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NUCLEAR ENERGY AGENCY
NUCLEAR SCIENCE COMMITTEE

Working Party on International Nuclear Data Evaluation Co-operation

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

SUMMARY RECORD

24 June 2019
NEA Headquarters
Boulogne-Billancourt, France

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OECD/NEA Nuclear Science Committee

Working Party on International Nuclear Data Evaluation Co-operation (WPEC)

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NEA Headquarters Room BB12

46 quai Alphonse Le Gallo, 92100 Boulogne-Billancourt, France

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SUMMARY RECORD

1. Welcome

The Chair, **V. Sobes**, welcomed the participants (see ***Appendix 1***) and the WPEC Secretariat, **M. Fleming**. The Co-Chair, **Cyrille de Saint Jean**, was unable to attend in person but was available via WebEx connection.

2. Adoption of the agenda

The agenda as described in ***Appendix 2*** was adopted with additional presentations from D. Brown on the Nuclear Data Belief Network and C. Perfetti on Improved Calibration of Nuclear Resonance Parameters.

3. Progress on the Development of Thermal Scattering Covariance Formats

V. Sobes, on behalf of **A. Tumulak**, presented work done at U. Michigan and ORNL in defining formats for TSL covariances. It was noted that, since the ENDF-6 format does not possess a format for this covariance it cannot be proposed. However, `gridded2D` within `covarianceSections` in the GNDS specification can be used. For each β-β' pair can then have an α-α' covariance matrix. Using the 1000 TMC TSL files generated by **G. Noguere** that were available on the WPEC subgroup 42 webpage, the calculation of covariances were calculated and stored in GNDS format. These generated a large amount of data and it was realised that an eigenvalue decomposition could be a more suitable description that will be prototyped in future work.

4. New paradigm for nuclear data evaluation

M. Herman reviewed the state of current nuclear data evaluation practices and highlighted the major shortcomings that now must be addressed as the community attempted to improve upon the most recent evaluated libraries. The proposed 'new paradigm' is to store all evaluation input materials as a self-documented and reproducible repository (see WPEC subgroup 49 proposal made 27 June 2019) and to consistently adjust a fully library in a reproducible and automated way. It was argued that the existing evaluations and most reaction model codes are robust enough and, potentially with the addition of some model defect handling methodologies (e.g. energy-dependent input parameters or ENDF-6 file-space Gaussian processes) we are ready to perform carefully documented and understood integral adjustment.

5. The role of fission yield correlations to obtain realistic uncertainty values in the summation method

A. Sonzogni presented the application of fission yield covariances to summation calculations. He reviewed several recent experimental results related to anti-neutrinos and other fission observables and then demonstrated summation calculations that are used to simulate these phenomena. Using independent fission yield correlations from the GEF code, correlated uncertainty calculations were performed and compared with experimental results and uncertainties, obtaining much better agreement in the latter with correlations included with the uncertainty propagation. It was noted that no library possesses official covariances for fission yields and that the ENDF-6 format does not currently accommodate this, although it may be extended in future and/or GNDS may be used.

6. ENDF/B-VIII.0 Augmented Covariance Data

V. Sobes discussed the philosophy behind the ENDF/B-VIII.0 covariance evaluations, where the nominal values provide excellent agreement with many well-known integral benchmarks, yet the propagation of the covariances result in uncertainties that are much larger than the experimental uncertainties. While it may not be acceptable to reduce the uncertainties on the differential quantities below current values, cross-correlations between quantities may be inferred from integral experiments and these may reduce uncertainties to values that are in general agreement with integral uncertainties. A prototype study was performed with cross-correlations that reduced the ENDF/B-VIII.0 uncertainties for a set of benchmarks considered.

7. Status and Requirements of Nuclear Data Variance-Covariance Matrices for the Neutronic Assessment of Fast Reactor Cores

G. Rimpault presented work calculating key neutronic parameters in SFR cores, with uncertainties propagated from major libraries to these integral quantities. Sensitivities were calculated for various quantities and used to propagate uncertainties from the nuclear data covariances. ENDF/B-VII.1, COMAC and JENDL-4.0 were considered for k_{eff}, β_{eff}, $\rho_{Doppler}$ and $\rho_{Na\text{-}Void}$. There are significant differences between covariances coming from COMAC, ENDF BVII.1 and JENDL4.0. These differences are partly due to the way the evaluation process has been done. For instance:

- The differences in the ^{238}U inelastic cross section are presumably due to optical models being used, differential measurements being scarce.
- The differences in the ^{23}Na cross sections are due to the use of more recent differential measurements performed at IRMM (inelastic) and Oak Ridge (total).

