TMC adjustment of nuclear data libraries using integral benchmarks

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SG46: Definition of the project and of proposed activities

• "Performing new generalized adjustments to provide unambiguous feedbacks. Some approaches has been proposed (Yokoyama, Palmiotti, and Ivanov) but not yet finalized or widely used. **Other approaches could be proposed** and compared. The use of reaction cross correlations and of covariance data for angular distributions, secondary energy distribution from inelastic scattering should be done as far as these data will be made available in the different nuclear data projects”
Uncertainty reduction using benchmarks

• Idea of using benchmarks for randomfile calibration is not new.
  – Petten method for best estimates
• Here:
  – Multiple correlated benchmarks
  – Multiple isotopes within one benchmark
Benchmarks from ICSBEP Handbook were used in this work.

• Method 1: Pu-Met-Fast
  – Re-evaluation of previously obtained data. (TENDL2012)

• Method 2: IEU-Met-Fast and HEU-Met-Fast
  – Courtesy of Steven Van Der Marck
  – TENDL2014
Uncertainty reduction

Random nuclear data from the 1st step is used as the prior for the 2nd step.

**1st level of constraint:** Differential data

- A large set of acceptable ND libraries
  - Simulations: MCNP etc.
  - Applications: Criticality, burnup, Fuel cycle etc.

**2nd level of constraint:** Integral benchmarks

- Assign weights to random files
  - Validation with a set of benchmarks
  - Simulations: MCNP
  - Posterior

**Physical models parameters:** TALYS based system (T6)

**Prior k_{eff} distribution**
The posterior is constrained by both the differential and integral data.

**1st level of constraint:** Differential data

- Physical models parameters: TALYS based system (T6)
- A large set of acceptable ND libraries

**2nd level of constraint:** Integral benchmarks

- Assign weights to random files
- Weighted random files

**Applications:** Criticality, burnup, Fuel cycle etc.

\[ w_i = e^{-\frac{\chi^2_i}{2}} \]

Rather complete on uncertainties, correlations and higher moments.
Benchmark consists of multiple isotopes contributing to the ND uncertainty. 

- $^{239,240,241}$Pu nuclear data uncertainties for a set of plutonium sensitive benchmarks computed using the TMC method. Only case one of each benchmark and 300 random nuclear data files were used for all isotopes. Note that, PU-MET-FAST-035 does not contain $^{241}$Pu.

<table>
<thead>
<tr>
<th>Benchmark category</th>
<th>$\sigma_{ND}(^{239}\text{Pu})$</th>
<th>$\sigma_{ND}(^{240}\text{Pu})$</th>
<th>$\sigma_{ND}(^{241}\text{Pu})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>PU-MET-FAST-001</td>
<td>962 ± 42</td>
<td>178 ± 8</td>
<td>36 ± 3</td>
</tr>
<tr>
<td>PU-MET-FAST-002</td>
<td>826 ± 36</td>
<td>833 ± 34</td>
<td>254 ± 11</td>
</tr>
<tr>
<td>PU-MET-FAST-005</td>
<td>954 ± 42</td>
<td>192 ± 8</td>
<td>31 ± 4</td>
</tr>
<tr>
<td>PU-MET-FAST-008</td>
<td>939 ± 41</td>
<td>195 ± 8</td>
<td>28 ± 4</td>
</tr>
<tr>
<td>PU-MET-FAST-009</td>
<td>925 ± 41</td>
<td>186 ± 8</td>
<td>33 ± 3</td>
</tr>
</tbody>
</table>

I.e., a deviation between C and E can be due to any of these isotopes.
Important to also include the calculation uncertainty

Method 1: Use benchmarks to calibrate the ND for a specific isotope (here Pu$^{239}$). Varying a single isotope at a time (here Pu$^{239,240,241}$).

\[
\chi^2_{i,j} = \sum_B \frac{(C_{B,i} - E_B)^2}{\sigma_{B,j}^2}, \; i = \text{randomfile}, \; j = \text{isotope}, \; B = \text{benchmark}
\]

\[
\sigma_{B,j}^2 = \sigma_E^2 + \sigma_{C,j}^2 = \sigma_E^2 + \sigma_{stat}^2 + \sum_{\text{overall } p \neq j} \sigma_{ND,p}^2 + \sigma_{other}^2
\]
Important to also include the calculation uncertainty

- Main idea: if the calculation deviates from the benchmark value it can be due to $\sigma_E$, $\sigma_{\text{stat}}$, an error in the isotope / (observable) that we are calibrating, any of the other isotopes / (observables) in the benchmark, or other errors not accounted for.

