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Whisper updates

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Overview

- Completed
  - Compared USLs calculated using existing BLO and new ENDF/B-VIII.0 nuclear data
  - Transitioned from Makefile to CMake build system
- In progress
  - Investigating erroneous ENDF/B-VIII.0 U-235 covariance data
  - Connecting the MCNP verification and validation framework and Whisper
- Planned
  - Modularize components of Whisper
  - Implement method[1] for computing c_k's accounting for benchmark correlations
- Conclusions

1. B. C. Kiedrowski, "Uniformly Ordered Binary Decision Algorithm for Benchmark Experiment Correlations in Whisper Validation", Transactions of the American Nuclear Society, 124:1, 379-382, June 2021

Completed

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 the 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 covariance 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.

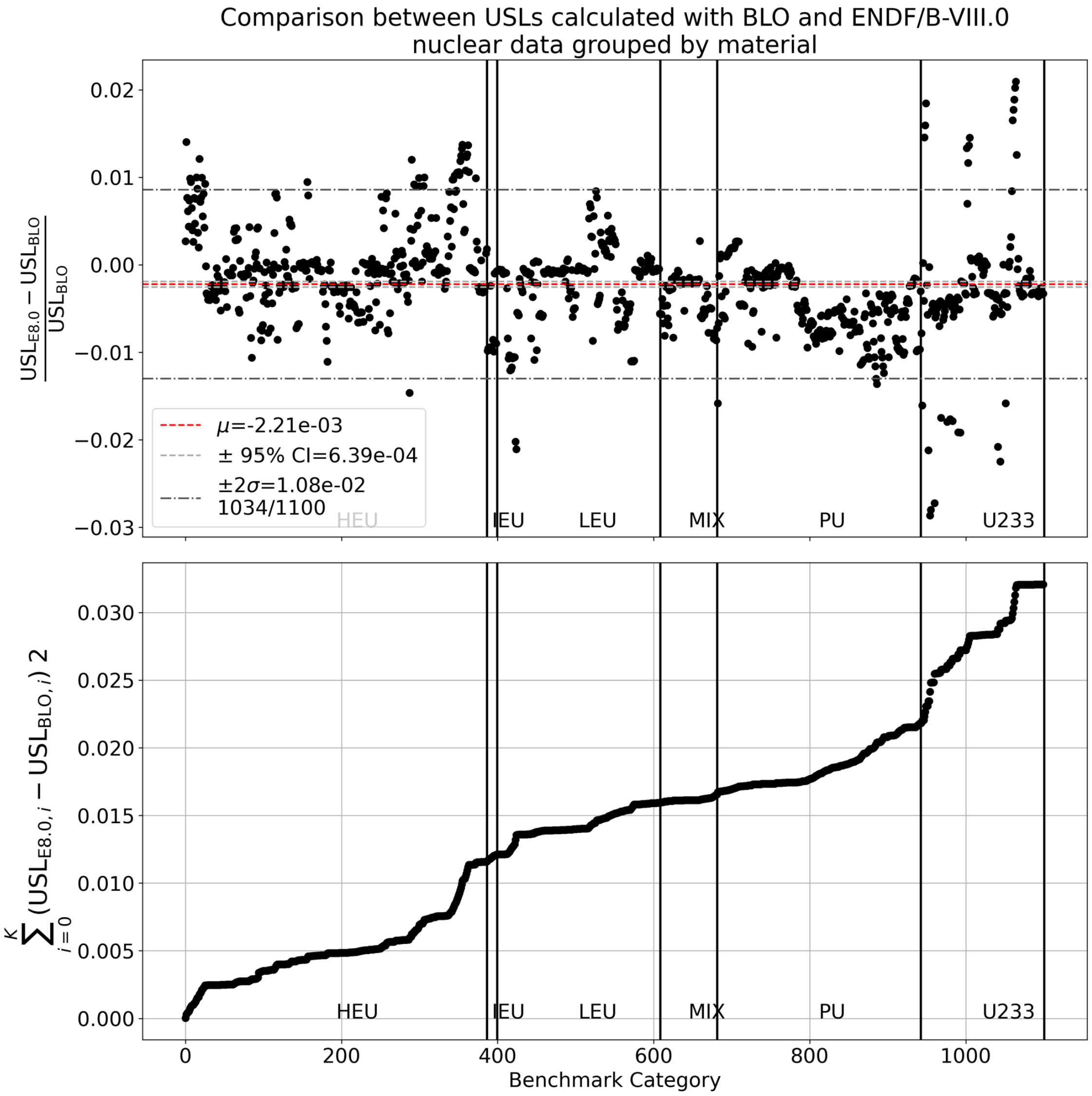
Sublibrary	VIII.0	VII.1	VII.0	VI.8
Neutron	557	423	393	328
Thermal n-scattering	33	21	20	15
Proton	49	48	48	35
Deuteron	5	5	5	2
Triton	5	3	3	1
Helium3	3	2	2	1
Alpha	1	n/a	n/a	n/a
Photonuclear	163	163	163	n/a
Atomic relaxation	100	100	100	100
Electron	100	100	100	100
Photoatomic	100	100	100	100
Decay 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*

