Integral adjustment and fine structure treatment for fusion evaluations

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Evaluation system

Overview

• Overarching goal: a general-purpose nuclear data evaluation pipeline with capability to address all fusion-relevant isotopes.

• Strong focus on evaluation of nuclear data uncertainties.
Updates 2023:

• New flexible covariance function in GP-parameter domain.
• Description of model defects in the resonance region - heteroscedastic GP.

Alf Göök et al., WONDER23, A Nuclear Data Evaluation Pipeline for the Fast Neutron Energy Range – using heteroscedastic Gaussian processes to treat model defects.

Presented today:
• Method for integral calibration.
• Treatment of fine-structure.
Integral calibration

• 2022 deliverable: Report on how to integrate integral calibration into the pipeline.
Total Monte Carlo - BMC

Random file #1
Random file #2
Random file #N

Integral experiment

MC-Calculation #1
MC-Calculation #2
MC-Calculation #N

Output file #1
Output file #2
Output file #N

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

New Random files produced

\[ \vec{p}_{upd}, P_{upd} \]
Half Monte Carlo (HMC)

Matrix calculations

Integral response for central file. Nuclear data file 0 (central file)

\[ R_i = R_0 + \text{Jacobian} \times [\text{ND}_i - \text{ND}_0] \]

Integral response file i.

Sensitivity matrix. A Jacobian for the integral experiment of interest

Random file i

Half Monte Carlo - HBMC

Random file #1
Random file #2
Random file #N

Integral experiment.
Sensitivity matrix.
Central value.

Matrix-Calculation #1
Matrix-Calculation #2

MC-Calculation #N

Output file #1
Output file #2
Output file #N

\( w_i = e^{\frac{-\chi^2}{2}} \)

New Random files produced

\( \vec{p}_{\text{upd}}, P_{\text{upd}} \)
Status and outlook

- Python framework developed.
- Tested on Godiva (DICE sensitivity matrix).
- Presented at WONDER23: E. Andersson Sundén et al., *Evaluation of nuclear data using the Half Monte Carlo technique*.

Next step
- Test on Fe56 (SINBAD together with EPFL).
- Feedback to model parameters.
The ratio of the best estimates of the (n,fission) cross section before and after the weights of the Half Monte Carlo method has been applied.
The relative uncertainties of the (n,fission) cross section before (red) and after (blue) the weights of the Half Monte Carlo method has been applied.
Correlation: **Before** integral adjustment

As we include the integral data in the evaluation the correlation between the reaction channels changes.
As we include the integral data in the evaluation the correlation between the reaction channels changes.

Correlation: \textbf{After} integral adjustment

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{correlation_plot.png}
\caption{Correlation plot showing changes in correlation before and after integral adjustment.}
\end{figure}
Comparisons of Sandwiches, Halfway Monte Carlo and Total Monte Carlo

<table>
<thead>
<tr>
<th>Sandwich</th>
<th>TMC</th>
<th>HMC</th>
</tr>
</thead>
<tbody>
<tr>
<td>● Linear assumption.</td>
<td>● Non-linear behaviors are covered.</td>
<td>● Linear assumption</td>
</tr>
<tr>
<td>● Sensitivity matrices for UQ</td>
<td>● Transport codes for UQ.</td>
<td>● Sensitivity matrices for UQ</td>
</tr>
<tr>
<td>● Fast.</td>
<td>● Computationally expensive.</td>
<td>● Fast</td>
</tr>
<tr>
<td>● Uncertainties described by normal distributions.</td>
<td>● Random files describe uncertainties</td>
<td>● Random files describe uncertainties</td>
</tr>
</tbody>
</table>
Deliverable 2023

- Develop a methodology to implement fine structure data in the energy range 1-6 MeV.
Energy-dependent Talys parameters cannot reproduce rapid variation in low energy region (1-5MeV).
New discrepancy model

\[ y_j = f(E_j; \beta + \delta(E_j)) + d(E)_j + \varepsilon; \]

\[ d_{j,\text{ch}} \sim GP(E) \]

\[ d_{\text{sum}} = \sum_{\text{ch}} d_{\text{ch}} \]

Similar to how it is solved in
G. Schnabel et al., Nuclear data evaluation with Bayesian networks
Reconstructed low-energy structures in the cross-section.
To do

• GP-regression on large data sets is slow.
  – Speed-up is needed.
• Solution?: Sparse covariance function\(^a\)
• Truncation → very sparse covariance matrices

\(^a\)A. Melkumyan and F. Ramos, A Sparse Covariance Function for Exact Gaussian Process Inference in Large Datasets in: IJCAI 2009, 1936-1942
Challenge!

• How to integrate into T6 framework?
  – Updating the TALYS randomfiles.
  or
  – Updating TEFAL to handle discrepancy files.
Summary 2023

• Pipeline update with new and improved methods.
  ➢ New flexible covariance function in GP-parameter domain.
  ➢ Description of model defects in the resonance region - heteroscedastic GP.
• New method for integral calibration.
• New method for fine-structure treatment.
Questions
References

- E. Andersson Sundén et al., WONDER23, *Evaluation of nuclear data using the Half Monte Carlo technique*