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Title: Computing upper subcritical limits via Whisper using ENDF/B-VIII.0 nuclear data

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Computing upper subcritical limits via Whisper using ENDF/B-VIII.0 nuclear data

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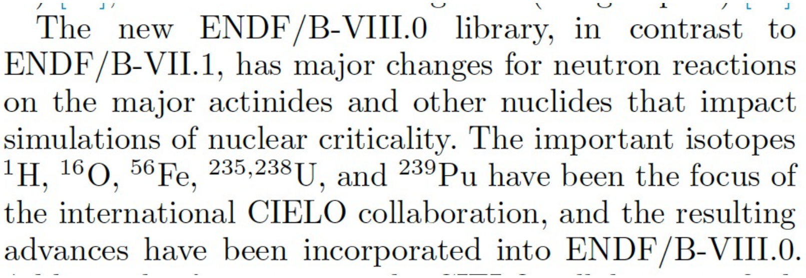
Overview

- Motivation
- Updating benchmark inputs to compute sensitivities
- Obtaining covariances in ACE format
- BLO- vs ENDF/B-VIII.0-calculated USL comparison
- Conclusions
- Future work and outlook

ENDF/B-VIII.0 release provided significant nuclear data improvements relevant to nuclear criticality safety

- Whisper USL calculations are an important component of nuclear criticality safety operations at LANL
- Nuclear data covariances provided with Whisper 1.1 are from BLO project and ENDF/B-VII.0 library
- Making ENDF/B-VIII.0 nuclear data available to Whisper is long overdue
  - USL calculations will include recent advances in important reflector, moderator, and actinide nuclides
  - Providing multiple nuclear data libraries will facilitate V&V for nuclear criticality safety applications



The new ENDF/B-VIII.0 library, in contrast to ENDF/B-VII.1, has major changes for neutron reactions on the major actinides and other nuclides that impact simulations of nuclear criticality. The important isotopes ^{1}H, ^{16}O, ^{56}Fe, ^{235,238}U, and ^{239}Pu have been the focus of the international CIELO collaboration, and the resulting advances have been incorporated into ENDF/B-VIII.0.

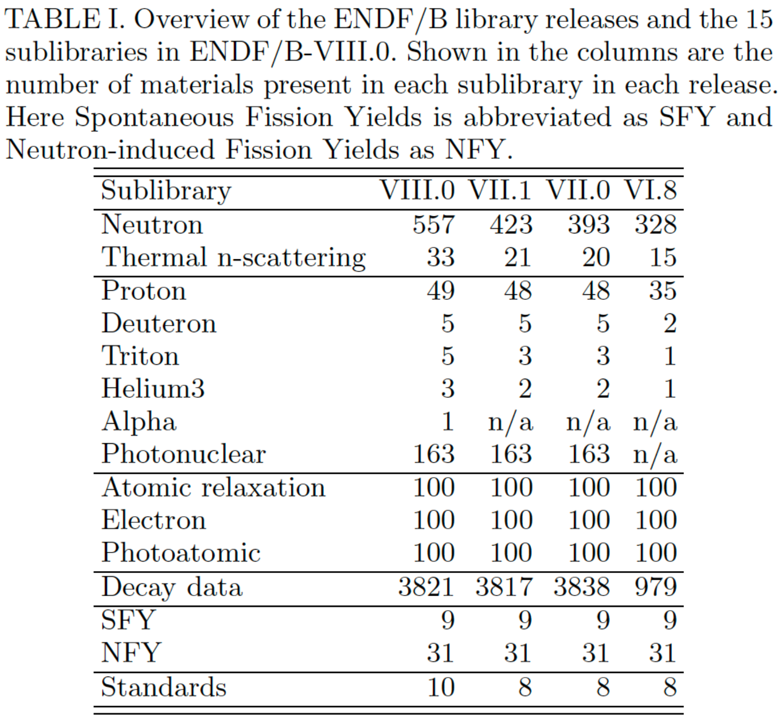


TABLE I. Overview of the ENDF/B library releases and the 15 sublibraries in ENDF/B-VIII.0. Shown in the columns are the number of materials present in each sublibrary in each release. Here Spontaneous Fission Yields is abbreviated as SFY and Neutron-induced Fission Yields as NFY.