Obtaining covariances in ACE format

- Used Python-based covariance processing tool (Nathan Gibson; XCP-5) that invoked NJOY to obtain JSON-format covariances
- Used CovVal (Denise Neudecker; XCP-5) to check JSON-format covariances for errors or unrealistic values
- Used ACEtk (Wim Haeck; XCP-5) to convert JSON-format covariances into ACE-format
- Caveats
  - ENDF/B-VIII.0 provides nuclear data covariances for only half (250) of all available nuclides
  - Covariances obtained via the above tools will not be distributed until they have been SQA'd
- Used Whisper benchmark suite to recompute the adjusted nuclear data covariances
- This process demonstrates progress toward a more cohesive framework for providing nuclear data covariances to Whisper

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



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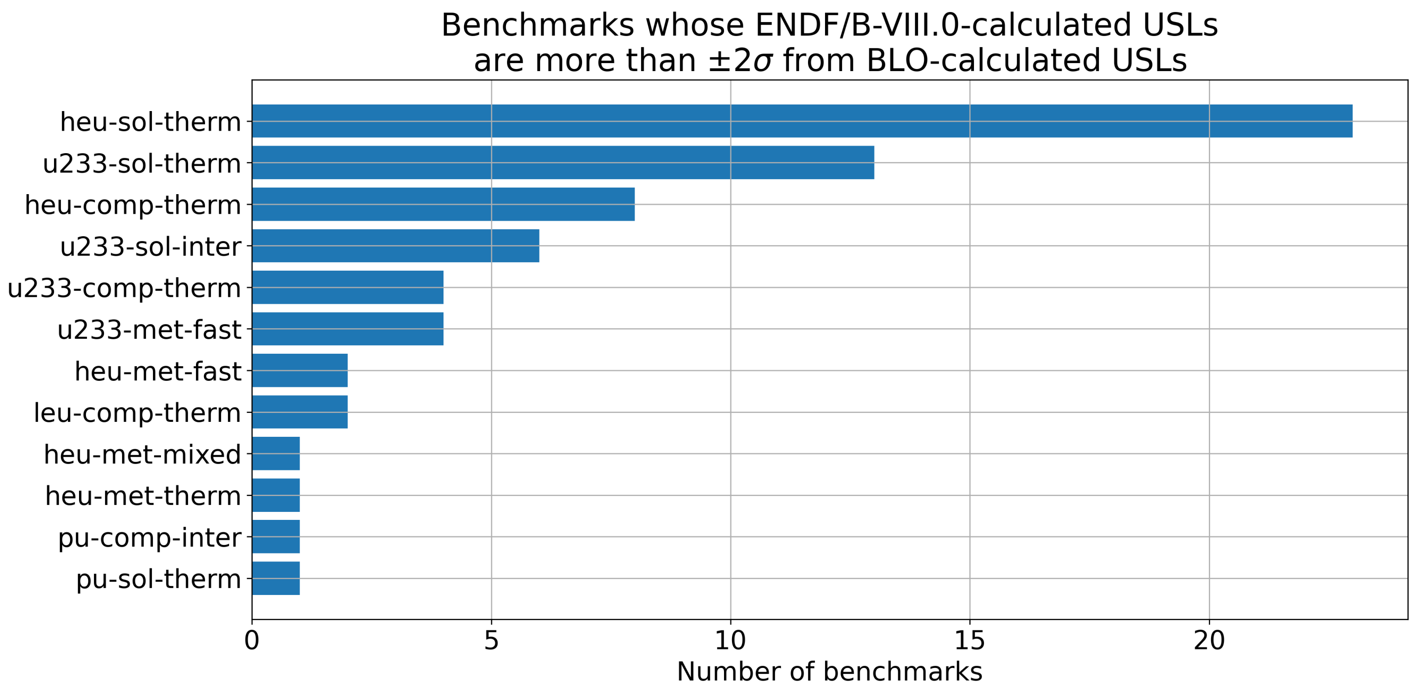
There are a statistically significant number of outliers when comparing BLO- vs ENDF/B-VIII.0-calculated USLs