However, several nuclear data covariance data are not reliable enough and better understanding of the differences are required (for PFNS and some capture cross sections, for instance). This is needed for assessing safety dossiers directly or through integral data assimilation. By using integral assimilation with well-regarded experiments (e.g. PMF-1), the uncertainties with several of these parameters can be reduced. It was noted that, in part due to a lack of differential experimental data, ^{238}U inelastic scattering, ^{23}Na cross sections and some PFNS, the uncertainties are relatively large and impact the propagated uncertainties. Covariances on delayed neutron constants and scattering distributions are lacking in some evaluations and are required for complete uncertainty propagation.

8. The identification and treatment of unrecognized uncertainties and the impact on evaluated uncertainties

H. Sjöstrand presented work done to address unreported systematic uncertainties (USU) that manifests as inconsistent data. Following previous work to address this issue, the technique of Marginal Likelihood Optimisation (MLO) has been employed to identify and correct erroneous experimental uncertainties in synthetic data studies. Three studies were shown to demonstrate interpretations of the approach in different circumstances, e.g. where all measurements are systematically wrong by a similar factor. It was stressed that this technique requires expert judgement and cannot replace knowledge of the underlying data.

9. Improved Calibration of Nuclear Resonance Parameters

C. Perfetti presented a work plan that will focus on the generation of sensitivity profiles not based exclusively on energy-averaged multigroup nuclear data, but on fundamental parameters such as resonance parameters. As part of a 5-year plan, the first steps will consider resolved resonance parameters and modifications to the TSURFER code to allow resolved resonance sensitivities and assimilation of integral benchmarks. This will be followed by unresolved and potentially fast energy range sensitivity studies.

10. Report on mini-CSEWG meeting and other covariance developments

D. Neudecker presented a review of the recent mini-CSEWG meeting that discussed the status of uncertainty templates for a range of different nuclear observables. The nature of a template is a reference of all typical measurement types for a specific observable with a comprehensive list of typical uncertainty sources, reasonable ranges for these values based on expert judgement and estimated correlation information. This has built upon earlier work done under the auspices of the IAEA and earlier work from D.L. Smith at ANL. The status and future work planned for templates for different obervables were reviewed, including several that will be the subject of a upcoming NDS publication.

11. The Nuclear Data Belief Network

D. Brown gave a presentation reviewing the nature of Gaussian Process Regression (GPR) and the ways that the nuclear data community are already employing this through various aspects of the evaluation procedures in place within each nuclear data programme. The network including (differential and integral) experimental data, input parameter libraries, model codes, evaluated files and libraries represents a large, interwoven Gaussian Belief Network that specialists have been applying Machine Learning (ML) techniques to for many years. One complication makes the automation of ML algorithms problematic: in order to improve performance in nuclear data evaluation, files and various other parts of this network have already been adjusted to ensure good performance on important quantities.

12. Discussion and other business

As this will be the final year of the subgroup 44, the group starting planning the activities to wrap up the subgroup and prepare a summary report. A draft outline was circulated in advance of the meeting and this was discussed in detail. Participants pledged to provide contributions on the sections defined. ***Appendix 3*** includes the draft document, including changes made during the meeting in red and the original in black.

An additional cross-comparison study will be run on the correlation between fission cross sections and nubar. Multiple participants expressed their interest in this study, in part due to the lack of dependence upon any specific integral benchmarks and the availability of data that has already been evaluated.

The subgroup may have an additional meeting during 25-29 November 2019, in parallel to the JEFF meetings, and the final subgroup meeting will take place in the week of 11-15 May 2020.