Sublibrary	VIII.0	VII.1	VII.0	VI.8
Neutron	557	423	393	328
Thermal n-scattering	33	21	20	15
Proton	49	48	48	35
Deuteron	5	5	5	2
Triton	5	3	3	1
Helium3	3	2	2	1
Alpha	1	n/a	n/a	n/a
Photonuclear	163	163	163	n/a
Atomic relaxation	100	100	100	100
Electron	100	100	100	100
Photoatomic	100	100	100	100
Decay data	3821	3817	3838	979
SFY	9	9	9	9
NFY	31	31	31	31
Standards	10	8	8	8

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, Volume 148, 2018, Pages 1-142, ISSN 0090-3752*

Updating benchmark inputs to compute sensitivities

- Whisper benchmark database is standalone
  - Incorporating revisions and updates must be done manually
  - History and pedigree of changes has been difficult to demonstrate
- Changes to benchmark inputs for ENDF/B-VIII.0 sensitivity calculations were specific to nuclear data
  - Update $S(\alpha, \beta)$ identifiers and ZAIDs
    - lwtr.20t -> h-h2o.40t
    - 94239.80c -> 94239.00c
  - Split elemental carbon via mattool
    - 6000 1. -> 6012 9.893000e-01 6013 1.070000e-02
- “whisper_mcnp.pl” and ”whisper_get_sens.pl” were run for all 1101 updated benchmark inputs

Obtaining covariances in ACE format

- Used Python-based covariance processing tool (Nathan Gibson; XCP-5) to obtain JSON-format covariances
  - Runs NJOY to provide ENDF-format covariances in ERRORR format
  - Parses ERRORR-format covariances into JSON format
  - Only used for MF31, 33, and 35 nuclear data
- Used ACEtk (Wim Haeck; XCP-5) to obtain ACE-format covariances
  - Provides a Python API for parsing and writing ACE files
  - Parses the JSON-format covariances into an ACE format
- Caveats
  - ENDF/B-VIII.0 nuclear data covariance library is incomplete
    - MF33 covariances are available for only about half (250) of all nuclides
    - Current BLO covariances supplement the missing ENDF/B-VIII.0 covariances
  - Covariances obtained via the above tools have not been SQAed
- Used Whisper to recompute the adjusted nuclear data covariances

Definition of Whisper-calculated USL – caculational margin

- Whisper uses non-parametric methods and extreme-value theory to compute a USL

$$USL = 1 - CM - MOS$$

- The calculational margin accounts for the effect of k-eigenvalue bias and uncertainty

$$CM = m + \Delta m, \qquad \Delta m = \max\{0, \beta\}$$

  - m is the bias such that $F(m) = q$, where $q = 0.99$
  - The bias is treated as an extreme-value-distributed random variable

$$F(x) = \prod_i F_i(x), \qquad f(x) = \frac{dF}{dx} = F(x) \sum \frac{f_{i(x)}}{F_i(x)}$$

  - For a particular benchmark i, the bias, variance, weight, and CDF are

$$\beta_i = k_{i,\mathrm{c}} - k_{i.\mathrm{b}}, \qquad \sigma_i^2 = \sigma_{k_{i,\mathrm{c}}}^2 + \sigma_{k_{i,\mathrm{b}}}^2, \qquad w_i = \frac{1}{\sigma_i^2},$$

$$F_i(x) = (1 - w_i) + \frac{w_i}{2}\left[1 + \operatorname{erf}\left(\frac{x + \beta_i}{\sqrt{2\sigma_i^2}}\right)\right]$$

  - The opposite-signed bias is the mean of the extreme-value PDF

$$\beta = -\int_{-\infty}^{\infty} x f(x) = x F(x) \sum \frac{f_{i(x)}}{F_i(x)}$$

Definition of Whisper-calculated USL – margin of subcriticality

- Whisper uses non-parametric methods and extreme-value theory to compute a USL

$$USL = 1 - CM - MOS$$

- The margin of subcriticality accounts for the effect of nuclear data uncertainty, errors in software implementation, and how well the application is represented by the benchmark suite

$$MOS = MOS_{\mathrm{data}} + MOS_{\mathrm{software}} + MOS_{\mathrm{application}}$$

  - $MOS_{\mathrm{application}}$ is determined by the nuclear criticality safety analyst
  - $MOS_{\mathrm{software}} = 0.005$ due to the maturity of the MCNP code k-eigenvalue capability
  - MOS_{data} is determined via GLLS
    - $\chi^2 = [\Delta \boldsymbol{k}]^{\mathrm{T}} \mathbf{C}_{kk} [\Delta \boldsymbol{k}] + [\Delta \boldsymbol{x}]^{\mathrm{T}} \mathbf{C}_{xx} [\Delta \boldsymbol{x}]$
    - $MOS_{\mathrm{data}} = n_\sigma C^{\frac{1}{2}}_{k'k',ii}$, where $n_\sigma = 2.6$ and $C^{\frac{1}{2}}_{k'k',ii}$ is the standard deviation of the i^{th} application after adjusting the nuclear data covariances