- 66/1100 (6%) benchmarks are outside $\pm 2\sigma$



- ENDF/B-VIII.0 USLs tend to be lower than BLO USLs ($\mu = -2.21 \times 10^{-3}$) with high confidence ($95\%\ CI = 6.39 \times 10^{-4}$), but the standard deviation is significant ($1\sigma = 5.04\text{x}10^{-3}$)

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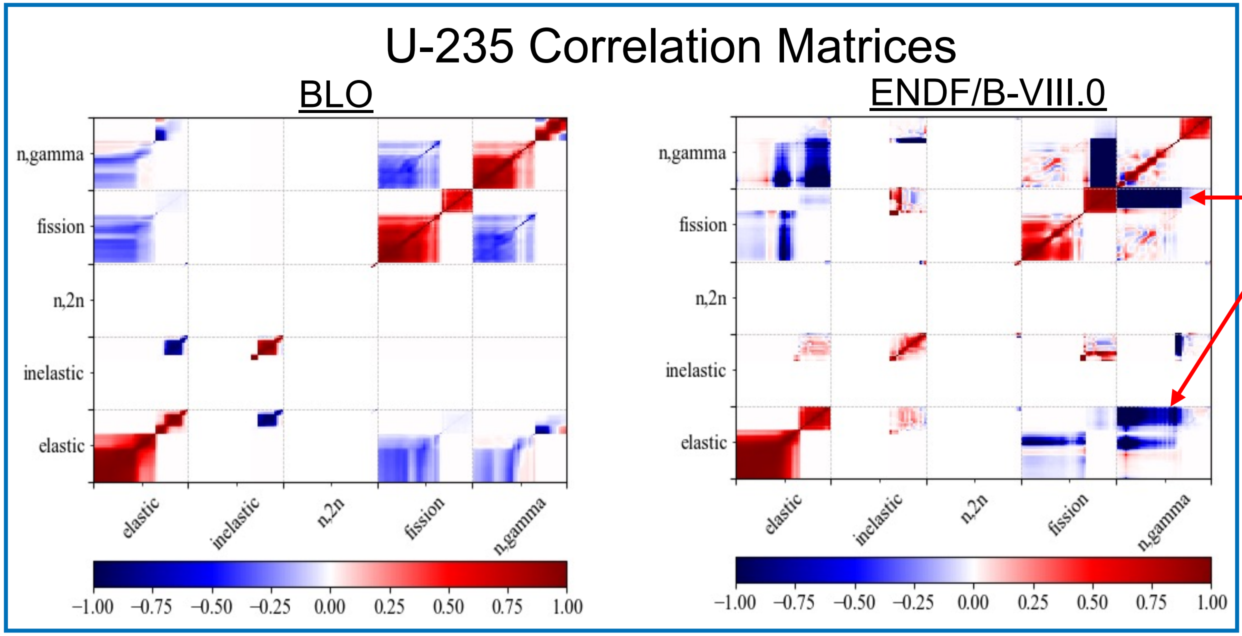
Transitioned from Makefile to CMake build system

- Generates build files automatically and handles compiling and installation on different systems
- Provides robust framework for testing
- Gives greater control over build and test options
- Currently reproduces previous Makefile but will make improvements easier
  - Support a greater number of compilers and operating systems
  - Easier to integrate library dependencies
  - Finer control over testing
- Promotes better consistency across the MCNP team's projects, as MCNP6 has already transitioned to a CMake build system

In progress

Non-physical correlations identified in ENDF/B-VIII.0 U-235 covariance data

- Processed ENDF/B-VIII.0 covariance matrices for Whisper
- The calculated c_k between Godiva and Krusty benchmarks
  - $c_{k,BLO} = 0.91911$ ✓, $c_{k,ENDF/B\text{-}VIII.0} = 1.08511$ ✗



These correlations between low-energy n,gamma and high energy fission and elastic scattering are mathematically unrealistic ($\rho \ll -1$).

