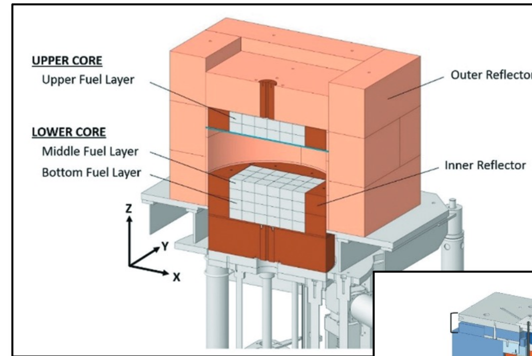
Legacy Benchmark Suite

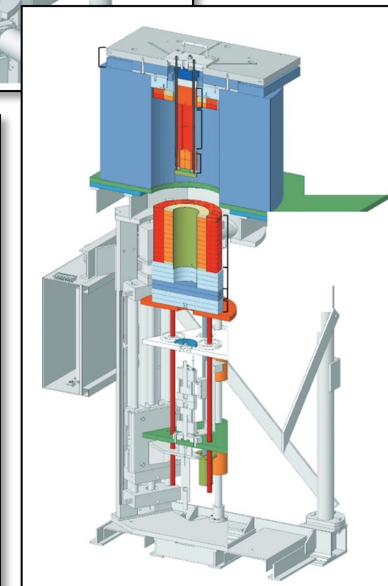


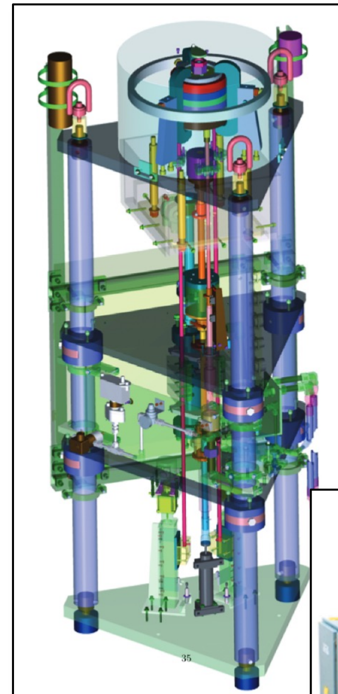
- This suite provides an overview of accuracy for fast/intermediate cross sections of $^{235,238}U$, ^{239}Pu as well as ^{233}U and ^{232}Th
- Good agreement between simulated and experimental criticality for HEU/Pu “bare” systems (i.e., Lady Godiva and Jezebel)
- Flattop-23 bias not necessarily bad… ^{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

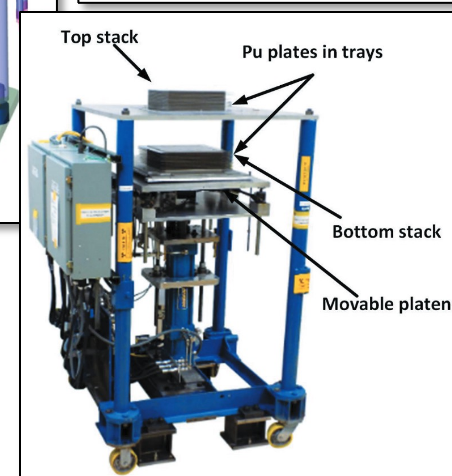
Modern Benchmark Suite











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

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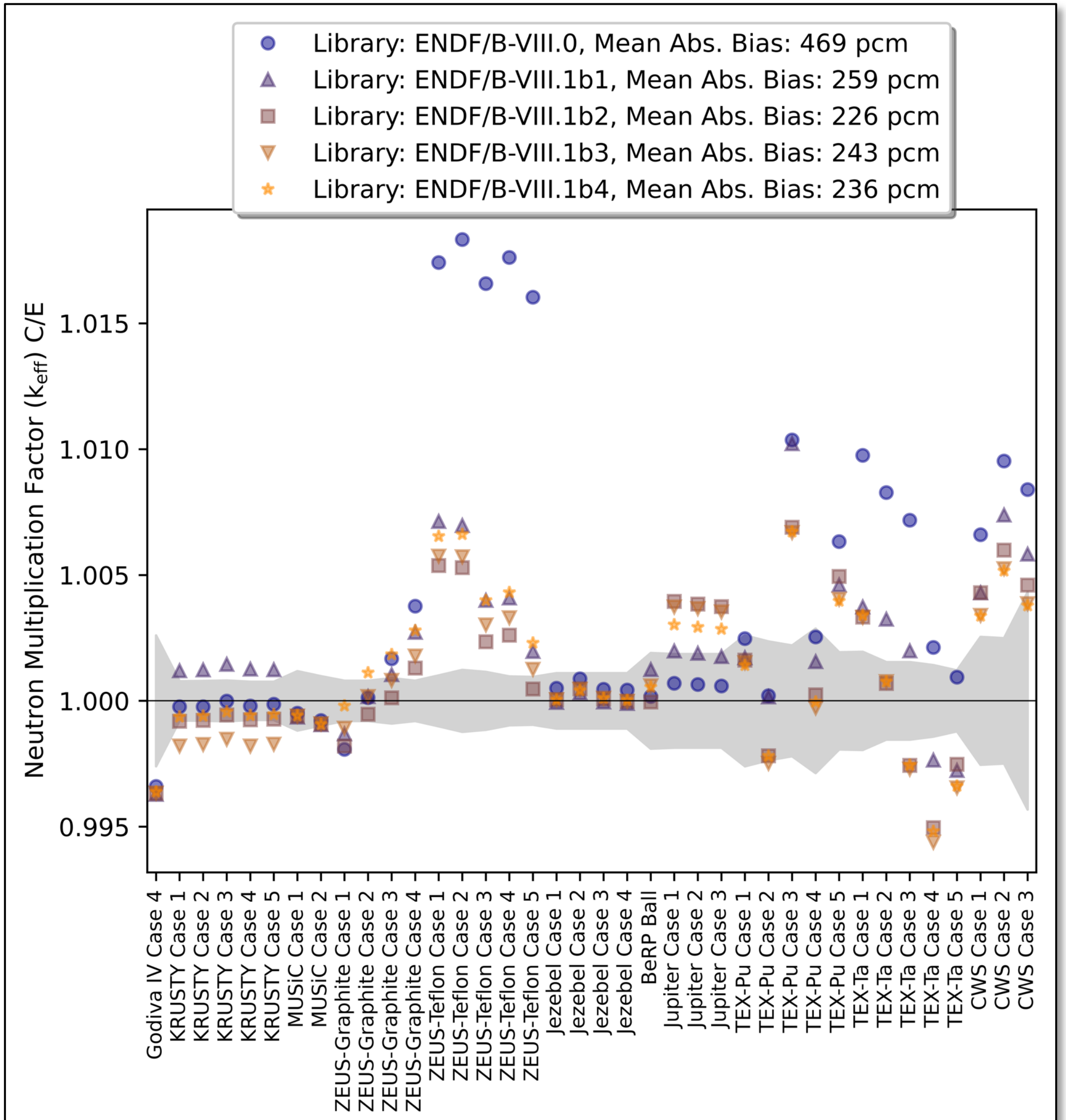
"National Criticality Experiments Research Center (NCERC): The First 10 Years of Operation," *Nuclear Science and Engineering* **195** Supplement 1 (2021)

