Meeting of the WPEC Subgroup 44 on the Investigation of Covariance Data in General Purpose Nuclear Data Libraries

Summary Record

26 November 2019, NEA Headquarters, Boulogne-Billancourt, France

Information Note: Use this area to provide a brief summary of the document or highlight any important information. This text will be displayed on the document page in O.N.E for Members and Partners.

Dr. Michael Fleming
+33 1 73 21 28 22
michael.fleming@oecd-nea.org
OECD/NEA Nuclear Science Committee

Working Party on International Nuclear Data Evaluation Co-operation (WPEC)
Meeting of the WPEC Subgroup 44 on the Investigation of Covariance Data in General Purpose Nuclear Data Libraries

NEA Headquarters Room BB10
46 quai Alphonse Le Gallo, 92100 Boulogne-Billancourt, France

SUMMARY RECORD

1. Welcome
The Chair, V. Sobes, welcomed the participants (see Appendix 1) and the WPEC Secretariat, M. Fleming, noting that the subgroup monitor, C. de Saint Jean, sent his apologies for his absence.

2. Adoption of the agenda
The agenda (see Appendix 2) was adopted without modification.

3. Review of action items
Two general sets of actions were raised in the previous meeting (see Appendix 3 of NEA/NSC/WPEC/DOC(2019)7) related to the summary report of the subgroup and all participants had been invited to participate in the inter-comparison study considering cross-correlations between reaction channels and isotopes in integral benchmarks. These are the subject of the following two sections of the summary record of this meeting.

4. Inter-comparison of correlations study
4.1. Subgroup 44 Computational Inter-comparison Exercise – Nuclear data libraries correlation estimates

V. Sobes presented work done at ORNL for the inter-comparison study that was agreed at the previous meeting. This includes correlations between the CIELO isotopes: \( ^1H, ^{16}O, ^{56}Fe, ^{235}U, ^{238}U \) and \( ^{239}Pu \), using the available correlations in the library of the participant’s choice (ENDF/B-VII.0 in this case) and a suite of integral benchmarks as selected by the participants. In the work shown, the ORNL VALID suite was used for the integral benchmarks. The OECD-NEA DICE sensitivity database for over 4000 benchmarks were reviewed to determine regions of sensitivity variation and for those reaction channels and energy ranges the correlations were excluded. Results obtained with the TSURFER code were shown graphically and had been sent to the SG44 participants in advance of the meeting for comparison. I. Hill proposed that the exercise...
be run with integral benchmarks removed that were not in agreement with the nominal calculation values, indicating that they were not used in any explicit or implicit fitting of the original evaluation.

4.2. Preliminary results on SG44 covariance inter-comparison study using JENDL-4.0 and JAEA’s integral database

K. Yokoyama presented the results of correlation calculations done at JAEA using the JENDL-4.0 covariances, ADJ2017 adjusted cross-sections and three different sets of integral experiments: (1) the ZPPR-9 $k_{\text{eff}}$, (2) the PMF-1 $k_{\text{eff}}$ and (3) the full set of 620 fast integral experiments used to create ADJ2017, including criticality, reaction rates, control rod worth, void coefficients, Doppler reactivity and more. Select results were shown for each of the cases, demonstrating the expected result that the use of benchmarks that are not sensitivity to different energies and/or isotopes/reactions will not generate similar correlations. Some comparisons between the results from V. Sobes were discussed, demonstrating that in cases with significant sets of benchmarks, some correlations would definitively be in disagreement. However, some correlation terms were in general agreement, such as the fission cross section and nubar, and this suggested a refinement of the original, broad hypothesis. It was agreed to narrow the scope of the inter-comparison study.

4.3. Monte-Carlo sampling: Lessons learnt from the past 3 years at PSI and CEA

D. Rochman reviewed work done in a partnership between CEA and PSI over the past years using Bayesian Monte-Carlo and Backward-Forward Monte Carlo approaches. Multiple cases had been considered, including individual benchmarks, suites of a few or dozens, and other experiment types such as boron letdown curves in reactor analyses. The graphical results shown in the presentation demonstrated that the set of integral benchmarks used, amongst other things, will determine the correlations that result. Ultimately, integral benchmarks have been and will continue to be used as part of the process to make evaluated nuclear data libraries and it was strongly recommended that evaluators take these into account during the evaluation process and document the process.

