The status of nuclear data uncertainty libraries

and the problem of too small uncertainties on differential data and too large uncertainties on integral data


WANDA
January 22 – 24, 2019
Washington
Difference between predicted and measured criticality is much smaller than predicted by nuclear data uncertainty.
The response from the European nuclear data community to large propagated uncertainties

Differences between JEFF-3.3T4 and JEFF-3.3T3

- **JEFF-3.3T3**: uncertainty in the fast range was based on microscopic experiment only. See files at: [http://www.oecd-nea.org/dbdata/jeff-beta/JEFF33T3/neutrons/](http://www.oecd-nea.org/dbdata/jeff-beta/JEFF33T3/neutrons/)

- **JEFF-3.3T4**: reduced uncertainties to reflect adjustment (e.g. fast range to JEZEBEL). See files at: [http://www.oecd-nea.org/dbdata/jeff-beta/JEFF33T4/neutrons/](http://www.oecd-nea.org/dbdata/jeff-beta/JEFF33T4/neutrons/)
The US nuclear data community has (generally) increased uncertainties in the new library (red)

Slides from P. Palmiotti, WPEC 2018
The current official guidance from the US nuclear data center

Comments about the covariance in current ENDF evaluations

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1. The covariance data in the ENDF evaluations represents uncertainties and correlations in differential data.

2. The use of this covariance to calculate uncertainties for integral quantities such as $K_{\text{ef}}$ will usually result in an overestimate of the uncertainty. That said, comparisons to integral data are essential during the evaluation process and users should not be surprised if the *mean value* nuclear data allow for the accurate prediction of $K_{\text{ef}}$, even if the covariances do not reflect this consideration.

3. The recommended methodology to overcome this problem is to adjust the covariance to add information from a set of integral data that represents the physics of the system for which the adjusted covariance will be used.


5. CSEWG is currently studying the best covariance representation for future releases.
HEU Benchmark C/E:
Prior vs Posterior Uncertainties

- prior C/E
- posterior C/E
- prior C/E unc.
- posterior C/E unc.

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<thead>
<tr>
<th>case</th>
<th>benchmark</th>
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<tr>
<td>1-10</td>
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<td>HST 9-001 - 9-004</td>
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Slide from
M. Williams,
CSEWG 2017
There are minimum bounds on realistic uncertainty estimates and adjustment methodologies often violate these.

(5) The conservative bound of PUBs is close to the ENDF/B-VIII.0 evaluated uncertainties.
The problem of too small uncertainties on differential data and too large uncertainties on integral data

Nuclear data uncertainties are in danger of being smaller than what can be measured experimentally

Nuclear data uncertainties are too large to reflect how well we actually know critical systems

(5) The conservative bound of PUBs is close to the ENDF/B-VIII.0 evaluated uncertainties.

Variation in C/E Values is Much Less Than Predicted by ENDF/B Covariances

Slide from of D. Neudecker, WPEC 2018

Slide from of M. Williams, CSEWG 2017
Have your cake and eat it too: solving the discrepancy with nuclear data correlations

We cannot experimentally measure nuclear data to precision below 1%,
\[ \delta \bar{v} > 1\%, \quad \delta \sigma_f > 1\% \]

But, only 1% uncertainty in \( \bar{v} \) results in 1% uncertainty in \( k_{eff} \) (more than $1$ of reactivity),
\[
k_{\infty} = \frac{(\bar{v} \pm 1\%) \Sigma_f}{\Sigma_a} \rightarrow 1\% \text{ uncertainty in } k_{\infty}
\]

However, the ability to predict \( k_{eff} \) with better accuracy than 1% does not imply the knowledge of the cross sections to better than 1%.

It only says that we know the integral of the cross sections (in the appropriate spectra) to better than 1%.
Approach philosophy

- The discrepancy comes from non-systematic treatment
- The solution will be non-systematic, (no one mathemagical equation)
- However, we promise to
  1. Document exactly what is done, therefore, everything will be reproducible
  2. Test and iterate with the nuclear data community and users
<table>
<thead>
<tr>
<th>Philosophy</th>
<th>Realization</th>
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<tbody>
<tr>
<td>1. 20/80 rule, start with only on the most impactful cross-correlations</td>
<td>1. $^{239}\text{Pu}$, $^{235}\text{U}$, $^{238}\text{U}$ $\sigma_{fis} - \bar{\nu}$</td>
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<tr>
<td>2. Augment the ENDF/B-VIII.0 covariance matrix (not adjust)</td>
<td>2. Only add new cross-correlations, do not adjust variances or existing correlations</td>
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<tr>
<td>3. Estimate the bulk correlation coefficient (coarse group structure)</td>
<td>3. Fast group $\quad$ 20 MeV - 50 keV*  &lt;br&gt;Inter. group $\quad$ 50 keV - 0.625 eV  &lt;br&gt;Thermal group $\quad$ 0.625 eV - 10^{-5} eV</td>
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The goal of the first iteration was not to “solve” the problem outright, but to show conservative progress in the right direction.

