Generation of fission yield covariances to correct discrepancies in the JEFF fission yield library

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ENDF-6-format libraries (JEFF, ENDF/B, ...):

- Independent Fission Yields \([Y]\)
- Cumulative Fission Yields \([C]\)
  - Best estimate
  - Uncertainties

No covariance matrix
- ENDF-6-format libraries (JEFF, ENDF/B, ...):
  - Independent Fission Yields \([Y]\)
  - Cumulative Fission Yields \([C]\)
    - Best estimate
    - Uncertainties

- Physical constraints:

  **Charge conservation**
  \[ \sum_i Z_i Y_i = Z_{CN} - Z_{LCP} \]

  **Mass conservation**
  \[ \sum_i A_i Y_i = A_{CN} - \bar{v}_p(E) - A_{LCP} \]

  **Individual charge conservation**
  \[ \sum_{Z=Z_1} Y = \sum_{Z=Z_2} Y \quad Z_1 + Z_2 = Z_{CN} \]

  **Number of fission products**
  \[ \sum_i Y_i = 2 \]

  **Asymmetry**
  \[ \sum_{A_i > \frac{A_{CN}-\bar{v}_p(E)}{2}} Y(A_i) = 1 \]
ENDF-6-format libraries (JEF)

- Independent Fission Yields
- Cumulative Fission Yields
  - Best estimate
  - Uncertainties

Physical constraints:

<table>
<thead>
<tr>
<th>Charge conservation</th>
<th>Number of fission products</th>
</tr>
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<tbody>
<tr>
<td>$\sum_i Z_i Y_i = Z_{CN} - Z_{LCP}$</td>
<td>$\sum_i Y_i = 2$</td>
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Mass conservation

$$\sum_i A_i Y_i = A_{CN} - \bar{\nu}_p(E) - A_{LCP}$$

Individual charge conservation

$$\sum_{Z=Z_1} Y = \sum_{Z=Z_2} Y \quad Z_1 + Z_2 = Z_{CN}$$
ENDF-6-format libraries (JEFF, ENDF/B, ...):

- Independent Fission Yields \([Y]\)
- Cumulative Fission Yields \([C]\)
  - Best estimate
  - Uncertainties
- Chain yields \([Ch]\)
  - Best estimate and uncertainties available in the literature (but not in the ENDF-6 library)


\[
Q Y = C
\]

\[
\sum_{A_i=A^*} Y(A_i) = Ch(A^*)
\]
Need for correlations

- Best-estimate values comply with the constraints
- Uncertainty data show discrepancies ($S^TV_S$)
- Example:
  - Calculation of burnup indicators
    \[ N_{Nd^{148}}(t) \approx \frac{\sum_f \phi C_{Nd^{148}}}{\sigma_c^{Nd^{148}} \phi} \left( 1 - e^{\sigma_c^{Nd^{148}} \phi t} \right) \]
  - Uncertainty on $^{148}$Nd cumulative fission yield
    \[ QY = C \quad \Rightarrow \quad V_C = Q^t V_Y Q \]
- Inconsistency in the moment propagation formula

<table>
<thead>
<tr>
<th></th>
<th>JEFF-3.1.1</th>
<th>ENDF/B-VII.1</th>
</tr>
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<tbody>
<tr>
<td>Library</td>
<td>0.7%</td>
<td>0.35%</td>
</tr>
<tr>
<td>Calculated</td>
<td>9.67%</td>
<td>21.42%</td>
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No correlation between fission yields
Discrepancy in the library (U235-th)

- Chain yields
- Cumulative yields
Covariance matrix generation

- Generalised least square approach

\[ \chi^2 = (\vartheta - \vartheta_a)^+ V_a^{-1} (\vartheta - \vartheta_a) + (\eta - y)^+ V^{-1} (\eta - y_a) = \text{minimum} \]

- Updating procedure

PRIOR

\[ \vartheta_a \]
\[ V_a \]

CONSTRAINT

\[ y = S \vartheta \]
\[ V_y = SV \vartheta S^+ \]

OBSERVABLE

\[ y_a = y(\vartheta_a) \]
\[ V_y = SV_a S^+ \]

