Monte Carlo integral adjustment of nuclear data libraries – experimental covariances and inconsistent data

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MC uncertainty reduction using integral data

- Idea of using benchmarks for random-file calibration is not new.
  - Petten method for best estimates
- Here:
  - Multiple correlated benchmarks
  - Multiple isotopes within one benchmark
  - Addressing inconsistencies
Uncertainty reduction

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

Physical models parameters: TALYS based system (T6)

1\textsuperscript{st} level of constraint: \textbf{Differential data}

A large set of acceptable ND libraries

2\textsuperscript{nd} level of constraint: \textbf{Integral benchmarks}

Assign weights to random files

Weighted random files

Simulations: MCNP etc.

Applications: Criticality, burnup, Fuel cycle etc.

\[ w_i = e^{-\frac{\chi^2}{2}} \]
The posterior is constrained by both the differential and integral data.

Rather complete on uncertainties, correlations and higher moments. Improvements possible.
Important to also include the calculation uncertainty

- C/E ≠ 1 can be due to $\sigma_E$, $\sigma_{stat}$, an error in the isotopes that we are calibrating, any of the other isotopes in the benchmark, or other errors not accounted for.

\[
\chi^2_{i,J} = \sum_B \frac{(C_{B,i} - E_B)^2}{\sigma^2_{B,J}}, i = \text{randomfile}, J = \text{isotopes}, B = \text{benchmark}
\]

\[
\sigma^2_{B,J} = \sigma^2_E + \sigma^2_{C,J} = \sigma^2_E + \sigma^2_{\text{stat}} + \sigma^2_{\text{defects}} + \sigma^2_{\text{other}} + \sum_{\text{overall } p, \text{ where } p \neq J} \sigma^2_{ND,p}
\]
Method

- Major isotopes are varied simultaneously.
- MCNP6 and TENDL2014
- Investigated for U8 and U5.
- \( k_{\text{eff},i} = f(U8_i, U5_i) \).
  \( i \) = random file number
- Intrinsically the uncertainty of the different isotopes are taking into account simultaneously

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

\[
\text{COV}_{B,J} = \text{COV}_E + \text{COV}_{\text{stat}}
\]

\[
w_i = e^{-\frac{\chi_i^2}{2}}
\]
Before and after calibration

IEU-Met-Fast and HEU-Met-Fast\(^1\)
1000 TENDL2014 files

\(^1\)Curtesy of Steven Van Der Marck
Difficult to fit the experimental data
- prior correlations

ND (U5U8) prior correlations

IMF7_4
IMF3_2
IMF2
HMF8
HMF1_1

HMF1_1 HMF8 IMF2 IMF3_2 IMF7_4

0.0 0.2 0.4 0.6 0.8 1.0
Difficult to fit the experimental data - inconsistent data

- Model defects.
  - E.g., ND uncertainties not taking into account
  - Models inability to reproduce the true ND
- Unaccounted experimental uncertainties or covariances.
- Underestimated statistical uncertainties.
- Isotopes not taken into account

\[
\sigma_{B,J}^2 = \sigma_E^2 + \sigma_{\text{stat}}^2 + \sigma_{\text{defects}}^2 + \sigma_{\text{other}}^2 + \sum_{\text{overall } p \text{ where } p \neq J} \sigma_{\text{ND},p}^2
\]

\(^1\)See, e.g., Gerald Rimpaults presentation: *Trends on major actinides from an Integral data assimilation.*
Marginalized Likelihood Optimization

• We add an extra uncertainty to each experiment.

\[
\sigma_{B,J}^2 = \sigma_E^2 + \sigma_{stat}^2 + \sigma_{defects}^2 + \sigma_{other}^2 + \sum_{p \neq J} \sigma_{ND,p}^2
\]

\[
\sigma_{B,l,J}^2 = \sigma_E^2 + \sigma_{stat}^2 + \sigma_{extra,l}^2
\]

• $\sigma_{extra}$ found by maximising$^1$ L:

\[
L = \frac{1}{\sqrt{2\pi n n|\text{cov}_{\text{exp,stat,extra}}|}} \sum_i e^{-\frac{\chi_i^2}{2}}
\]

n = number of parameters

$^1$ Here MC and integral information. Compare with G. Schnabel’s presentation.