Modern Benchmark Suite



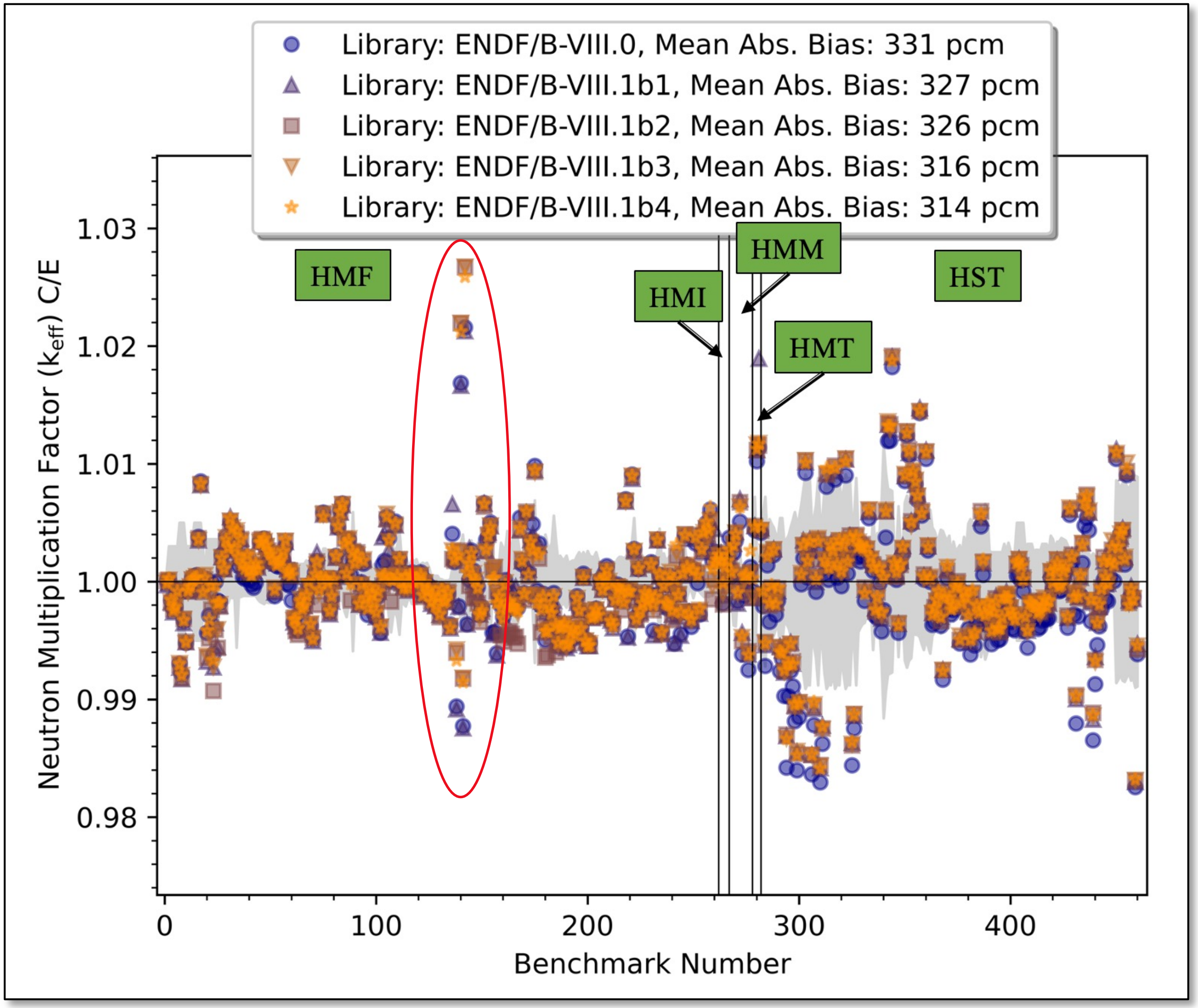
- *NEW* well-characterized experiments recently accepted into ICSBEP Handbook
- This suite provides an overview of accuracy for modern thermal/intermediate/fast cross sections of fuel/moderator/reflector materials
- Significant reduction in bias using ENDF/B-VIII.1 b/c of multiple evaluation updates:

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:

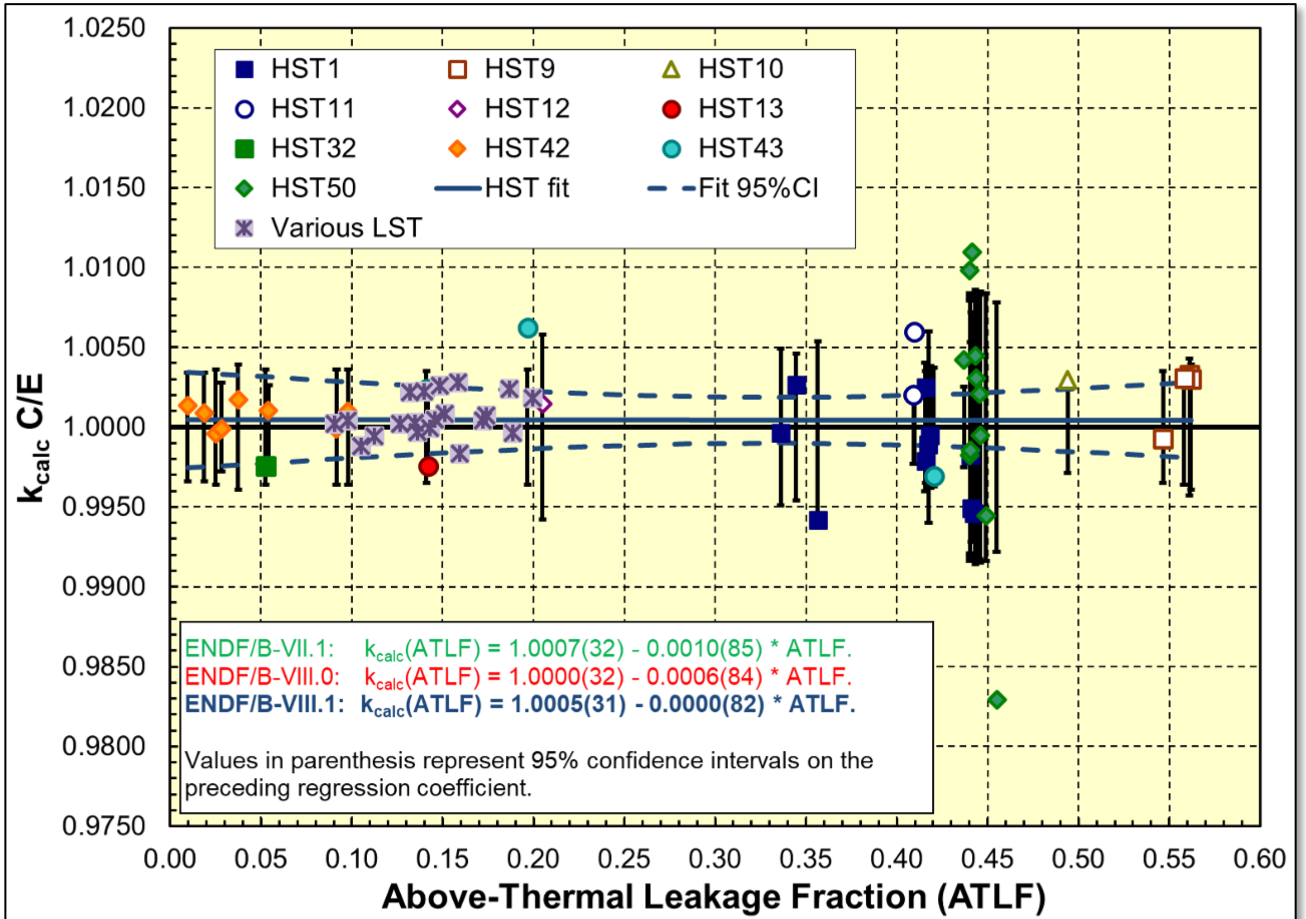
1. ^{9}Be (KRUSTY, BeRP Ball)
2. Pb (Jupiter) – discussions w/ IAEA
3. Ta in thermal energy region/h-poly TSL File/$S(\alpha,\beta)$ (TEX-Ta)

