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Los Alamos NATIONAL LABORATORY

Updating Covariance Data for Use in MCNP-related Tools

2024 MCNP® User Symposium

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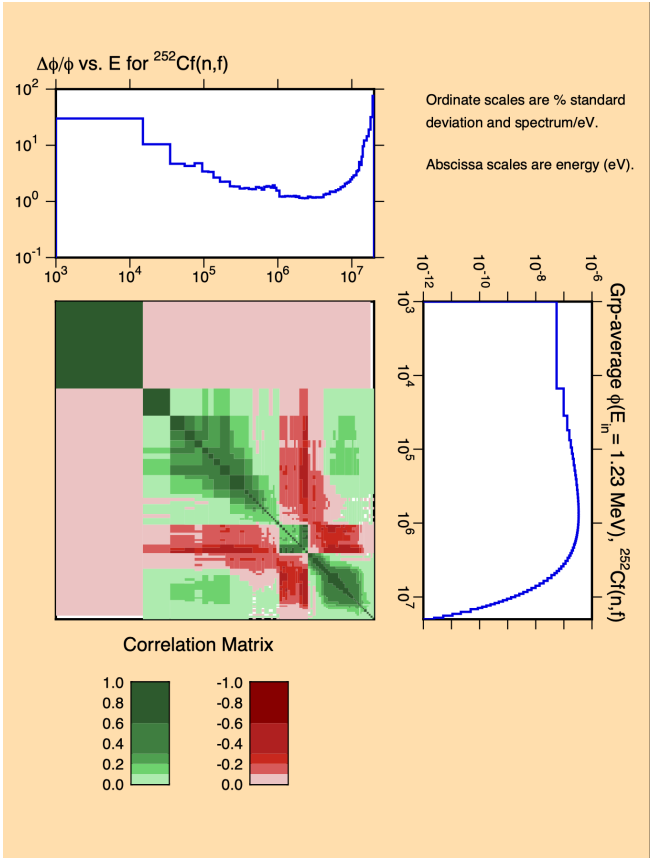
Covariance Data Tabulates Uncertainties and Correlations in Nuclear Data

The nuclear data community is fortunate to have evaluated covariance data available for many reactions

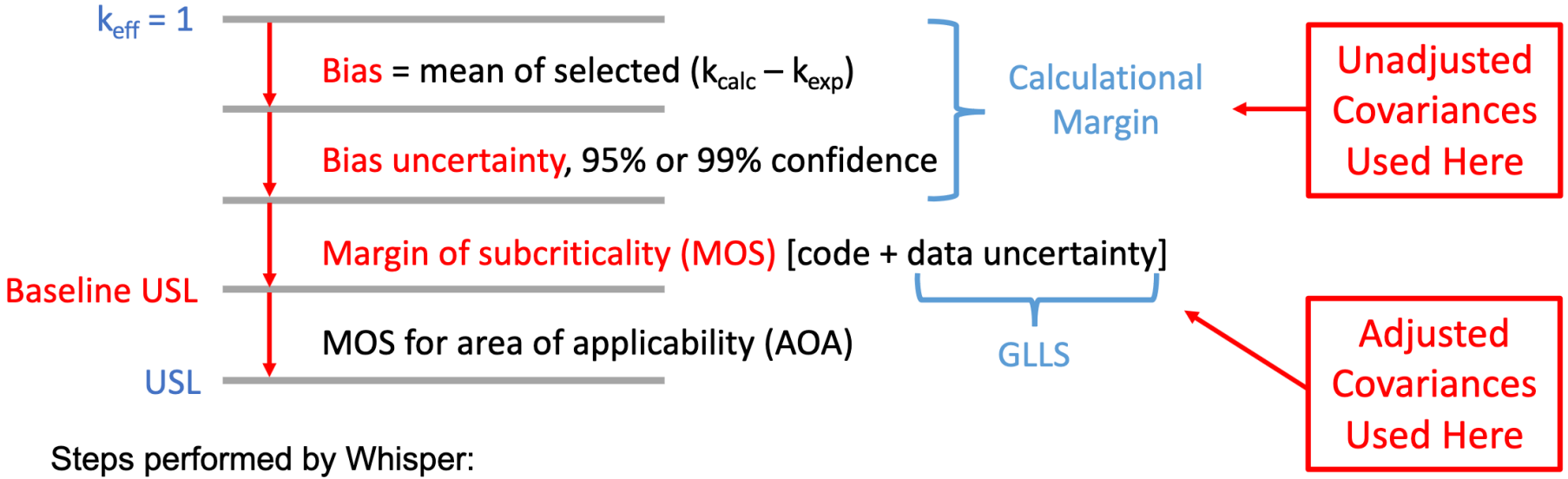
- Evaluators include uncertainties and energy correlations associated with their evaluations
- Available in 251/557 neutron files in ENDF/B-VIII.0