*Selected to match the boundary of the SCALE 56-group structure
### Philosophy

1. 20/80 rule
2. Do not change uncertainty on differential data
3. Include benchmarks beyond ICSBEP (e.g. shielding and transmission)
4. Iterate with testing community frequently. Increase the number of cross-correlations and fidelity in energy domain.
5. Do not aspire to reduce propagated uncertainty to level of C/E discrepancy in integral data

### Realization

1. Prioritize work on only the most impactful cross-correlations. The vision is not to have a full covariance matrix for the library
2. Only add cross-correlations, do not adjust variances
3. Collaboration with community
4. Test that uncertainty on “unstudied” integral systems is not significantly reduced
5. Reduce uncertainty as possible by realistic estimation of “generic” cross-correlations independent of integral system
\[ ^{235}\text{U} \sigma_{fis} - \bar{\nu} \] (bulk cross-correlations are only weakly dependent on choice of integral system)

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<th>nu-bar intermediate</th>
<th>nu-bar thermal</th>
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Results for HEU-MET-FAST systems
Results for PU-MET-FAST systems

- C/E
- SCALE 6.2 Covariance Library
- ENDF/B-VIII Covariance Library
- Adj v0
Through a careful examination of nuclear data correlations (energy, reaction, isotope), propagated uncertainties for well known systems can be small and large for systems without vast validation data.
ENDF/B-VIII.0 augmented uncertainty data

• The first demonstration augmented ENDF/B-VIII.0 uncertainty data make progress in the right direction

• More work and collaboration with the international community is necessary for further progress

Thermal Scattering Law uncertainty data

• Currently there is no uncertainty data for thermal scattering in ENDF and the impact on applications is unknown

• University of Michigan and ORNL are developing a format for TLS covariance in new nuclear data format (GNDS)
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Nuclear data cycle

Nuclear Data Needs

Differential Data Measurements

Validation and Applications (SCALE)

Data Evaluation (SAMMY)

Nuclear Data Processing (AMPX)

Evaluated Nuclear Data Files (ENDF)

Nuclear Data

Oak Ridge National Laboratory
The EXFOR library contains an extensive compilation of experimental nuclear reaction data. Neutron reactions have been compiled systematically since the discovery of the neutron, while charged particle and photon reactions have been covered less extensively. The EXFOR library contains data from 22563 experiments (see statistics and recent database updates).

EXFOR Reference Paper: Nucl. Data Sheets 120(2014)272

EXFOR data base: http://www-nds.indcentre.org.in/exfor/exfor.htm
Different cross section uncertainty
Missing correlations
JEFF-3.3

33g energy grid

Uncertainty drop?

Different correlations

ENDF/B-VIII.0

Correlation Matrix

0.0 0.2 0.4 0.6 0.8 1.0

-0.8 -0.6 -0.4 -0.2 0.0 1.0
Have your cake and eat it too: solving the discrepancy with nuclear data correlations

- A negative correlation coefficient between multiplicative terms allows you to keep realistic uncertainties for differential nuclear data which will propagate to realistic uncertainties on integral applications.

- Example:

$$\frac{k_{\infty}}{\Sigma_a} = \frac{\bar{\nu}}{\Sigma_f}, \quad \frac{\delta \bar{\nu}}{\bar{\nu}} = 1\%, \quad \frac{\delta \Sigma_f}{\Sigma_f} = 1\%$$

$$\frac{\delta k_{\infty}}{k_{\infty}} = \sqrt{\left(\frac{\delta \bar{\nu}}{\bar{\nu}}\right)^2 + \left(\frac{\delta \Sigma_f}{\Sigma_f}\right)^2 - 2 \rho_{\bar{\nu}, \Sigma_f} \left(\frac{\delta \bar{\nu}}{\bar{\nu}}\right) \left(\frac{\delta \Sigma_f}{\Sigma_f}\right)}$$