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Refactoring V&V Python tool to compute sensitivities required by Whisper

- Improving interface
  - Run via command line or JSON file
  - Generate template for doing a default run
  - Obtain machine-specific arguments
  - Option to run inputs as user-defined suite type

```
:~/projects/vnvstats_runs% python -m vnvstats criticality -h

The simplest way to do a run is to first generate an "arguments.template.json" file:

    `python -m vnvstats criticality --generate`

After defining the "-suite_dir" and "-run_dir" fields and customizing
any other fields, do:

    `python -m vnvstats criticality -args_path arguments.template.json`
```

- Preparing VnVstats to be the engine for the MCNP runs required by Whisper

Planned

Modularizing components of Whisper

- Extract Whisper components into individual library files
- Provide Python API for running desired Whisper components
- Merge Whisper and Whisper-tk capabilities
- Allow users to
  - Run specific components of Whisper (e.g. do only the nuclear data adjustment)
  - Compute USLs with different methodologies (e.g. parametric vs non-parametric)
  - Specify nuclear data covariances from different libraries (e.g. BLO vs ENDF/B-VIII.0)

Implement method for computing c_k's that account for benchmark correlations

- Whisper currently computes c_k's for an application without considering benchmark correlations
- Benchmarks that are highly correlated provide lower information content than those that are uncorrelated
- B. Kiedrowski's patch implements[1] the Uniformly Ordered Binary Decision algorithm
  - Identify and randomly order clusters of highly-correlated benchmarks
  - Decide if
    - A pair of benchmarks will be included together
    - If the pair of benchmarks are redundant
  - Adjust included benchmark weights to account for redundant information
- Implementing this patch into production will make available benchmark correlations immediately useful.

Table I. HEU-SOL-THERM-001 Correlation Matrix

	HST-001-001	HST-001-002	HST-001-003	HST-001-004	HST-001-005	HST-001-006	HST-001-007	HST-001-008
HST-001-001	1.00	0.47	0.46	0.44	0.42	0.42	0.46	0.57
HST-001-002	0.47	1.00	0.42	0.58	0.42	0.42	0.41	0.44
HST-001-003	0.46	0.42	1.00	0.46	0.43	0.43	0.46	0.46
HST-001-004	0.44	0.58	0.46	1.00	0.44	0.42	0.42	0.44
HST-001-005	0.42	0.42	0.43	0.44	1.00	0.54	0.48	0.47
HST-001-006	0.42	0.42	0.43	0.42	0.54	1.00	0.48	0.47
HST-001-007	0.46	0.41	0.46	0.42	0.48	0.48	1.00	0.51
HST-001-008	0.57	0.44	0.46	0.44	0.47	0.47	0.51	1.00

Table II. Results for HEU Solution Application Cases

Application	# (orig.)	# (corr.)	$\sum w_i$	Δm
HST-001-001	55	68	34.5	0.0022
HST-001-002	52	62	31.0	0.0002
HST-001-003	49	69	34.7	0.0023
HST-001-004	53	66	31.2	0.0002
HST-001-005	41	72	34.1	0.0040
HST-001-006	43	73	34.0	0.0040
HST-001-007	49	69	34.6	0.0024
HST-001-008	51	69	34.6	0.0020
HST-001-009	53	66	31.4	0.0002
HST-001-010	41	72	34.2	0.0049

1. B. C. Kiedrowski, "Uniformly Ordered Binary Decision Algorithm for Benchmark Experiment Correlations in Whisper Validation", Transactions of the American Nuclear Society, 124:1, 379-382, June 2021