Statistical measures for comparing calculated USLs

$USL_{BLO,i}$ and $USL_{E8.0,i}$ are USLs calculated using BLO and ENDF/B-VIII.0 nuclear data, respectively, for the i^{th} benchmark

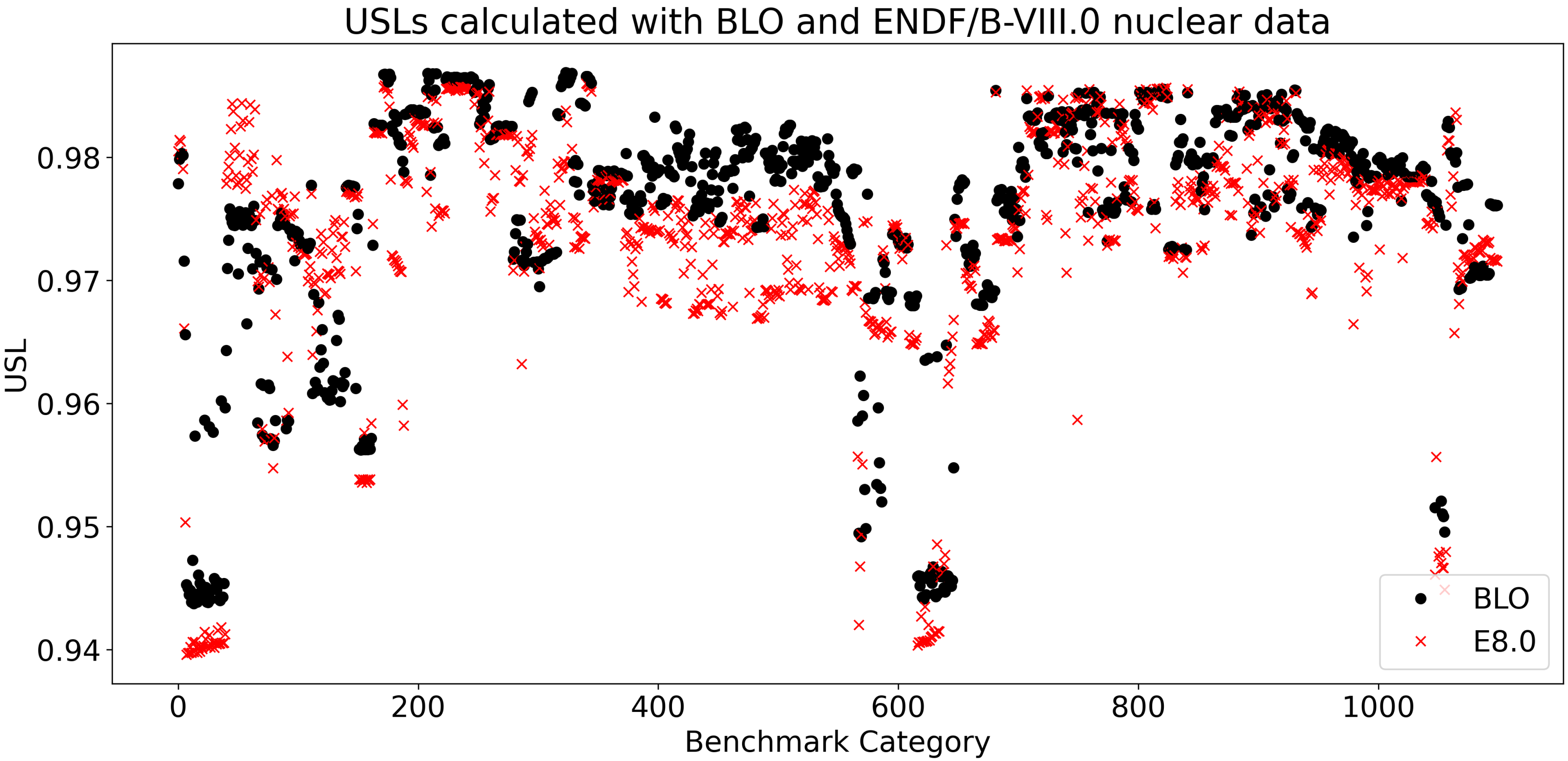
$$R_i = \frac{USL_{E8.0,i} - USL_{BLO,i}}{USL_{BLO,i}}$$