from M. Rising

MCNP-Companion Whisper Uses Covariances for USL

- Statistical analysis code using sensitivity/uncertainty-based methods to determine baseline upper subcritical limit (**USL**) for nuclear criticality safety



Steps performed by Whisper:

1. Benchmark selection
2. Compute bias and bias uncertainty
3. Estimate additional margin of subcriticality

Many More Applications of Covariance Data!

Applications

- Design and estimating impact of new experiments
- Safety and operating margins for reactor systems
- Adjusted nuclear data to incorporate integral data
- Nuclear non-proliferation and forensics
- …

Methods

- Sensitivity/Uncertainty
  - "Sandwich Rule" $\delta\rho = S\Sigma S^T$
  - ksen card / Finite differences
- Monte Carlo
  - Simulate ensembles of data realizations

Whisper Ships with ACE-formatted Covariances from SCALE-6.0

Content

- SCALE 44-group structure
- ENDF/B-VII.0
- BLO “LoFi” supplement

Format

- Ad-hoc format similar to existing ACE files
- Not supported by NJOY or used elsewhere
- LANL Tech Report LA-UR-17-20098

Many improvements to nuclear data have been made in the decades since this covariance data was developed which need to be realized!

Common Request: Covariances Consistent with Latest ENDF Data

Many in the user community are interested in uncertainties for all sorts of applications, rightfully requesting new data!

Goal:
Release covariance data based on ENDF/B-VIII.1 on nucleardata.lanl.gov

How to make updated data more useful?

- Format?
- Group structures?
- Corrections and other deviations from ENDF?
- Documentation and warnings?

Covariance Data is Less Mature and Less Tested – But Improving Quickly!

Possible issues

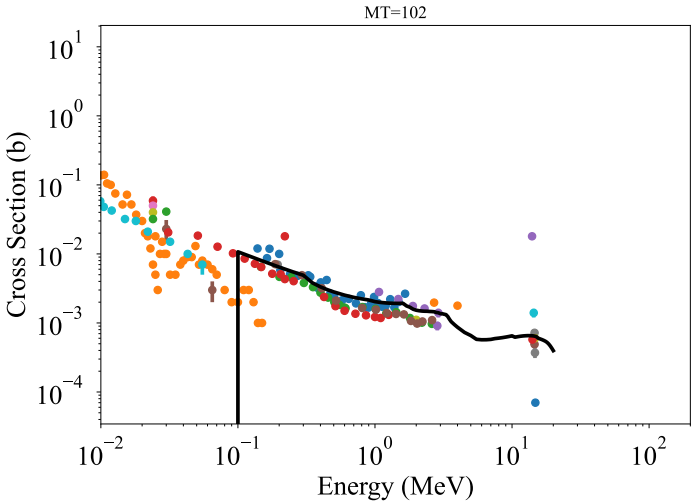
- Mathematical
  - Negative eigenvalues
  - Correlations outside of [-1,1]
- Physical
  - Too small (based on templates, standards, spread of experimental data)
  - Not updated with mean values
  - Incomplete coverage