Conclusions

- USLs calculated with ENDF/B-VIII.0 have significant deviations with respect to those computed with BLO, which warrants further investigation
- Moving to a CMake build system allows for greater flexibility in build and testing options
- Non-physical correlations in the ENDF/B-VIII.0 U-235 covariances have had a significant impact in recent Whisper c_k's calculations for LANL internal studies
- Letting VnVstats compute sensitivities for Whisper improves interconnectivity between our tools
- Modularizing components of Whisper will make it easier to change what method gets used or only run specific capabilities
- Implementing the Uniformly Ordered Binary Decision algorithm will allow for USL calculations that account for benchmark correlations

Future work and outlook

- Provide new nuclear data covariances in future Whisper release after appropriate SQA process
- Look for other opportunities to connect Whisper to other tools that the MCNP team provides
- Benchmark and nuclear data inputs to Whisper need to be connected to databases that are subject to review and version control
  - Benchmark inputs pulled from ICSBEP and/or LABS databases
  - Nuclear data covariances that are in ACE format with appropriate SQA procedures
- The LABS project is already subject to these constraints and provides an example for what other databases can do

Acknowledgements

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Backup slides

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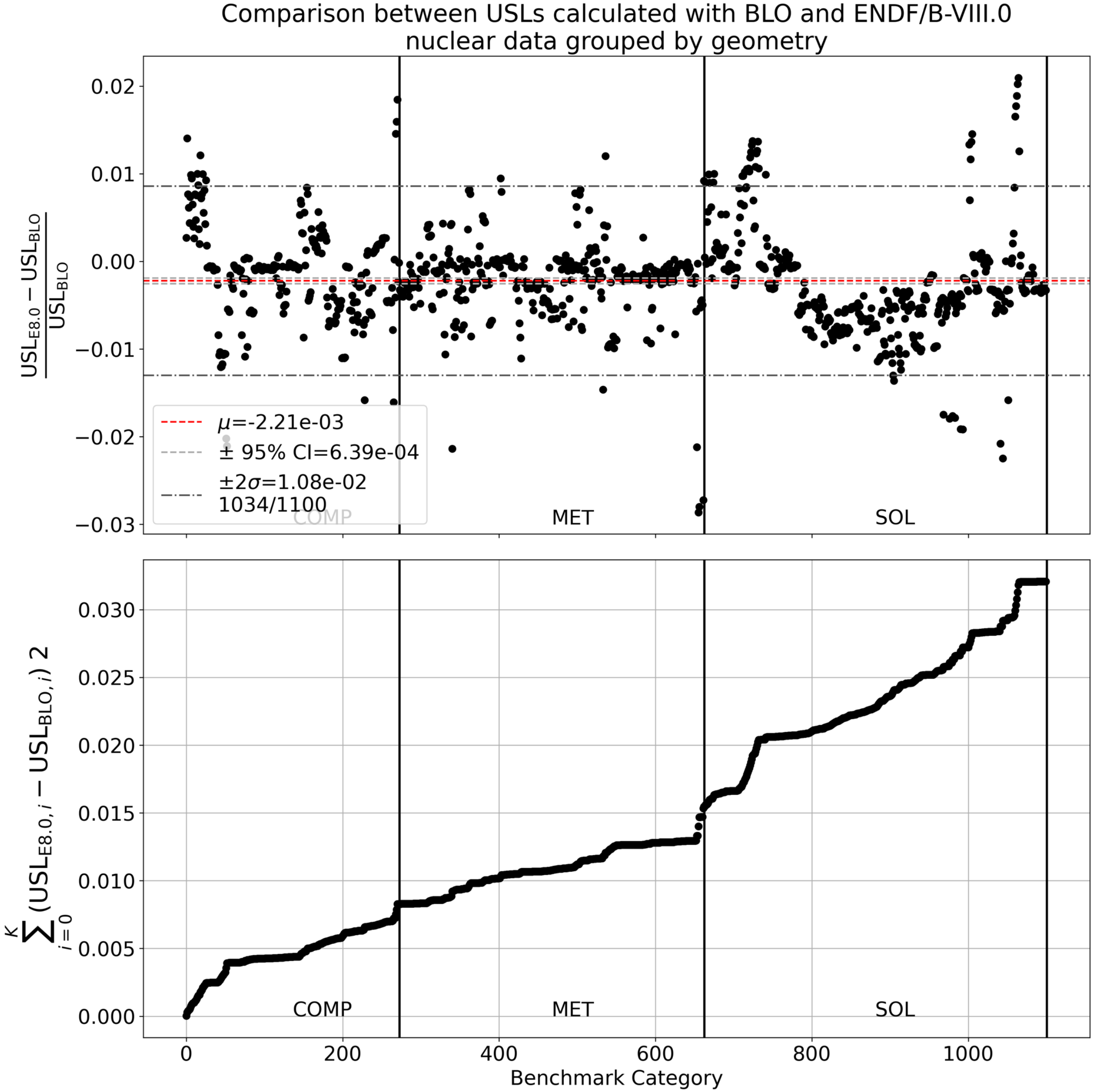
BLO- vs ENDF/B-VIII.0-calculated USL comparison