- Note: the $\sigma_E$ in, e.g., ICSBEP, includes both the actual experimental uncertainty, but also uncertainties in transferring the experiment to a benchmark (e.g., densities).

$$\chi^2_{i,j} = \sum_B \frac{(C_{B,i} - E_B)^2}{\sigma^2_{B,j}}, i = \text{randomfile}, j = \text{isotope}, B = \text{benchmark}$$

$$\sigma^2_{B,j} = \sigma^2_E + \sigma^2_{C,j} = \sigma^2_E + \sigma^2_{\text{stat}} + \sum_{\text{overall } p} \sigma^2_{ND,p} + \sigma^2_{\text{other}}$$
Benchmark exp. errors are correlated

Working with covariances

How can $\text{COV}_E$ be determined?

1. Careful analysis of the experiments.
2. Using DICE.
3. Here: checking sensitivity of results, and try to be conservative.

$\text{COV}_C$ is also strongly correlated

$$\text{COV}_{C,j} = +\text{COV}_{\text{stat}} + \sum_{\text{overall } p \neq j} \text{COV}_{ND,p}$$

$$\chi_i^2 = (C - E)^T \text{COV}_{B,j}^{-1} (C - E)$$

$$\text{COV}_{B,j} = \text{COV}_E + \text{COV}_{C,j}$$
Before and after calibration

Before calibration + Pu239 + unc.
After calibration + Pu239 unc.
Benchmark uncertainty (exp+Pu240+241)

TENDL2012
250 randomfiles

Calibration
Validation
Comment on results

- Decreased ND uncertainty to more ‘realistic values’.
- Small improvement of the best-estimates.
  - Strong correlations
- The inclusion of $\text{COV}_c$ and $\rho_{\text{exp}}=0.5$ affects the ND uncertainty but not the mean values.
- Old version of TENDL!
Method 2

- All isotopes of interest are varied simultaneously
- Intrinsically the uncertainty of the different isotopes are taking into account simultaneously
- Investigated for U8 and U5.

\[ w_i = e^{-\frac{\chi_i^2}{2}} \]

\[ \chi_i^2 = (C - E)^T \text{COV}_{B,j}^{-1} (C - E) \]

\[ \text{COV}_{B,j} = \text{COV}_E + \text{COV}_{\text{stat}} \]
Importance of benchmark exp. correlation
Importance of benchmark exp. correlation 2
Before and after calibration

\[ \rho_{\text{exp}} = 0.6 \]

1000 TENDL2014 files

- Calibration
- Validation
Difficult to fit the experimental data?

- Wrong model parameter distribution?
- Model defects?
- To small experimental uncertainties or wrong experimental covariance matrix.
Adding 80 pcm experimental uncertainty to hmf1 and imf7_4

TENDL2014
1000 random files

C-E [PCM]

Before calibration + U5U8 unc.
After calibration + U5U8 unc.
Benchmark uncertainty

Calibration  Validation
Method 1 vs. Method 2

Method 2 - hypothesis

- Better calibration of the best estimate - due to higher degree of freedom
- Smaller posterior ND uncertainty – negative correlations between isotopes.
- Higher cost in terms of random files needed. I.e., the method produce lower average weights.

Proposal

Use Method 1 to determine the uncertainty for minor isotopes (e.g. $^{234}$U) and Method 2 for the major isotopes ($^{235}, ^{238}$U).

Limitation of this work

- To few effective random files
- ENDF/B-VII.0 used as background library
How is the uncertainty reduced?

E. Bauge. "Correlations in nuclear data from integral constraints: cross-observables and cross-isotopes", CW2017

- Using integral data introduce correlations: between isotopes and between different parts of the ND file.
- The integral weighing only slightly change the best estimate <1% and std dev < 10%

D. Rochman: Nuclear data correlation between different isotopes via integral information

Conclusion

• Random file integral calibration possible.
• Results still constrained by differential data and the model.
• Calculation uncertainties should be included
  – e.g., take into account multiple isotopes within the benchmarks (and observables not accounted for).
• The correlation between the benchmarks are important.
• Robust techniques to account for discrepant integral data needs to be developed.

\[ \sigma_{C,j}^2 = \sigma_{stat}^2 + \sum_{\text{overall } p \text{ where } p \neq j} \sigma_{ND}^2 \]
THANK YOU FOR YOUR ATTENTION!


Cross-isotope correlations

D. Rochman: Nuclear data correlation between different isotopes via integral information
Fig. 11. Comparison between the posterior (weighted), prior (unweighted) and the IAEA standard $^{235}$U(n,f) cross section and uncertainties (the lines denotes the cross sections whereas the bands are the uncertainties).