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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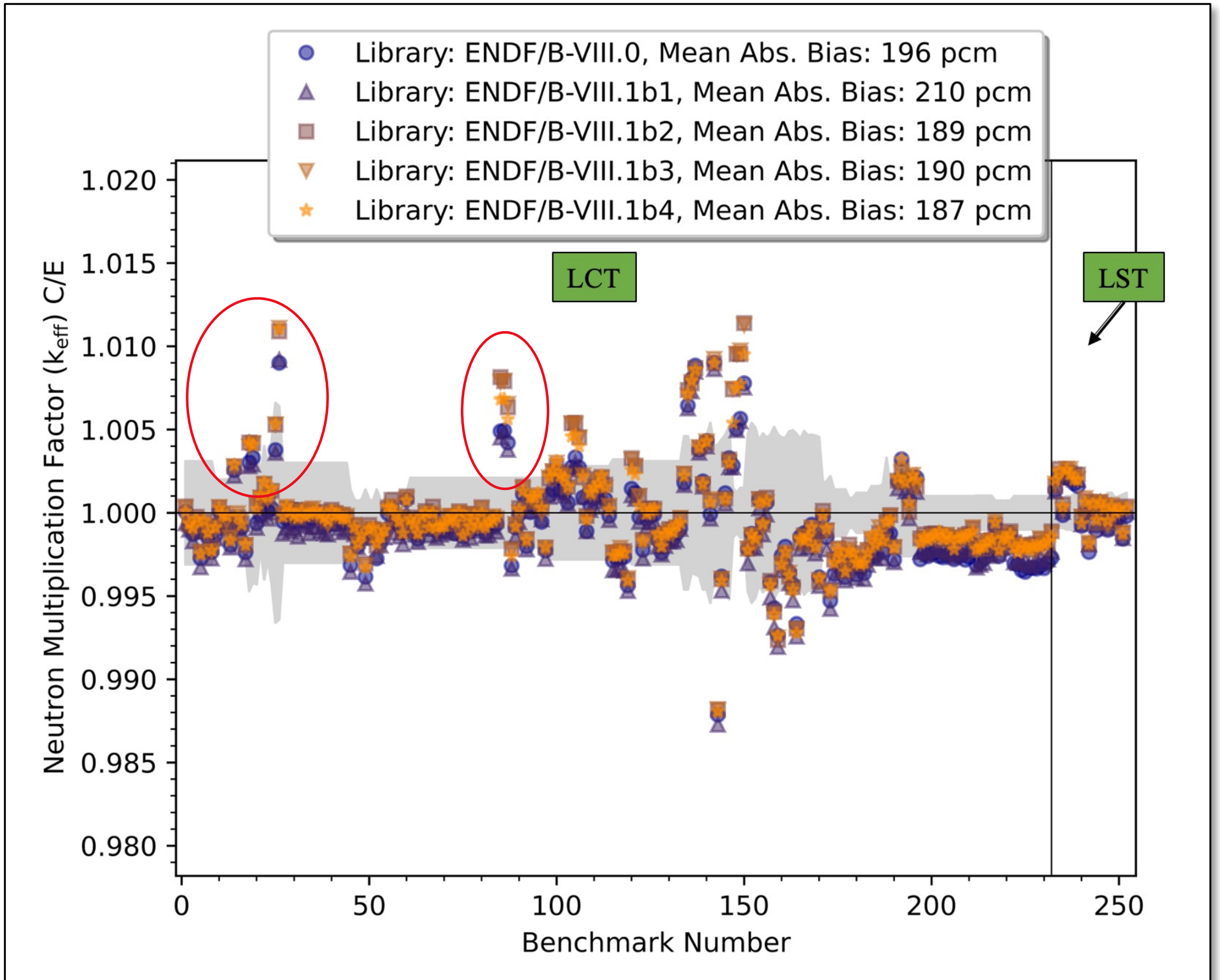
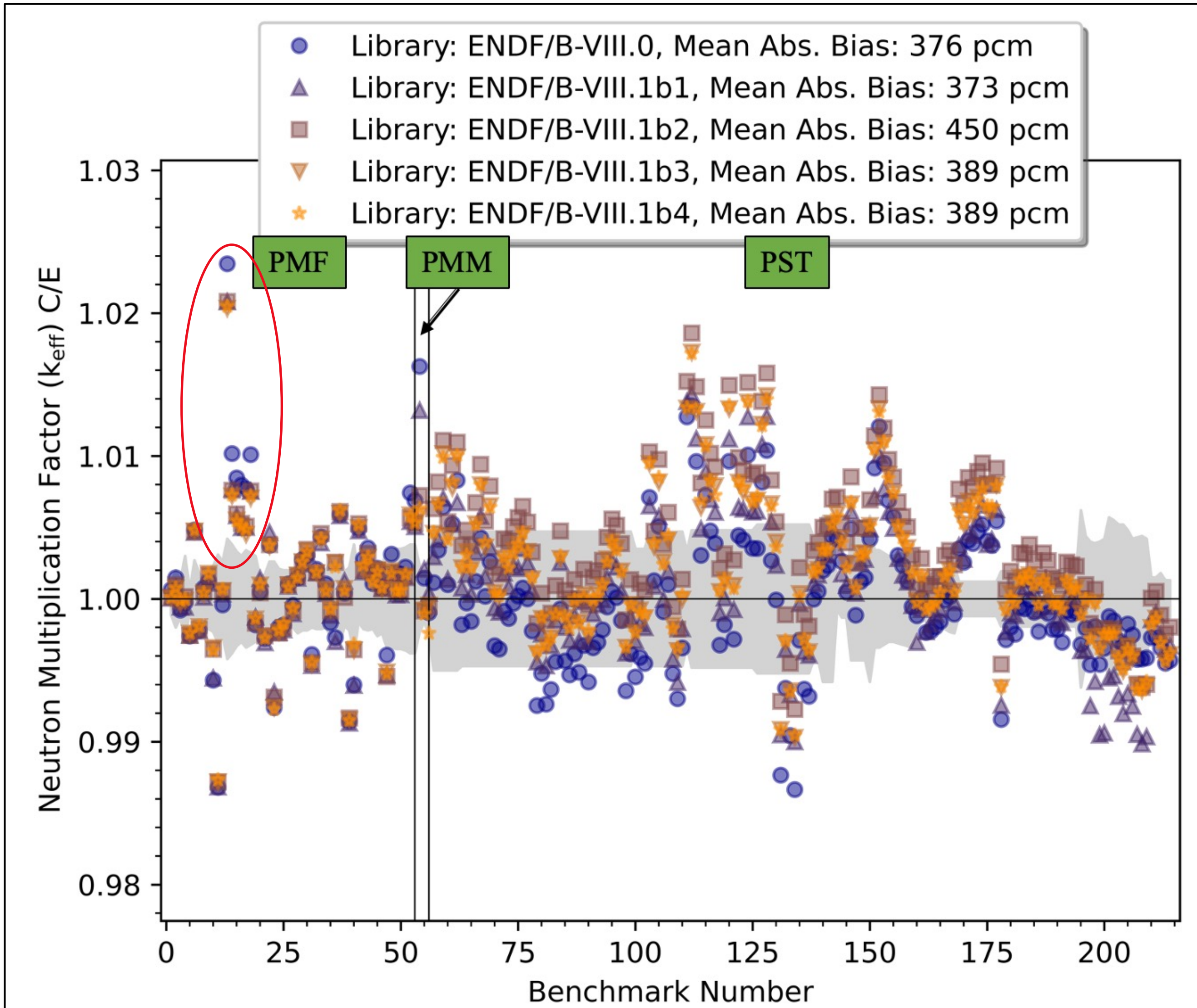
LEU Benchmark Suites