GLS METHOD

\[ \vartheta_{\text{upd.}} = \vartheta_a + V_a S^+ (SV_a S^+ + V)^{-1} (\eta - y_a) \]
\[ V_{\text{upd.}} = V_a + V_a S^+ (SV_a S^+ + V)^{-1} SV_a \]

NEW INFORMATION

\[ y_{\text{new}} \]
\[ V_{y,\text{new}} \]
Iterative updating process

\[ y = Sv\theta \]

\[ V_y = SV\theta S^+ \]

**NEW INFORMATION**

\[ y_{\text{new}} \]

\[ V_{y,\text{new}} \]

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<th>Constraint</th>
<th>( y_{\text{new}} )</th>
<th>( V_{y,\text{new}} )</th>
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<tr>
<td>Independent to Chain</td>
<td>Evaluations*</td>
<td>Evaluations*</td>
</tr>
<tr>
<td>Charge conservation</td>
<td>( Z_{CN} - Z_{LCP} )</td>
<td>0.01%</td>
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<tr>
<td>Mass conservation</td>
<td>( A_{CN} - \bar{v}<em>p(E) - A</em>{LCP} )</td>
<td>( \text{cov} \ \bar{v}_p(E) )</td>
</tr>
<tr>
<td># of fission products</td>
<td>2</td>
<td>0.01%</td>
</tr>
<tr>
<td>Asymmetry</td>
<td>1</td>
<td>0.01%</td>
</tr>
<tr>
<td>Ind. charge conserv.</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Independent to Cum</td>
<td>Measurements?</td>
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*IAEA, Handbook of Nuclear Data for Safeguards (2008)*
Example of correlation matrix (U235-th)

- Independent yields
- Cumulative yields
Double effect of the updating process

Charge yields = \( \sum_{Z_i=Z^*} Y(Z_i) \)
Need for correlations

Example:

- Calculation of burnup indicators

\[ N_{Nd^{148}}(t) \approx \frac{\Sigma_f \phi C_{Nd^{148}}}{\sigma_c^{Nd^{148}} \phi} \left( 1 - e^{\sigma_c^{Nd^{148}} \phi t} \right) \]

- We introduced correlations amongst the independent fission yields
- Uncertainty on \(^{148}\text{Nd}\) cumulative fission yield

\[ QY = C \quad \Rightarrow \quad V_C = Q^t V_Y Q \]

WITH CORRELATIONS

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- Now the moment propagation formula is consistent
Discrepancy in the library (U235-th)

- **Chain yields**

- **Cumulative yields**
Discrepancy in the library (U235-th)

- Chain yields

- Cumulative yields
Summary

- Generation of correlations between fission yields
- Covariances represent physical constraints and evaluated uncertainties
- Correlations solve the discrepancies in the libraries
- We applied our covariance update procedure to **14 systems of the JEFF-3.1.1 library:**
  - Th-232 fast, 14-MeV
  - U-233 thermal, fast, 14-MeV
  - U-235 thermal, fast, 14-MeV
  - U-238 fast, 14-MeV
  - Pu-239 thermal, fast
  - Pu-241 thermal, fast
- Attempt to create inter-energy correlations using $\tilde{\nu}$ correlations
- **New ENDF-like format to store covariances** (mix MF=8, MF=33) MF=38 MT=454
Impact on FPDH calculations

![Graph showing impact on FPDH calculations](image)

- **VARIANCE**
- **CORRELATIONS**
REBUS: irradiation of samples ($\text{UO}_2$ fuel elements among them) in commercial PWR at Neckarwestheim NPP (Germany)
Gamma spectroscopy $\rightarrow$ burn-up profile
Radiochemical analysis $\rightarrow$ inventories of radionuclides

Impact on $k_{\text{eff}}$
Impact on nuclide density uncertainties
Conclusions

- Discrepancies in uncertainties
- Covariance generation by GLS method
- We generated covariance matrices for (almost) all the systems in JEFF-3.1.1
- Covariance matrices are stored in new format \( MF=38, MF=454 \)
- Fission yield covariance matrices help reduce the response uncertainties to acceptable values