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

Simulations: mcnp etc.

Applications: Criticality, burnup, Fuel cycle etc.

\[ W_i = e^{\frac{-x_i^2}{2}} \]

Prior $k_{\text{eff}}$ distribution

Posterior
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.

Validation with a set of benchmarks

Simulations: mcnp etc.

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

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

- \( C/E \neq 1 \) 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.

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

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

where \( p \neq J \).
Method

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

$$w_i = e^{-\frac{\chi_i^2}{2}}$$

$$\chi_i^2 = (C - E)^T COV_{B,i}^{-1} (C - E)$$

$$COV_{B,i} = COV_E + COV_{stat}$$
Before and after calibration

IEU-Met-Fast and HEU-Met-Fast

1000 TENDL2014 files

Curtesy of Steven Van Der Marck
Difficult to fit the experimental data - prior correlations

ND (U5U8) prior correlations
Difficult to fit the experimental data - inconsistent data

- Model defects.
  - E.g., ND uncertainties not taking into account\(^1\)
  - Models inability to reproduce the true ND
- Unaccounted experimental uncertainties or covariances.
- Underestimated statistical uncertainties.
- Isotopes not taken into account

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

\(^1\)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.

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

\[ \sigma^2_{B,I,J} = \sigma^2_E + \sigma^2_{stat} + \sigma^2_{extra,I} \]

- \( \sigma_{extra} \) found by maximizing\(^1\) \( L \):

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

\( n = \) 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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<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>Uptated uncertainties</td>
<td>153</td>
<td>204</td>
<td>300</td>
<td>580</td>
<td>390</td>
</tr>
</tbody>
</table>

**Legend:**
- Red dot: Before calibration + USU8 unc.
- Blue dot: After calibration + USU8 unc.
- Orange line: Benchmark uncertainty
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.

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

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

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

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<tr>
<td>With correlation</td>
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<td>333</td>
<td>591</td>
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Adding a prior

$prior(\sigma_{extra}) = e^{-\beta\sigma_{extra}^2}$ or,

$prior(\sigma_{extra}) = e^{-\beta\sigma_{extra}}$

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

$\beta$ 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

### Benchmark uncertainties [PCM]

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<tr>
<td>With prior</td>
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<td>263</td>
<td>366</td>
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### Posterior

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<td>103</td>
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<td>2,1</td>
<td>6%</td>
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<td>Uptated uncertainties</td>
<td>139</td>
<td>131</td>
<td>234</td>
<td>183</td>
<td>273</td>
<td>0,38</td>
<td>86%</td>
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<td>With correlation</td>
<td>264</td>
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<td>351</td>
<td>0,4</td>
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<tr>
<td>With Prior</td>
<td>253</td>
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<td>0,58</td>
<td>72%</td>
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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%


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

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.

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$^{1}$G. Schnabel, *Fitting and analysis technique for inconsistent data*, MC2017
THANK YOU FOR YOUR ATTENTION!
References


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
\[ \log L = c - 0.5 \left| \text{cov}_{\text{exp}} + \text{cov}_{\text{extra}} \right| + \ln \left( \sum e^{\frac{-\chi^2}{2}} \right) \]

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