$$\mu = \frac{1}{N}\sum_i R_i$$

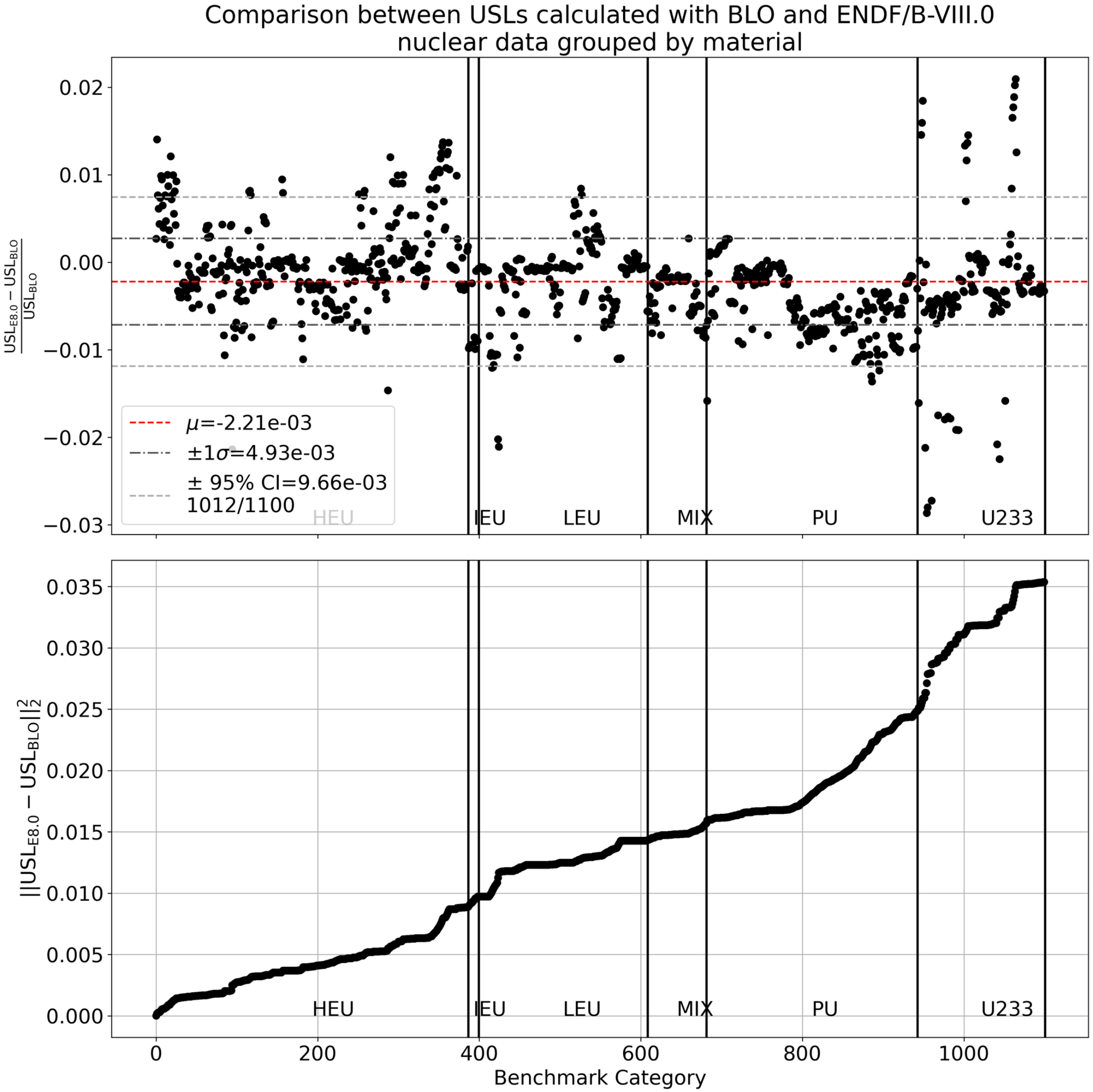
$$1\sigma = \sqrt{\frac{1}{N}\sum_i R_i^2 - \mu^2}$$