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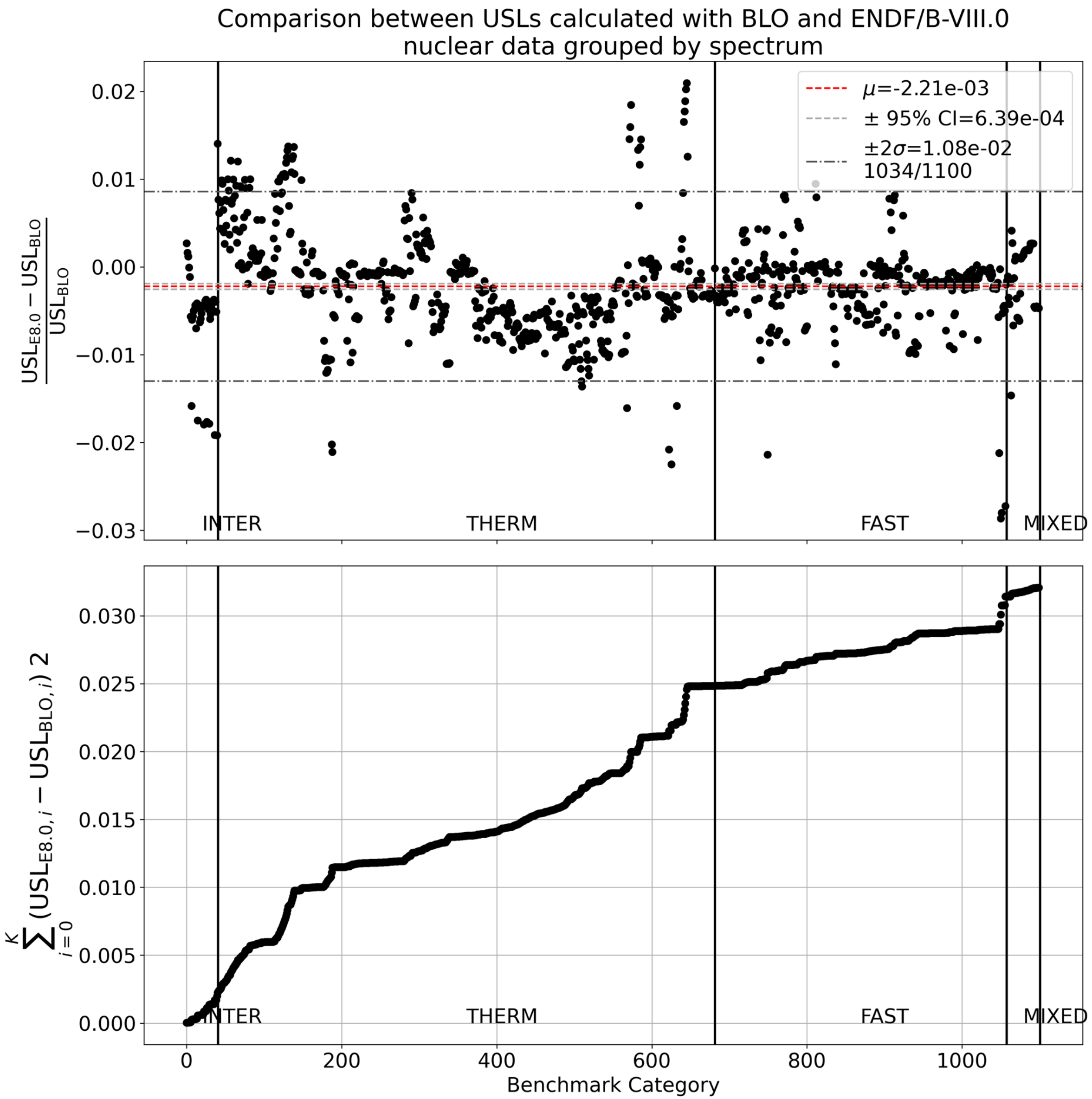