- 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

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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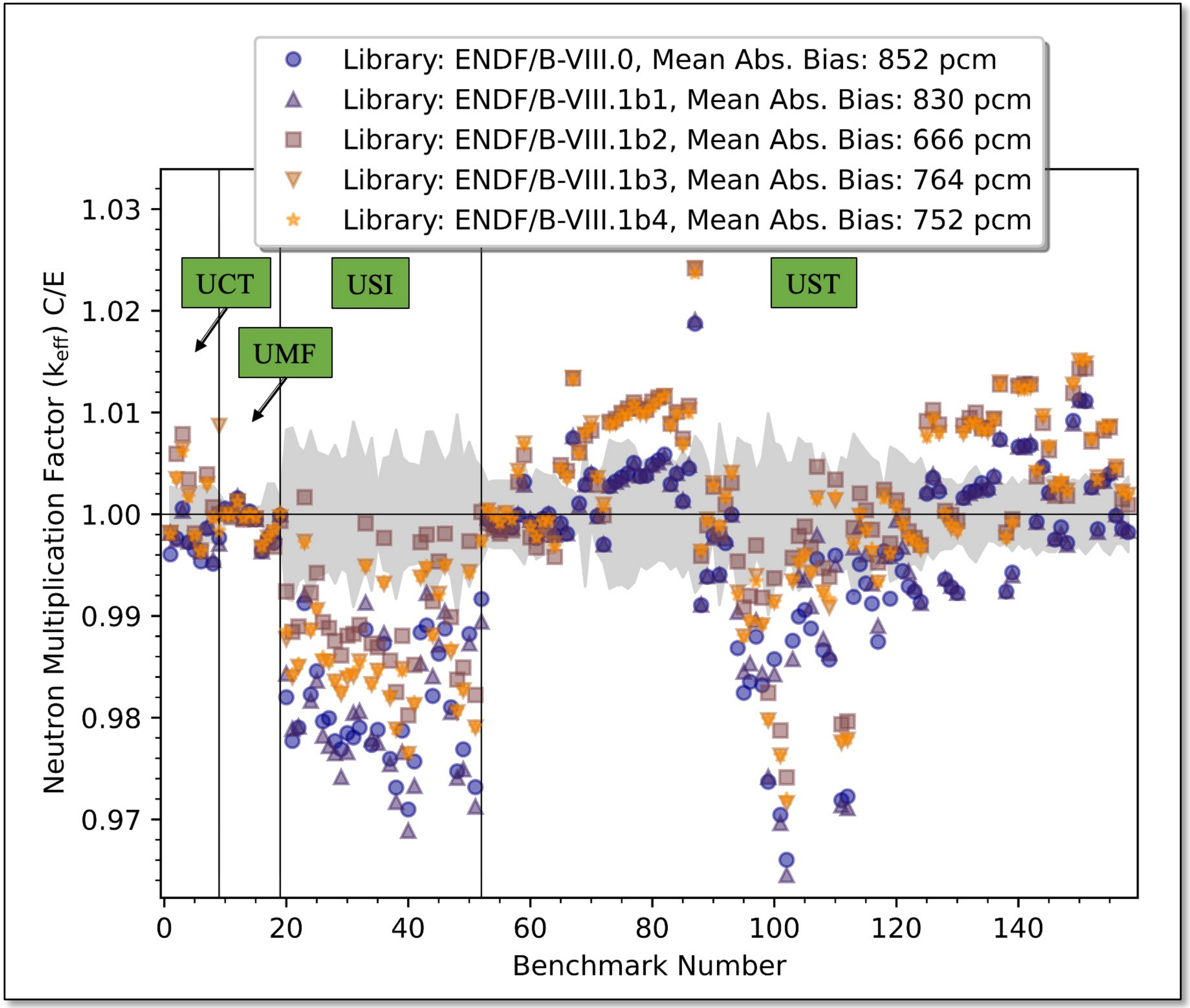
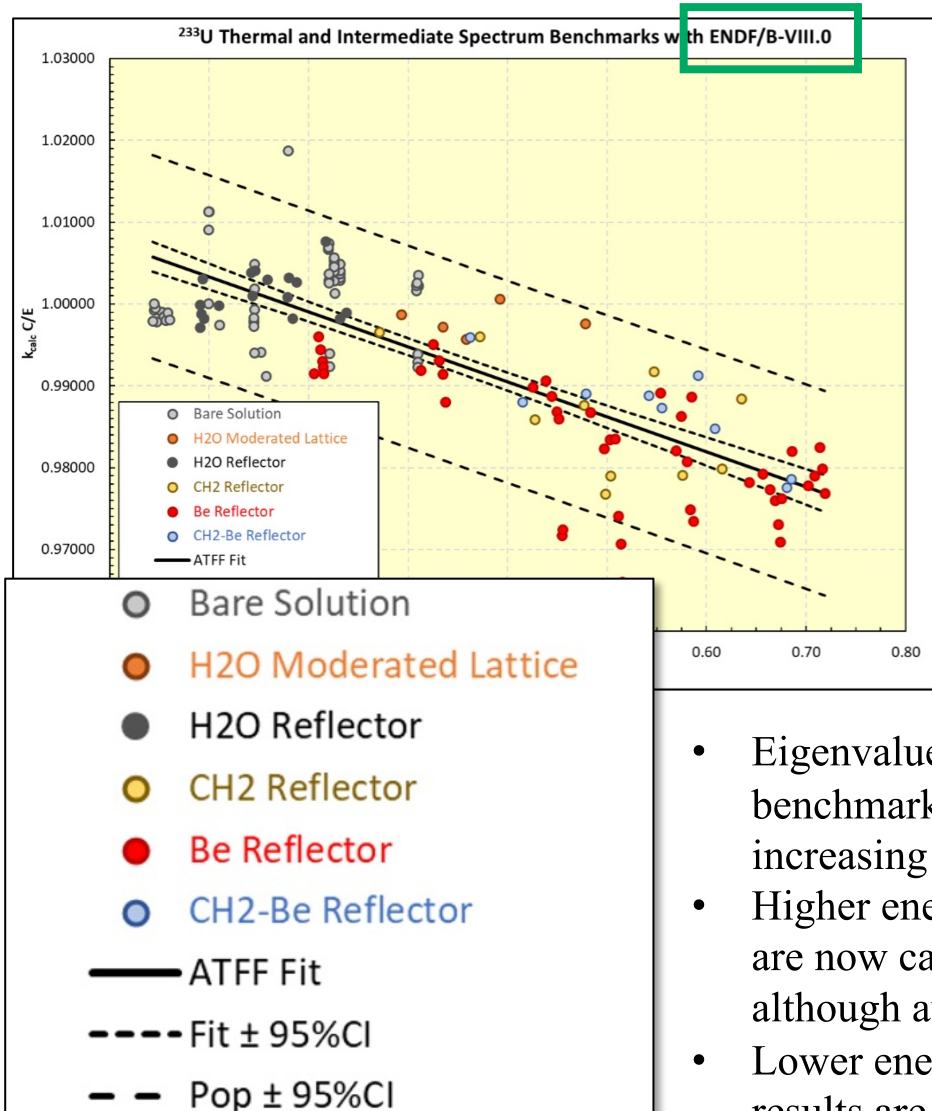
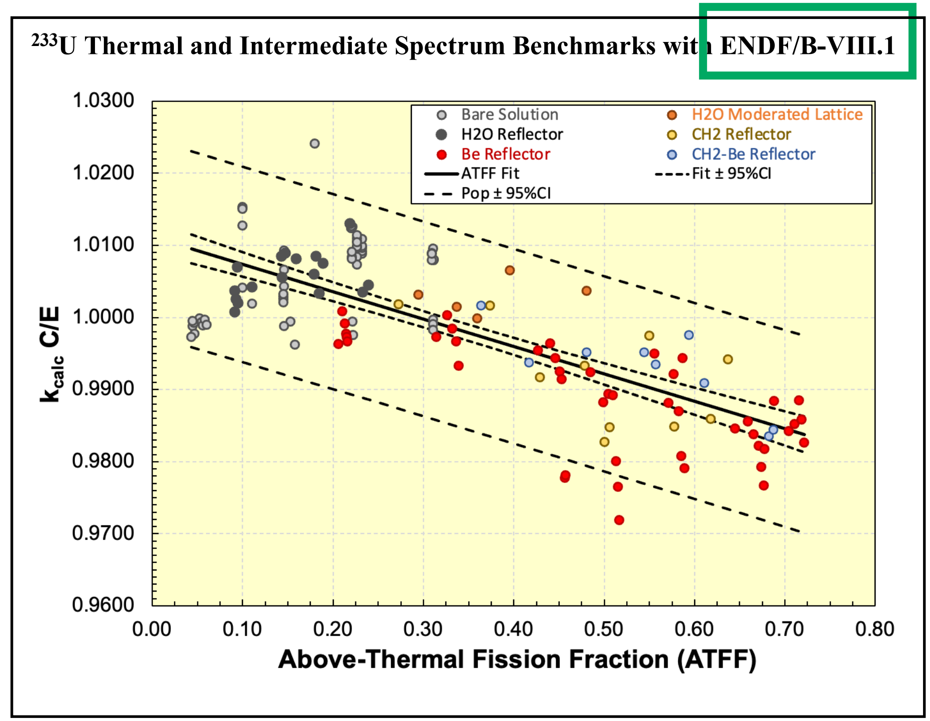
^{233}U Benchmark Suites



