The status of the nuclear data uncertainty libraries and the problem of too small uncertainties on differential data and too large uncertainties on integral data

Vladimir Sobes
sobesv@ornl.gov
Nuclear data is of fundamental importance in nuclear science and engineering.

Nuclear data includes all of the nuclear interaction information required for computational modeling.
1. Importance of nuclear data for advanced reactors
2. Uncertainty in differential nuclear data
3. Propagated uncertainty to integral applications
4. Have your cake and eat it too: nuclear data correlations
Nuclear data is necessary for reliable modeling and simulation of the next generation of nuclear reactors.
The problem of extrapolating nuclear data to new designs
Nuclear data uncertainty dominates:

- Beginning-of-Life (BOL) $k_{\text{eff}}$
- Coolant temp. feedback
- Doppler feedback
- Control rod worth
- Void worth
Nuclear data effecting reactor design (2/2)
Molten Chloride Fast Reactor

A change in absorption cross section of $^{35}\text{Cl}$ resulted in 2000 pcm change in BOL $k_{\text{eff}}$. 
Importance of angular distribution nuclear data

- Exact Angular Distributions for Copper
- Small Resonances Eliminated from Angular Distributions but not from Angle-Integrated Cross Sections only in Copper

Different Critical Experiments (Fuel, Geometry, Neutron Spectrum)
1. Importance of nuclear data for advanced reactors
2. Uncertainty in differential nuclear data
3. Propagated uncertainty to integral applications
4. Have your cake and eat it too: nuclear data correlations
We cannot solve the cross sections from first principles because the nuclear potential, $V(r)$, is not well understood!

\[
\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \psi(r) = E\psi(r)
\]
Experiments to measure cross sections are complex.

Capture measurement set up

Scattering measurement set up
Nuclear data measurements come with uncertainties
Nuclear data evaluation come with more uncertainties
Nuclear data uncertainties are not certain

ENDF Expert

JENDL Expert
1. Importance of nuclear data for advanced reactors
2. Uncertainty in differential nuclear data
3. Propagated uncertainty to integral applications
4. Have your cake and eat it too: nuclear data correlations
Variation in C/E Values is Much Less Than Predicted by ENDF/B Covariances
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

---------------------------------------------------------

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 $K_{eff}$ 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 $K_{eff}$, 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 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.**

<table>
<thead>
<tr>
<th>Case</th>
<th>Benchmark</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-10</td>
<td>HST 1-001 - 1-010</td>
</tr>
<tr>
<td>11-14</td>
<td>HST 9-001 - 9-004</td>
</tr>
<tr>
<td>15-18</td>
<td>HST 10-001 - 10-004</td>
</tr>
<tr>
<td>19-20</td>
<td>HST 11-001 - 11-002</td>
</tr>
<tr>
<td>21</td>
<td>HST 12-001</td>
</tr>
<tr>
<td>22-25</td>
<td>HST 13-001 - 13-004</td>
</tr>
<tr>
<td>26</td>
<td>HST 32-001</td>
</tr>
<tr>
<td>27-29</td>
<td>HST 43-001 - 43-003</td>
</tr>
<tr>
<td>30</td>
<td>Godiva</td>
</tr>
</tbody>
</table>
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.

Slide from of D. Neudecker, WPEC 2018

Slide from of M. Williams, CSEWG 2017
1. Importance of nuclear data for advanced reactors
2. Uncertainty in differential nuclear data
3. Propagated uncertainty to integral applications
4. Have your cake and eat it too: nuclear data correlations
Have your cake and eat it too: solving the discrepancy with nuclear data correlations

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

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

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%. 
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:

\[
\kappa_\infty = \frac{\bar{\nu} \Sigma_f}{\Sigma_a}, \quad \frac{\delta \bar{\nu}}{\bar{\nu}} = 1\%, \quad \frac{\delta \Sigma_f}{\Sigma_f} = 1\%
\]

\[
\frac{\delta \kappa_\infty}{\kappa_\infty} = \sqrt{\left(\frac{\delta \bar{\nu}}{\bar{\nu}}\right)^2 + \left(\frac{\delta \Sigma_f}{\Sigma_f}\right)^2 - 2\rho_{\bar{\nu}, \Sigma_f} \left(\frac{\delta \bar{\nu}}{\bar{\nu}}\right) \left(\frac{\delta \Sigma_f}{\Sigma_f}\right)}
\]
Through a careful examination of nuclear data correlations (energy, reaction, isotope), propagated uncertainties on well known systems can be small and large for systems without vast validation data.
The status of the nuclear data uncertainty libraries
and the problem of too small uncertainties on differential
data and too large uncertainties on integral data

Vladimir Sobes
sobesv@ornl.gov