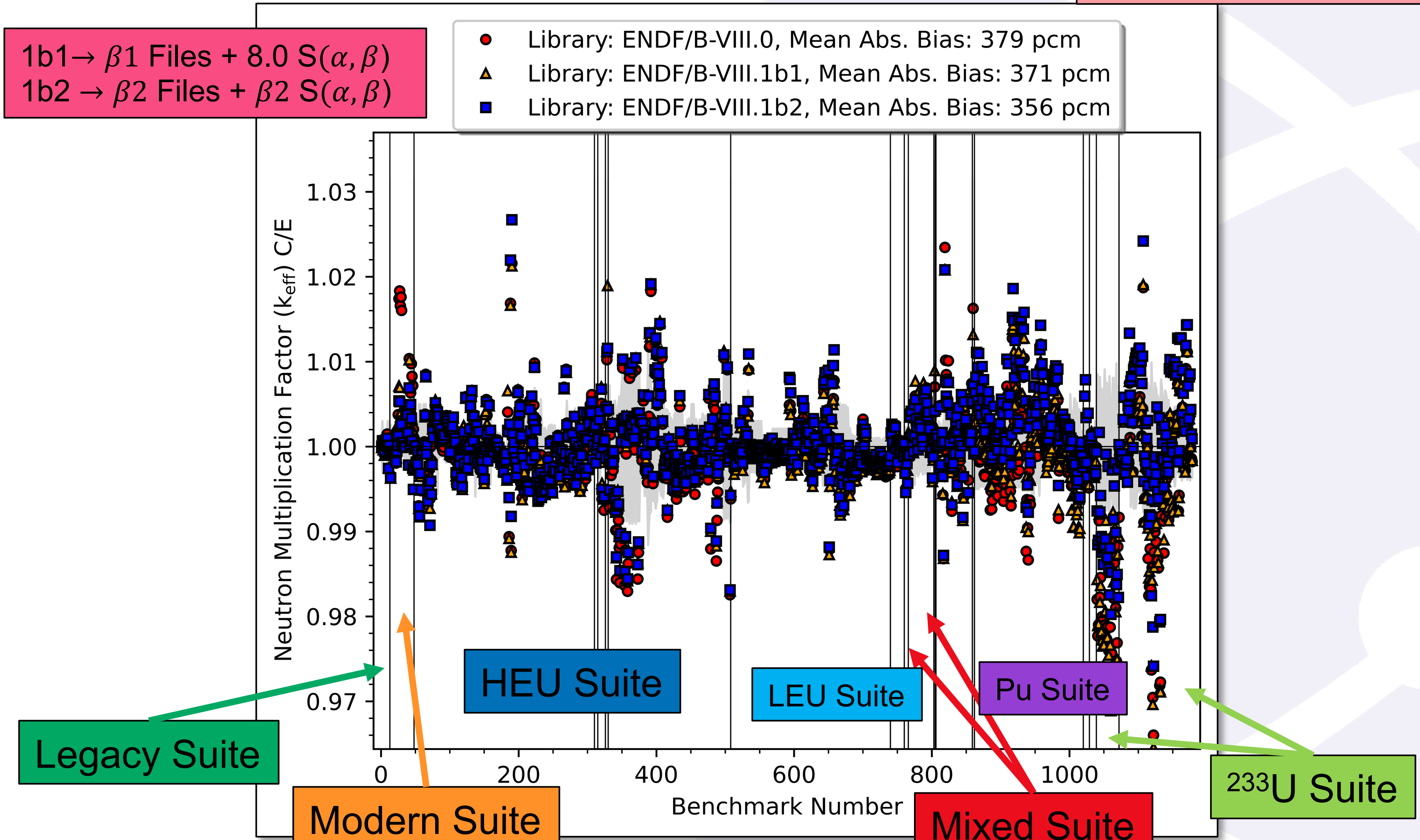
BLO- vs ENDF/B-VIII.0-calculated USL comparison