- 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…

^{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

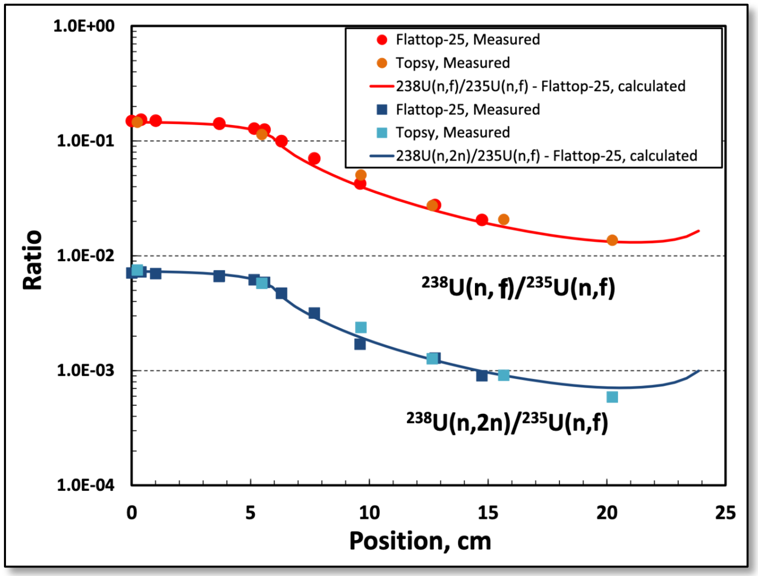
Reaction Rate Ratios

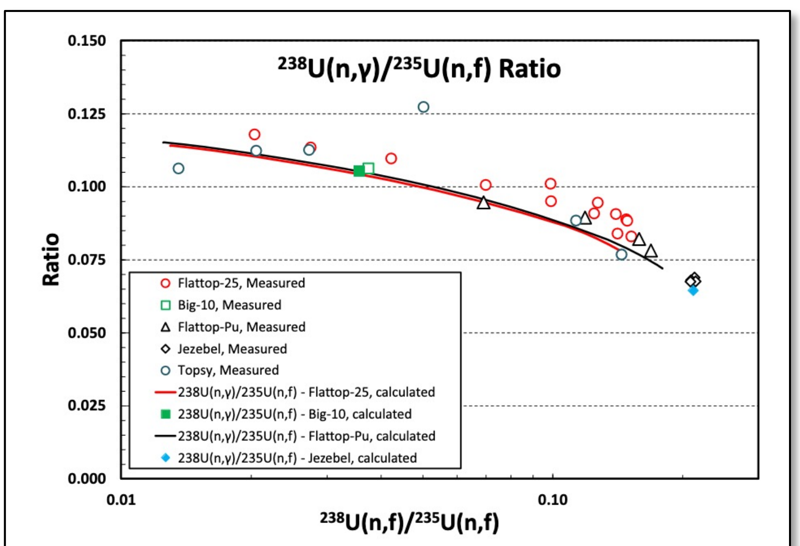
		Calculated Value	
Experiment, Ratio	**Measured Value**	**ENDF/B-VIII.0**	**ENDF/B-VIII.1**
Lady Godiva, $\frac{^{233}\mathrm{U(n,f)}}{^{235}\mathrm{U(n,f)}}$	1.59(3)	1.58	1.58
Lady Godiva, $\frac{^{237}\mathrm{Np(n,f)}}{^{235}\mathrm{U(n,f)}}$	0.8516(120)	0.8311	0.8307
Lady Godiva, $\frac{^{238}\mathrm{U(n,f)}}{^{235}\mathrm{U(n,f)}}$	0.1643(18)	0.1582	0.1580
Lady Godiva, $\frac{^{239}\mathrm{Pu(n,f)}}{^{235}\mathrm{U(n,f)}}$	1.4152(140)	1.3844	1.3832
Big Ten, $\frac{^{238}\mathrm{U(n,f)}}{^{235}\mathrm{U(n,f)}}$	0.0375(9)	0.0357	0.0362
Big Ten, $\frac{^{239}\mathrm{Pu(n,f)}}{^{235}\mathrm{U(n,f)}}$	1.198(28)	1.170	1.170
Jezebel, $\frac{^{233}\mathrm{U(n,f)}}{^{235}\mathrm{U(n,f)}}$	1.578(27)	1.566	1.566
Jezebel, $\frac{^{237}\mathrm{Np(n,f)}}{^{235}\mathrm{U(n,f)}}$	0.9835(14)	0.9768	0.9710
Jezebel, $\frac{^{238}\mathrm{U(n,f)}}{^{235}\mathrm{U(n,f)}}$	0.2133(23)	0.2119	0.2106
Jezebel, $\frac{^{239}\mathrm{Pu(n,f)}}{^{235}\mathrm{U(n,f)}}$	1.4609(130)	1.4273	1.4242
Jezebel, $\frac{^{239}\mathrm{Pu(n,2n)}}{^{239}\mathrm{Pu(n,f)}}$	None	0.0023	0.0022
Jezebel, $\frac{^{239}\mathrm{Pu(n,\gamma)}}{^{239}\mathrm{Pu(n,f)}}$	None	0.0345	0.0359
Jezebel-23, $\frac{^{237}\mathrm{Np(n,f)}}{^{235}\mathrm{U(n,f)}}$	0.997(15)	0.984	0.984
Jezebel-23, $\frac{^{238}\mathrm{U(n,f)}}{^{235}\mathrm{U(n,f)}}$	0.2131(26)	0.2116	0.2110
Flattop-Pu, $\frac{^{237}\mathrm{Np(n,f)}}{^{235}\mathrm{U(n,f)}}$	0.8561(120)	0.8569	0.8513
Flattop-Pu, $\frac{^{238}\mathrm{U(n,f)}}{^{235}\mathrm{U(n,f)}}$	0.1799(20)	0.1793	0.1779
Flattop-Pu, $\frac{^{239}\mathrm{Pu(n,2n)}}{^{239}\mathrm{Pu(n,f)}}$	None	0.0020	0.0019
Flattop-Pu, $\frac{^{239}\mathrm{Pu(n,\gamma)}}{^{239}\mathrm{Pu(n,f)}}$	None	0.0458	0.0468
Flattop-23, $\frac{^{237}\mathrm{Np(n,f)}}{^{235}\mathrm{U(n,f)}}$	0.910(13)	0.900	0.898
Flattop-23, $\frac{^{238}\mathrm{U(n,f)}}{^{235}\mathrm{U(n,f)}}$	0.1916(21)	0.1882	0.1869
Flattop-25, $\frac{^{233}\mathrm{U(n,f)}}{^{235}\mathrm{U(n,f)}}$	1.608(3)	1.578	1.578
Flattop-25, $\frac{^{237}\mathrm{Np(n,f)}}{^{235}\mathrm{U(n,f)}}$	0.7804(100)	0.7716	0.7712
Flattop-25, $\frac{^{238}\mathrm{U(n,f)}}{^{235}\mathrm{U(n,f)}}$	0.1492(16)	0.1445	0.1444
Flattop-25, $\frac{^{239}\mathrm{Pu(n,f)}}{^{235}\mathrm{U(n,f)}}$	1.3847(120)	1.3615	1.3602

- There are not significant changes in the reaction rate ratios from E8.0 to E8.1
- Some change is noticeable in spectral index (i.e., ^{238}U(n,f)/^{235}U(n,f)) for Big Ten