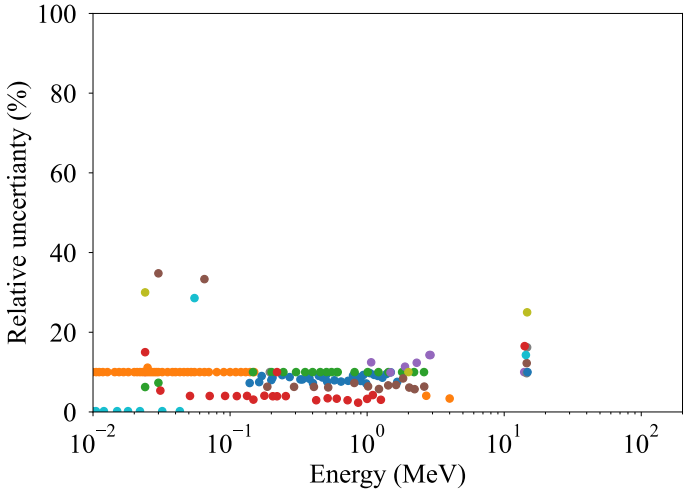
Community Development

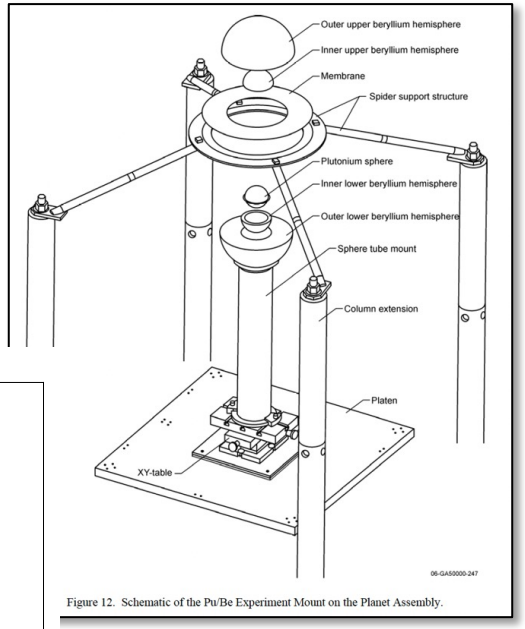
- CSEWG Covariance Committee
- Processing and physics testing at each beta release of ENDF/B-VIII.1
- Discussions and debates about evaluation techniques

Covariance Data Comes from Differential Data and Theory – Not Integral Data!

By design, covariances do not include all our knowledge about nuclear data. Missing correlations imposed by integral data may make naïve propagation yield unreasonable conclusions.







(left) from A. Lovell
(up) from ICSBEP

Unlike Typical ACE Files, Covariances Are Not General Purpose!

- Group structure
  - Covariance energy bins must match sensitivity energy bins or multigroup data
- Adjustment
  - Adjusting to irrelevant integral data not generally a good idea
  - Different users have different definitions of relevance
- Format
  - No widely used option everyone could agree on, even in MCNP user community

Many Covariance Formats Exist, None Are Universal

Available formats

- NJOY: ERROR, COVR/BOXER
- Whisper: ACE
- AMPX/SCALE
- Internal use: JSON

A new, easy to use format is my preference for updates, but requires documentation, interface development, etc.

Processing and Library Preparation Makes Data Usable

Evaluated nuclear data formats designed for ensuring physics consistency and faithful data representation, not use in application codes.

Neutron ACE files

- Reconstruct resonances
- Union energy grid
- Create PDF/CDFs from ENDF distributions

Processed Covariances

- Translate resonance parameter uncertainties to cross section uncertainties
- Union/user energy grid
- Apply summation rules

Conclusions and Outlook

- There is a need for updated covariances being released for the MCNP community on nucleardata.lanl.gov
- This is an unprecedented effort, due to concerns about ensuring it's as general purpose as possible
- Imminent release of ENDF/B-VIII.1 good excuse to do this now!
- Outstanding issues on formats, group structures, completeness, and other subtleties

Questions/Comments?
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