Simulations of keff have improved in more recent versions of ENDF/B-VIII

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

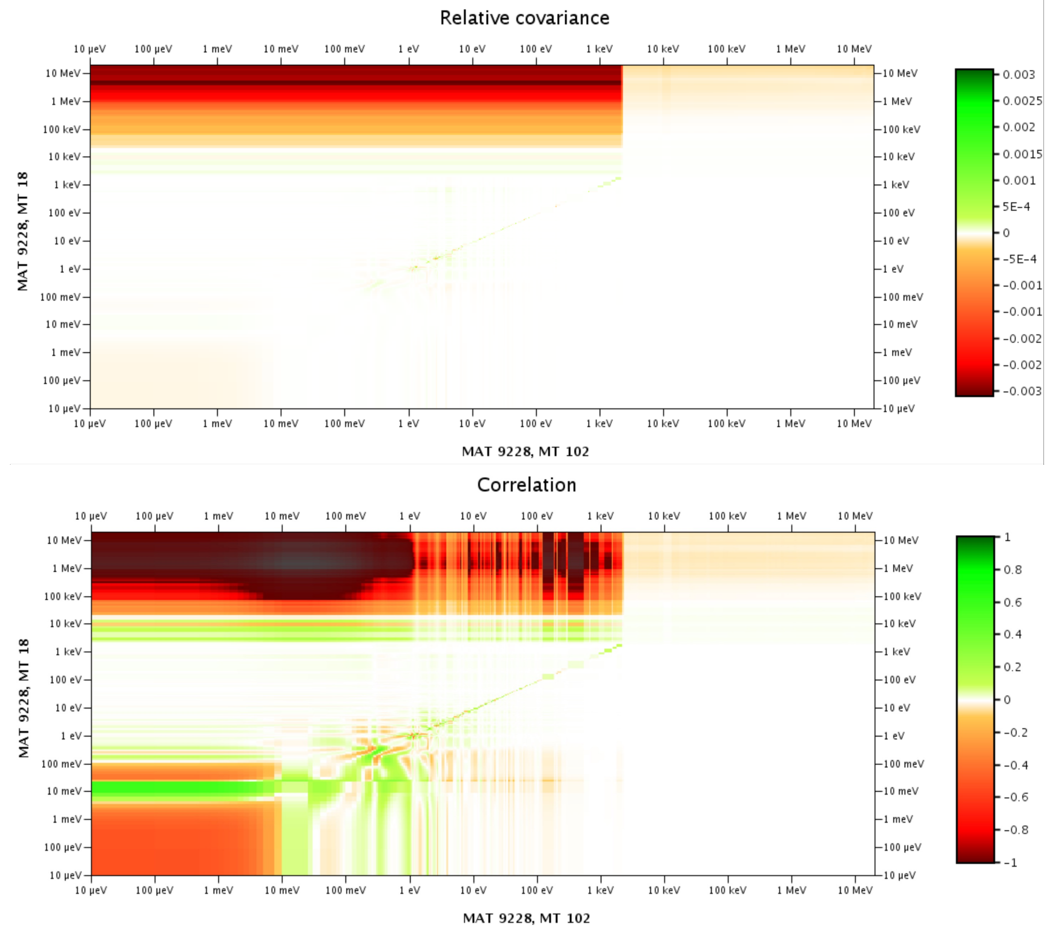
1b1→ β1 Files + 8.0 S(α,β)
1b2 → β2 Files + β2 S(α,β)



N. Kleedtke and A. C. Kahler, "Validation of ENDF/B-VIII.1β2 Files", presentation at the 2023 Cross Section Evaluation Working Group Meeting, LA-UR-23-32912

ENDF/B-VIII.0 U-235 non-physical correlations present in evaluation, before NJOY processing

- In this case, the correlations between the high-energy fission and low-energy capture should be 0
- To incorporate into Whisper, this will need to be manually corrected until it's fixed in the ENDF/B library



Plots from JANIS of the relative covariance (top) and correlation (bottom) between ^{235}U ENDF/B-VIII.0 MT 102 (radiative capture) and MT 18 (neutron-induced fission).

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