$^{1}$G. Schnabel, Fitting and analysis technique for inconsistent data, MC2017
Results

**Benchmark uncertainties [PCM]**

<table>
<thead>
<tr>
<th></th>
<th>HMF1_1</th>
<th>HMF8</th>
<th>IMF2</th>
<th>IMF3_2</th>
<th>IMF7_4</th>
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</thead>
<tbody>
<tr>
<td>No ML: Reported uncertainties</td>
<td>100</td>
<td>160</td>
<td>300</td>
<td>170</td>
<td>80</td>
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<tr>
<td>Updated uncertainties</td>
<td>153</td>
<td>204</td>
<td>300</td>
<td>580</td>
<td>390</td>
</tr>
</tbody>
</table>
Benchmark exp. errors are correlated
Adding a correlation term

- Correlations: $\sigma_E$, $\sigma_{\text{defect}}$, $\sigma_{\text{other isotopes}}$
- A fully correlated uncertainty to all experiments is added.

$$\sigma^2_{B,l,J} = \sigma^2_E + \sigma^2_{\text{stat}} + \sigma^2_{\text{extra},l} + \sigma^2_{\text{extra all}}$$

$$L = \frac{1}{\sqrt{2\pi n \left| \text{cov}_{\text{exp,stat,extra}} \right|}} \sum_i e^{-\frac{\chi_i^2}{2}}$$

$max(L) \rightarrow \sigma^2_{\text{extra},l} + \sigma^2_{\text{extra all}}$
Results – with correlation

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<th>Fully correlated</th>
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<td>170</td>
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<td>0</td>
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<tr>
<td>Uptated uncertainties</td>
<td>153</td>
<td>204</td>
<td>300</td>
<td>580</td>
<td>390</td>
<td>0</td>
</tr>
<tr>
<td>With correlation</td>
<td>267</td>
<td>329</td>
<td>333</td>
<td>591</td>
<td>409</td>
<td><strong>257</strong></td>
</tr>
</tbody>
</table>
Adding a prior

\[ \text{prior}(\sigma_{\text{extra}}) = e^{-\beta \sigma_{\text{extra}}^2} \]  

or,

\[ \text{prior}(\sigma_{\text{extra}}) = e^{-\beta \sigma_{\text{extra}}} \]

\[ L = \frac{1}{\sqrt{2\pi n |\text{cov}_{\text{exp,stat,extra}}|}} e^{-\beta \sum \sigma_{\text{extra}}^2} \sum_{i} e^{-\frac{\chi_{i}}{2}} \]

\( \beta \) is chosen **by expert judgement** or in a data-driven approach\(^1\).

\(^1\)G. Schnabel, *Fitting and analysis technique for inconsistent data*, MC2017
Results with an added prior

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<td>409</td>
<td>257</td>
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<tr>
<td>With prior</td>
<td>232</td>
<td>263</td>
<td>366</td>
<td>468</td>
<td>228</td>
<td>209</td>
</tr>
</tbody>
</table>

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<tr>
<th>Posterior</th>
<th>HMF1_1</th>
<th>HMF8</th>
<th>IMF2</th>
<th>IMF3_2</th>
<th>IMF7_4</th>
<th>Chi2</th>
<th>p_value</th>
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<tr>
<td>No ML</td>
<td>69</td>
<td>28</td>
<td>103</td>
<td>52</td>
<td>34</td>
<td>2,1</td>
<td>6%</td>
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<tr>
<td>Uptated uncertainties</td>
<td>139</td>
<td>131</td>
<td>234</td>
<td>183</td>
<td>273</td>
<td>0,38</td>
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<tr>
<td>With correlation</td>
<td>264</td>
<td>254</td>
<td>313</td>
<td>290</td>
<td>351</td>
<td>0,4</td>
<td>84%</td>
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<tr>
<td>With Prior</td>
<td>253</td>
<td>214</td>
<td>288</td>
<td>256</td>
<td>265</td>
<td>0,58</td>
<td>72%</td>
</tr>
</tbody>
</table>
Posterior correlations

ND (U5U8) prior correlations

ND (U5U8) posterior correlations
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%


Same conclusion from: C. De Saint Jean et al., Evaluation of Cross Section Uncertainties Using Physical Constraints: Focus on Integral Experiments, Nuclear Data Sheets, Volume 123, Pages 178-184
Conclusion

• MC - Marginalized Likelihood maximization to account for discrepant integral data.
• Results still constrained by differential data and the model.
  – improvements necessary (G. Schnabel’s presentation)
• Include calculation uncertainties
  – e.g., multiple isotopes (and observables not accounted for).
• The correlation between the benchmarks are important.
• Outlook: sampling of $L^1 +$ validation / transposition.

1G. Schnabel, Fitting and analysis technique for inconsistent data, MC2017
THANK YOU FOR YOUR ATTENTION!


4. C. De Saint Jean et al., Evaluation of Cross Section Uncertainties Using Physical Constraints: Focus on Integral Experiments, Nuclear Data Sheets, Volume 123, Pages 178-184

5. G. Schnabel, Fitting and analysis technique for inconsistent data, MC2017
Cross-isotope correlations

D. Rochman: Nuclear data correlation between different isotopes via integral information
\[\log L = c - 0.5 \cdot \left| \text{cov}_{\text{exp}} + \text{cov}_{\text{extra}} \right| + \ln \left( \sum e^{\frac{\chi^2}{2}} \right)\]