$$95\%\ CI = [R_i - 1.96\sigma, R_i + 1.96\sigma]$$

BLO- and ENDF/B-VIII.0-calculated USLs



BLO- vs ENDF/B-VIII.0-calculated USL comparison



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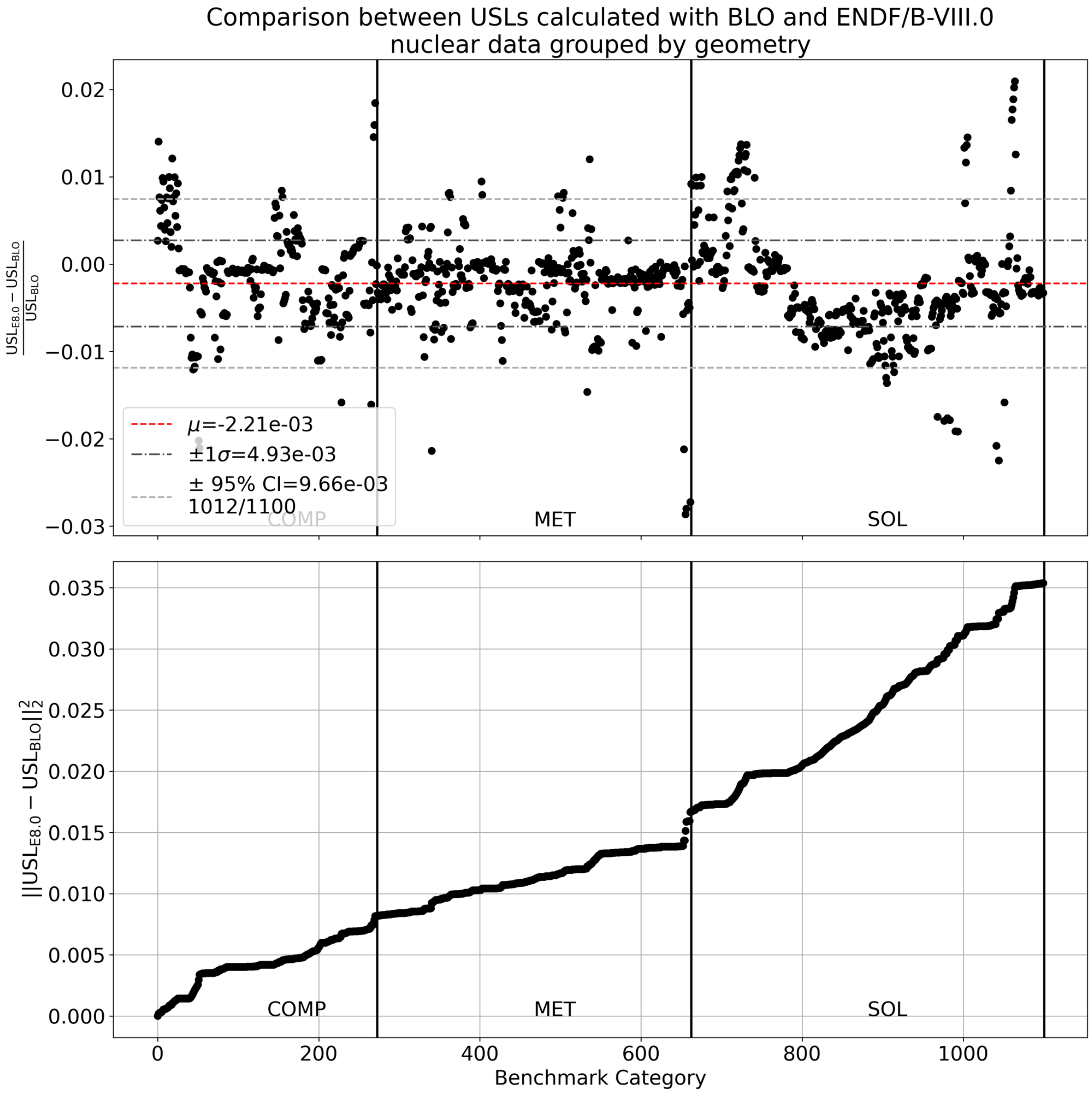