4.4. UPM/IAEA contributions to inter-comparison study

O. Cabellos presented a joint effort between the IAEA and UMP to generate correlations in the exercise, using a UMC-B method and GLLS, between fission cross sections, capture cross sections and nubar. The NJOY iwt=4 processing option was used, reflecting a thermalised system weighting function for the three-group cross section processing. Both the GLLS and UMC-B results were very similar and results using ENDF/B-VII.0 and JEFF-3.3 were compared alongside the results that V. Sobes had prepared. While the signs and rough magnitudes were similar between the different libraries and results from Sobes, the UPM/IAEA results showed no correlations between different energy groups and some values were as much as 50% different (e.g. thermal $^{235}$U capture to nubar). It was later shown that the method presented generated negative eigenvalues in the covariance matrix, as highlighted by using NDaST and considering correlations between this same nubar and capture of $^{235}$U. It was proposed that these data
be made available in the format proposed by the Chair or some other format so that further analysis may be performed.

4.5. Review of the status of the inter-comparison study

The group reviewed the findings from these presentations and analyses, concluding that the original hypothesis was, as designed, too broad and that some of the cross-correlations will necessarily depend on the integral benchmarks considered and, to some extent, on the methods and prior correlations. It was agreed that a revised description would be prepared by the Chair, V. Sobes, and circulated in early 2020 so that participants may refine their analyses and results in advance of the May 2020 meeting.

5. Contributions to the final report

The Chair, V. Sobes, reviewed the outline of the subgroup report that had been drafted in the previous meeting (see Appendix 3 of NEA/NSC/WPEC/DOC(2019)7) with various contributions agreed from the participants of that meeting. The progress was reviewed for all sections and is summarised below. Some sections were agreed to be re-organised and/or removed in a revised outline and all materials will be shared via a password-protected area of the NEA website for SG44. A brief summary of the status and changes to the document draft agreed in the previous meeting is provided in Appendix 3 of this document.

6. Next meeting and any other business

The next meeting will occur during the week of 11-15 May 2020 at the NEA Headquarters in Boulogne-Billancourt. The exact dates will be confirmed with all of the WPEC subgroup chairs and communicated in December 2020.
APPENDIX 1

List of participants to the 26 November 2019 Meeting of Subgroup 44 on the Investigation of Covariance Data in General Purpose Nuclear Data Libraries

<table>
<thead>
<tr>
<th>First Name</th>
<th>Last Name</th>
<th>Country</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Erwin</td>
<td>ALHASSAN</td>
<td>SWITZERLAND</td>
<td></td>
</tr>
<tr>
<td>2 Francisco</td>
<td>ALVAREZ VELARDE</td>
<td>SPAIN</td>
<td></td>
</tr>
<tr>
<td>3 Oscar</td>
<td>CABELLOS</td>
<td>SPAIN</td>
<td>Remote</td>
</tr>
<tr>
<td>4 Luca</td>
<td>FIORITO</td>
<td>BELGIUM</td>
<td></td>
</tr>
<tr>
<td>5 Michael</td>
<td>FLEMING</td>
<td>NEA</td>
<td>Secretariat</td>
</tr>
<tr>
<td>6 Ian</td>
<td>HILL</td>
<td>NEA</td>
<td></td>
</tr>
<tr>
<td>7 Robert</td>
<td>JACQMIN</td>
<td>FRANCE</td>
<td></td>
</tr>
<tr>
<td>8 Arjan</td>
<td>KONING</td>
<td>IAEA</td>
<td></td>
</tr>
<tr>
<td>9 Alexander</td>
<td>KONOBEV</td>
<td>GERMANY</td>
<td></td>
</tr>
<tr>
<td>10 Helmut</td>
<td>LEEB</td>
<td>AUSTRIA</td>
<td></td>
</tr>
<tr>
<td>11 Robert</td>
<td>MILLS</td>
<td>UNITED KINGDOM</td>
<td></td>
</tr>
<tr>
<td>12 Denise</td>
<td>NEUDECKER</td>
<td>UNITED STATES</td>
<td>Remote</td>
</tr>
<tr>
<td>13 Giuseppe</td>
<td>PALMIOTTI</td>
<td>UNITED STATES</td>
<td></td>
</tr>
<tr>
<td>14 Dimitri</td>
<td>ROCHMAN</td>
<td>SWITZERLAND</td>
<td></td>
</tr>
<tr>
<td>15 Pablo</td>
<td>ROMOJARO</td>
<td>SPAIN</td>
<td>Remote</td>
</tr>
<tr>
<td>16 Georg</td>
<td>SCHNABEL</td>
<td>AUSTRIA</td>
<td></td>
</tr>
<tr>
<td>17 Allan</td>
<td>SIMPSON</td>
<td>UNITED KINGDOM</td>
<td></td>
</tr>
<tr>
<td>18 Henrik</td>
<td>SJOSTRAND</td>
<td>SWEDEN</td>
<td></td>
</tr>
<tr>
<td>19 Vladimir</td>
<td>SOBES</td>
<td>UNITED STATES</td>
<td>Chair</td>
</tr>
<tr>
<td>20 Alejandro</td>
<td>SONZOGNI</td>
<td>UNITED STATES</td>
<td>Remote</td>
</tr>
<tr>
<td>21 Haicheng</td>
<td>WU</td>
<td>CHINA</td>
<td></td>
</tr>
<tr>
<td>22 Kenji</td>
<td>YOKOYAMA</td>
<td>JAPAN</td>
<td></td>
</tr>
</tbody>
</table>
APPENDIX 2

