Correlations in nuclear data from integral constraints: cross-observables and cross-isotopes

Eric Bauge : CEA DAM DIF, France  
Dimitri Rochman : PSI, Switzerland
σ – χ – ν correlations in the fast region via integral information

Cross-observables correlations

Correlation $\bar{\nu}_p – \sigma – \chi$ in the fast neutron range via integral information

Dimitri Rochman1, Eric Bauge2*, Alexander Vasiliev1, and Hakim Ferroukhi1

1 Laboratory for Reactor Physics Systems Behaviour, Paul Scherrer Institut, Villigen, Switzerland
2 CEA, DAM, DIF, 91297 Arpajon cedex, France

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Abstract. This paper presents a Bayesian approach based on integral experiments to create correlations which do not appear with differential data. Some quantities such as the fission cross section ($\sigma$), neutron multiplicity ($\bar{\nu}_p$), neutron spectra ($\chi$), etc. are usually neither modeled together nor measured in coincidence, thus there is no correlation matrices in evaluated nuclear data libraries. One can nevertheless use the information from integral experiments such as fast criticality-safety benchmarks to correlate such quantities for possible inclusion in nuclear data libraries. A simple Bayesian set of equations is presented with random nuclear data, similarly to the usual methods applied with differential data. An example for $^{239}$Pu is proposed.
Cross-observables correlations?

$\sigma$: cross sections (integrated $\sigma(E)$, simply differential $d\sigma/dE$, $d\sigma/d\Omega$, doubly differential $d^2\sigma/d\Omega dE$, for all reaction channels).

$\chi$: prompt fission neutron spectra (PFNS normalized to 1).

$\nu$: ($\bar{\nu}$) average number of prompt fission neutrons
Integral constraints?

\[ n + ^{239}\text{Pu} \]

\[ n,f \]

\[ \text{Cross Sections (barn)} \]

\[ \text{Neutron Energy (MeV)} \]

\[ \text{PMF1} \]

\[ 150 \text{ pcm} \]

\[ -20 \text{ keV on } V_A \approx 0.34\% \]

\[ 1000 \text{ pcm on } K_{\text{eff}} \]

+ Integral experiments produce strong constraints on model parameters and the resulting nuclear data.
In real life (ND evaluator’s perspective)

One model for cross sections, with parameters adjusted on differential measurements (a few % for fission, a few 10% for capture, inelastic, )

One model for PFNS, with parameters adjusted on differential measurements (<E> within a few %).

One model for nubar, with parameters adjusted on differential measurements (nubar within 2 %)

Integral experiments measured within 0.2-0.3 %

To reach the “good” integral performance, evaluators select the “good” $\sigma-\chi-\nu$ set.

$\sigma-\chi-\nu$ are strongly correlated, but that correlation is never quantified.
Quantification of $\sigma - \chi - \nu$ correlations

At PSI using the T6 system used to produce the TENDL library.

Total Monte-Carlo (TMC) approach: model (TALYS, TAFIS,...) parameter sampling such as differential data is accounted for ($\sigma$, $\chi$ and $\nu$).

10000 ENDF6 formatted files, with different combinations of $\sigma$, $\chi$ and $\nu$ and MCNP calculations for 9 fast spectrum $^{239}$Pu configurations. Bayesian-like weighting of samples according to $\chi^2$ between exp. and calc.

$i$: sample index

$$Q_i = \left(\frac{k_{\text{eff},i} - k_{\text{exp}}}{\Delta k}\right)^2$$

$$w_i = \exp\left(-\frac{Q_i}{2}\right)$$

$$\omega = \sum_{i=1}^{n} w_i$$

$$w_{\sigma} = \sum_{i=1}^{n} w_i \cdot \sigma_{\alpha,i}/\omega$$

$$\begin{align*}
\text{var}_{\sigma_\alpha} &= \sum_{i=1}^{n} \frac{[\sigma_{\alpha,i} - \omega_{\sigma_\alpha}]^2 \cdot w_i}{\omega} \\
\text{var}_{\sigma_\beta} &= \sum_{i=1}^{n} \frac{[\sigma_{\beta,i} - \omega_{\sigma_\beta}]^2 \cdot w_i}{\omega} \\
\text{cov}_{\sigma_\alpha\sigma_\beta} &= \sum_{i=1}^{n} \frac{[\sigma_{\alpha,i} - \omega_{\sigma_\alpha}] \cdot [\sigma_{\beta,i} - \omega_{\sigma_\beta}] \cdot w_i}{\omega}
\end{align*}$$

$$\rho(\sigma_\alpha, \sigma_\beta) = \frac{\text{cov}_{\sigma_\alpha\sigma_\beta}}{\sqrt{\text{var}_{\sigma_\alpha} \cdot \text{var}_{\sigma_\beta}}}$$

Good agreement = high weight
Bad agreement = low weight
Quantification of $\sigma-\chi-\nu$ correlations

At PSI using the T6 system used to produce the TENDL library.