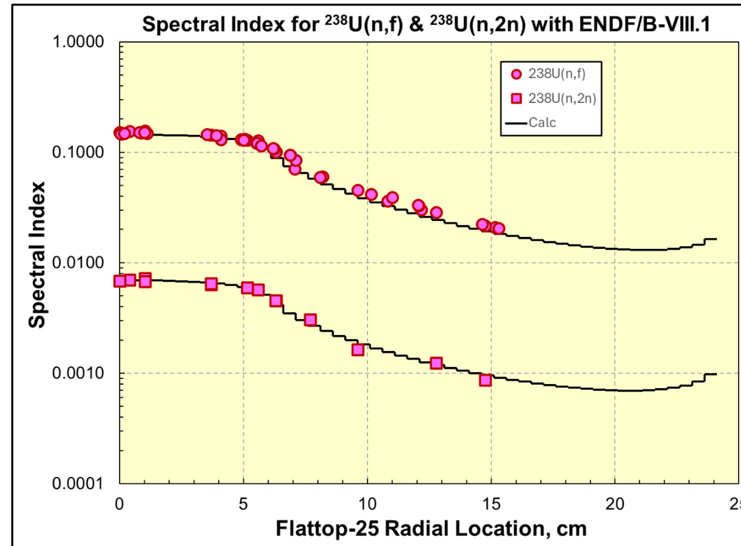
Reaction Rate Ratios

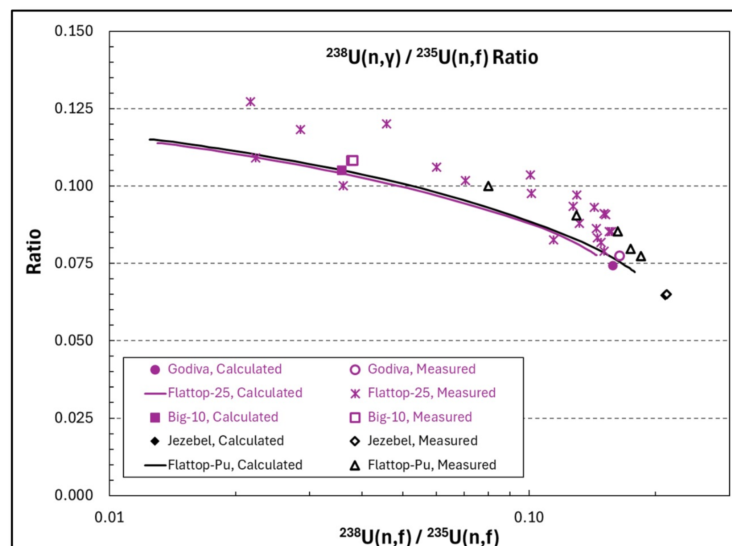
ENDF/B-VIII.0





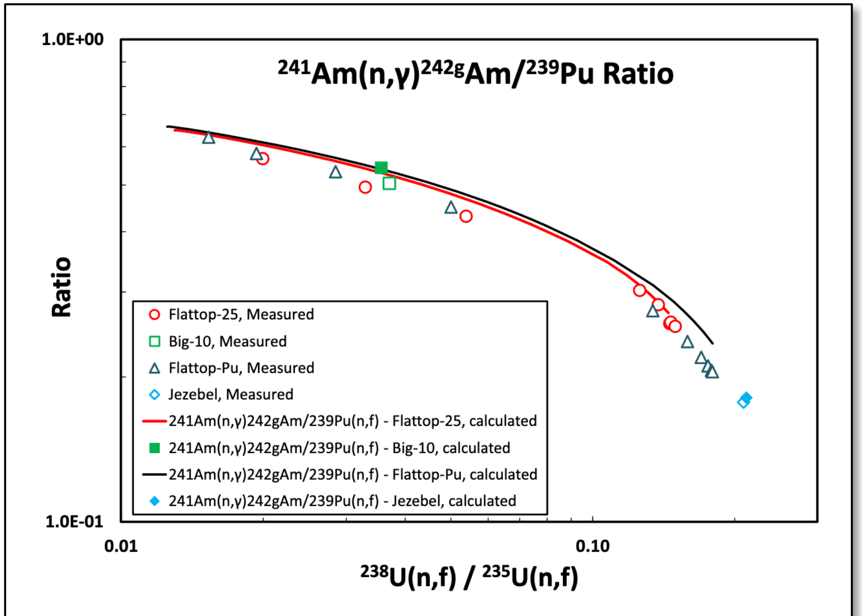
ENDF/B-VIII.1



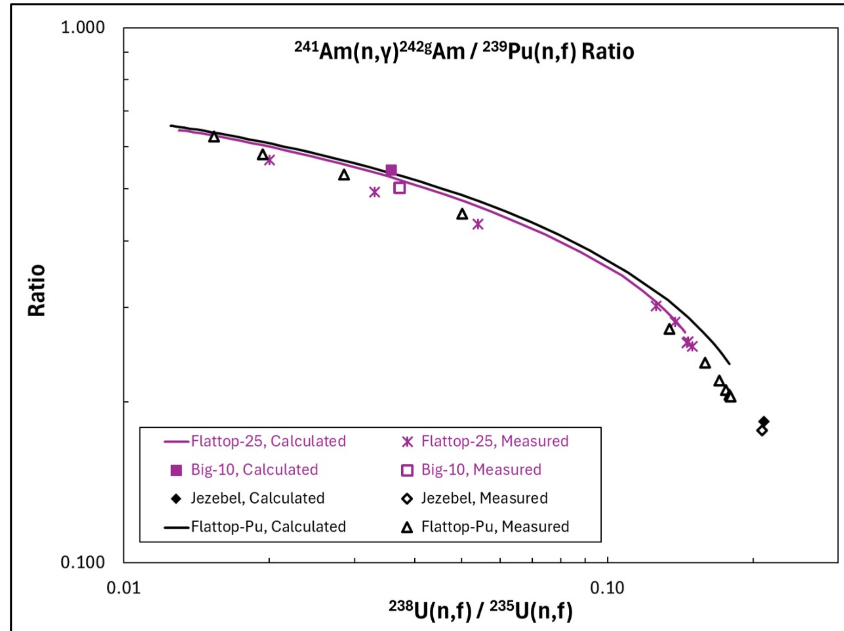


Reaction Rate Ratios

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)

Acknowledgments

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