Working Party on International Nuclear Data Evaluation Co-operation (WPEC)  
Meeting of the WPEC Subgroup 44 on the Investigation of Covariance Data in General Purpose Nuclear Data Libraries

NEA Headquarters Room BB10  
46 quai Alphonse Le Gallo, 92100 Boulogne-Billancourt, France

AGENDA

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
</tr>
</thead>
<tbody>
<tr>
<td>14:00</td>
<td>Welcome and introductions</td>
</tr>
<tr>
<td>14:10</td>
<td>Discussion of the inter-comparison study and ORNL contributions</td>
</tr>
<tr>
<td>14:30</td>
<td>JAEA contributions to inter-comparison study</td>
</tr>
<tr>
<td>14:50</td>
<td>Microscopic correlations from integral data through Monte-Carlo sampling: Lessons learnt from the past 3 years at PSI and CEA</td>
</tr>
<tr>
<td>15:10</td>
<td>Coffee Break</td>
</tr>
<tr>
<td>15:30</td>
<td>UPM/IAEA contributions to inter-comparison study</td>
</tr>
<tr>
<td>15:50</td>
<td>Discussion on the inter-comparison study</td>
</tr>
<tr>
<td>16:40</td>
<td>Discussion of draft of SG44 final report and writing assignments</td>
</tr>
<tr>
<td>17:45</td>
<td>Action items, next meeting and AOB</td>
</tr>
</tbody>
</table>

---

Chair  
V. Sobes  
K. Yokoyama  
D. Rochman  
O. Cabellos  
All  
All  
Chair
APPENDIX 3

Status report of and actions for the WPEC Subgroup 44 on the Investigation of Covariance Data in General Purpose Nuclear Data Libraries Summary Report

The format and outline of the WPEC Subgroup report was agreed at the meeting on 24 June 2019 (see Appendix 3 of NEA/NSC/WPEC/DOC(2019)7). The status of all sections were reviewed and are summarised below.

1. Section completed by V. Sobes

2. Section introduction to be completed by Chair when material is prepared.
   2.a. C. de Saint Jean is working on this section but no draft is available.
   2.b D. Neudecker is preparing material for this subsection and will integrate contributions from G. Schnabel and H. Leeb as and when they are prepared. It was agreed that all subsubsections (i-iii) are unnecessary and this will be completed with one subsection.

3. D. Neudecker has already prepared material for the upcoming paper on templates and will produce a summary for this section of the report.
   3.a.iii A. Koning confirmed that V. Zerkin, under his line management, will provide this section for the report.
   3.b In preparation by H. Sjöstrand
   3.c In preparation by H. Sjöstrand

4. Completed by V. Sobes
   4.a Completed by V. Sobes
   4.b.i Completed by V. Sobes
   4.b.ii V. Sobes to request a contribution from C. Mattoon
   4.c Completed by V. Sobes
   4.d I. Hill agreed to contribute on cross-correlations based on work done in SG33 and the WPNCS SG1.

5. 5.a Completed by V. Sobes and will be distributed for review by other participants. D. Rochman volunteered to review the content and provide feedback.
5.b R. Mills volunteered to provide a section on fission yield correlations based on the results of the WPEC SG37 report materials

6. The results from the inter-comparison study will be put in this section, but this activity will require a re-drafting of the specification for the inter-comparison by V. Sobes.

7.
7.a Completed by D. Neudecker
7.b L. Fiorito to provide content, integrating material provided by A. Trkov
7.c V. Sobes to contact C. Mattoon to request a contribution
7.d Activity completed and V. Sobes to finish existing draft

8.
8.a D. Neudecker to provide a short note on PFNS correlations based on existing work
8.b V. Sobes to request contribution from A. Trkov
8.c Removed
8.d Contributions to be provided by A. Koning, H. Sjöstrand and/or G. Schnabel