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$\sigma-\chi-\nu$ correlations

$E_n[\sigma(n,f)]=1.45$ MeV

NB: $<E_n>\approx 1.4$ MeV
Correlations resulting from model response to parameter variations

Without $\sigma-\chi-\nu$ correlation
(prior)

With $\sigma-\chi-\nu$ correlation
(posterior)

Correlations resulting from model response to parameter variations
+ 9 PMF configurations integral constraints

Such correlations allow for variance reduction of calculated $K_{\text{eff}}$!
Easy (1 slide) prompt neutronics with point geometry

\[
\Phi_{i}^{t+1} = \sum_{j} \nu_{ji} \Phi_{j} \sum_{f} j - \Phi_{i} \sum_{c} i - \Phi_{i} \sum_{i}^{inel} + \sum_{j \neq i} \Phi_{j} \sum_{j}^{inel \rightarrow i}
\]

with \( \nu_{ij} = \nu_{i} \chi_{ij} \)

Source term = \( \Phi \cdot \nu_{i} \cdot \chi_{ij} \cdot \sigma_{i} \)

\( \Phi^{t+1} > \Phi^{t} \) Runaway reaction

\( \Phi^{t+1} = \Phi^{t} \) Stable reaction

\( \Phi^{t+1} < \Phi^{t} \) Reaction stops

Typically measured with 0.2-0.3% precision (200-300 pcm)
Such correlations allow for variance reduction of calculated $K^{\text{eff}}!$
Some benchmarks exhibit strong sensitivity to several isotopes. Example: IMF7 « Big Ten » a highly enriched U core surrounded by a massive reflector made of depleted U.

It is sensitive to both $^{235}\text{U}$ and $^{238}\text{U}$ data. Its exp. Keff value (1.00450 (70 pcm)) cannot be reproduced by mixing different libraries.

<table>
<thead>
<tr>
<th>$^{238}\text{U} \rightarrow ^{235}\text{U}$</th>
<th>JEFF-3.3</th>
<th>ENDF/B-VII.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>JEFF-3.3</td>
<td>1.00522</td>
<td>1.01315</td>
</tr>
<tr>
<td>ENDF/B-VII.1</td>
<td>0.99617</td>
<td>1.00478</td>
</tr>
</tbody>
</table>

Therefore: $^{235}\text{U}$ and $^{238}\text{U}$ data are effectively correlated in evaluated libraries.

The same Bayesian weighting technique can be used to quantify those correlations.
Cross isotopes correlations

Unweighted (prior)
Correlations resulting from model response to parameter variations

With IMF7-derived weights (posterior)
Correlations resulting from model response to parameter variations + integral constraints
Cross-isotopes correlations from integral constraints

With IMF7-derived weights

Cross-observables correlations from integral constraints
Cross-isotopes and cross-observables correlations, zoom in...

With IMF7-derived weights

\[
\frac{^{235}\text{U}}{^{235}\text{U}}
\]

\[
\sigma_{(n,f)} \text{(keV)}
\]

\[
\sigma_{(n,y)} \text{(keV)}
\]

\[
\sigma_{(n,el)} \text{(keV)}
\]
The Bayesian weights slightly change the central values. Typically less than 1%
The Bayesian weights slightly change the std dev.

Mostly reduced by a few % up to ~10%

Diagram showing posterior/prior ratios for different energy-reactions and isotopes, with lines indicating changes in the posterior distribution over the prior.
Differential data

\( ^{235}\text{U}(n,f) \)

Posterior
Prior
IAEA Standard

\( \sigma_{(n,f)} \) (b.)

Energy (MeV)

0.8 1.6 3.2 6.4
The IMF7-derived weights do not degrade the agreement of other benchmarks, they even slightly improve the central value and calculated uncertainties!
A first attempt at the rigorous quantification of the $\sigma-\chi-\nu$ correlations existing in all the present evaluated nuclear data files

These correlations allow nuclear data files to reach target integral performance. (Evaluators have known that for a long time, but never advertised it).

A first demonstration is limited to a few PMFs (Eur. Phys. J. N 3, 14 (2017))

Cross isotopes correlations (IMF7: BIGTEN known to strongly depend on both $^{235}\text{U}$ and $^{238}\text{U}$) can be quantified (submitted to EPJ N).

The posterior (weighted) distributions are not inconsistent with the best differential experiments.

Adjusting for one integral exp. seems to improve agreement with other integral expt. (including with different neutronic spectra).

Do we learn anything about the fission process? NO!

The ENDF6 format does not allow for storage or processing of such correlations.
- New GND format will allow to store and process such correlations.
- New WPEC subgroup 44 starting on best practices for uncertainties evaluations
- Mix several integral constraints in the weights (ex HMF1 +IMT7 +LCT6 +…)
- Also add differential weights (EXFOR + AIEA Std)
- Extension to wider spectral constraints (thermal,…), other isotopes ($^{235}$U, $^{238}$U), other observables (spectral indices), all reaction channels is underway.
- Use better models (the models used for TENDL are quite simple)
Convergence of the sampling process?
Table 1. Average neutron energy in keV causing fission or capture in the two main zones of the imf7 benchmark.

<table>
<thead>
<tr>
<th></th>
<th>$^{235}\text{U}$</th>
<th></th>
<th>$^{238}\text{U}$</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>core</td>
<td>(n,f)</td>
<td>Blanket</td>
<td>(n,f)</td>
<td>Blanket</td>
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<tr>
<td>(n,γ)</td>
<td></td>
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<td>(n,γ)</td>
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