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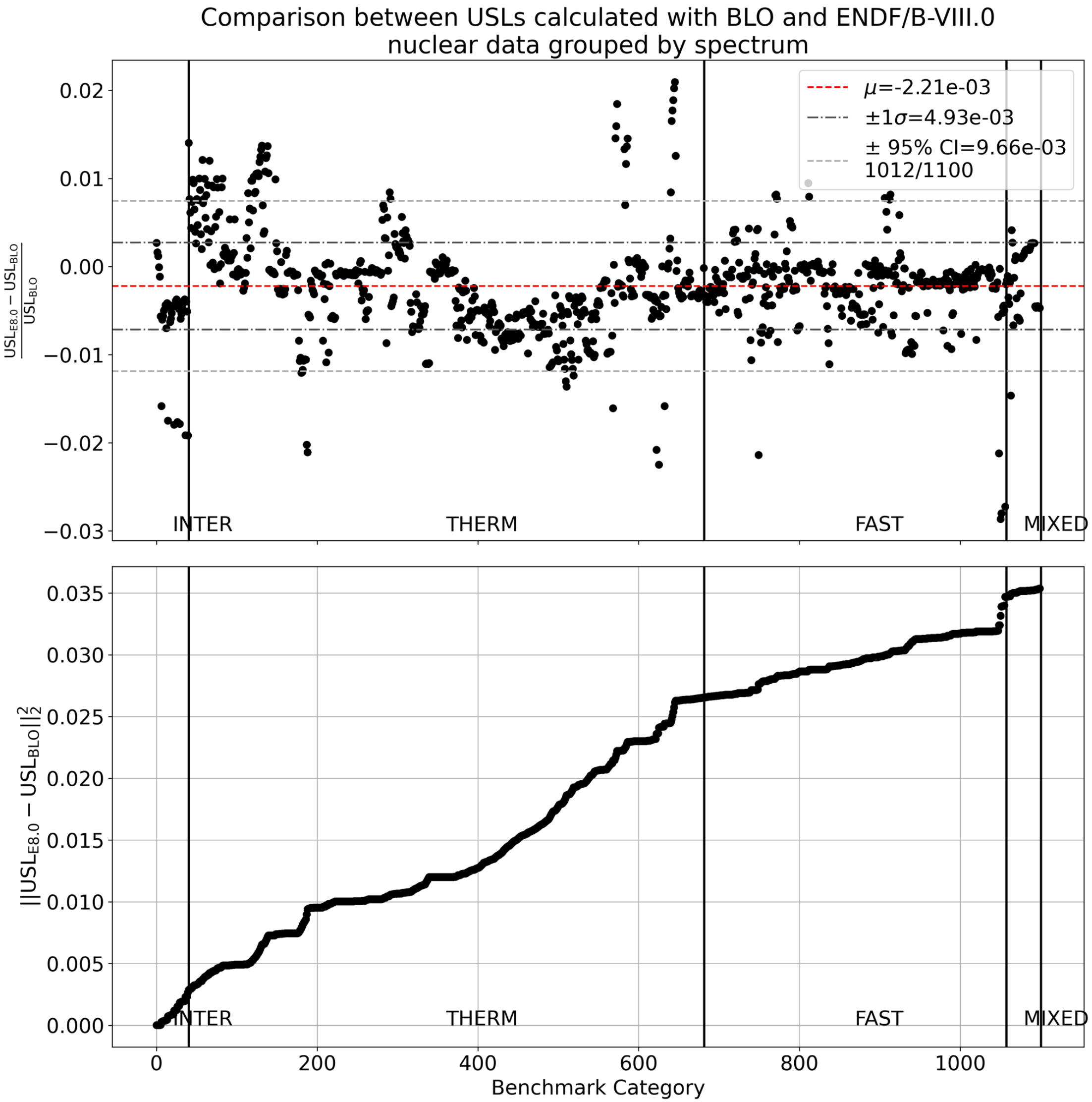

Conclusions

- There are 88 (8%) significant outliers in the set of ENDF/B-VIII.0-calculated USLs
  - Largest number of outliers are various geometries of HEU (40), LEU (6), PU (3), and U233 (18) THERM systems
  - Relatively few outliers have FAST (13), INTER (7), and MIXED (1) spectra

Material	**HEU**					**LEU**	**PU**		**U233**			
Geometry	MET			SOL	COMP	COMP	COMP	SOL	MET	COMP	SOL	
Spectrum	FAST	MIXED	THERM			THERM	INTER	THERM	FAST	THERM		INTER

- ENDF/B-VIII.0 USLs tend to be lower than BLO USLs (μ =-2.21e-03), but the deviation is significant ($1\sigma = 4.93\text{e} - 03$)

Future work and outlook

- The process described here is a significant step toward making several nuclear data libraries available
- Will need to determine if significant changes in USLs calculated with ENDF/B-VIII.0 covariances are reasonable
- Nuclear data covariances need to be provided in ACE format with appropriate SQA procedures
- Benchmark inputs need to be connected to version-controlled database
  - ICSBEP
  - LABS