APPENDIX 1

List of participants to the 24 June 2019 Meeting of Subgroup 44 on the Investigation of Covariance Data in General Purpose Nuclear Data Libraries

	First Name	Last Name	Country	Notes
1	David	BROWN	UNITED STATES	
2	Yaron	DANON	UNITED STATES	
3	Cyrille	DESAINTJEAN	FRANCE	*Remote*
4	Isabelle	DUHAMEL	FRANCE	
5	Luca	FIORITO	BELGIUM	
6	Michael	FLEMING	NEA	*Secretariat*
7	Zhigang	GE	CHINA	*Remote*
8	Michal	HERMAN	UNITED STATES	
9	Andrew	HOLCOMB	UNITED STATES	
10	Jesse	HOLMES	UNITED STATES	
11	Raphaelle	ICHOU	FRANCE	
12	Osamu	IWAMOTO	JAPAN	
13	Nobuyuki	IWAMOTO	JAPAN	
14	Luiz Carlos	LEAL	FRANCE	
15	Nicolas	LECLAIRE	FRANCE	
16	Caleb	MATTOON	UNITED STATES	
17	Denise	NEUDECKER	UNITED STATES	
18	Giuseppe	PALMIOTTI	UNITED STATES	
19	Chris	PERFETTI	UNITED STATES	
20	Gerald	RIMPAULT	FRANCE	
21	Pablo	ROMOJARO	SPAIN	
22	Evgeny	ROZHIKHIN	RUSSIA	
23	Xichao	RUAN	CHINA	*Remote*
24	Henrik	SJOSTRAND	SWEDEN	
25	Vladimir	SOBES	UNITED STATES	*Chair*
26	Alejandro	SONZOGNI	UNITED STATES	
27	Ian	THOMPSON	UNITED STATES	
28	Morgan	WHITE	UNITED STATES	
29	Dorothea	WIARDA	UNITED STATES	
30	Kenji	YOKOYAMA	JAPAN	

APPENDIX 2

OECD/NEA Nuclear Science Committee

Working Party on International Nuclear Data Evaluation Co-operation (WPEC)

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

NEA Headquarters Room BB12

46 quai Alphonse Le Gallo, 92100 Boulogne-Billancourt, France

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AGENDA

1. Welcome and introductions	Chair
2. Adoption of the agenda	All
3. Progress on the Development of Thermal Scattering Covariance Formats	A. Tumulak
4. New paradigm for nuclear data evaluation	M. Herman
5. The role of fission yield correlations to obtain realistic uncertainty values in the summation method	A. Sonzogni
6. ENDF/B-VIII.0 Augmented Covariance Data	V. Sobes
7. Status and Requirements of Nuclear Data Variance-Covariance Matrices for the Neutronic Assessment of Fast Reactor Cores	G. Rimpault
8. The identification and treatment of unrecognized uncertainties and the impact on evaluated uncertainties	H. Sjöstrand
9. Improved Calibration of Nuclear Resonance Parameters	C. Perfetti
10. Report on mini-CSEWG meeting and other covariance developments	D. Neudecker
11. The Nuclear Data Belief Network	D. Brown
12. Discussion and other business	

APPENDIX 3

Draft Summary Report Outline from the 24 June 2019 Meeting of Subgroup 44 on the Investigation of Covariance Data in General Purpose Nuclear Data Libraries

1. Introduction [Sobes]
2. Evaluation techniques proposed to break into two sections: (I) main techniques used [Cyrille] and (II) synthesize discussion from previous meetings/discussions on known problems (model defects/biases, (R/U)RR uncertainties) [Denise/Schnabel/Henrik/Leeb]
    a. Model defects: phenomenological models can be poor but with very low evaluated uncertainties
    b. Model biases: inference of biases from advanced models
    c. Treatment and representation of uncertainties in the unresolved resonance region where self-shielding is important for reactors
3. Analysis of experimental data results from the mini-CSEWG [Denise/Lewis], including experimental cross-correlations
    a. Sources of experimental uncertainty
        i. Catalogue
        ii. Publication requirements (not only numbers)
        iii. Recommendations for EXFOR database IAEA contribution on evaluated EXFOR [Zerkin]
        iv. Algorithms/methods Ni evaluation example [Sjöstrand/Schnabel]
    b. Commenting on autonomous/automatic methods See previous bullet [UU]
    c. Commenting on handling of discrepant data sets discrepant experiments work [UU]
4. Propagation of uncertainty and integral experiments - Collaboration with SG46
    a. Use of integral experiments in evaluations, documentation not guidance for whether or not to utilise IE, but comments regarding documentation [Sobes]
    b. Other probability distributions for nuclear data uncertainty review paper from CW to consider inclusion [Sobes]
        i. Document
        ii. Format
    c. Testing/comparison/consistency of covariance data pub methodology [Denise]
    d. IE cross-correlation [Hill]
5. Cross-correlation
    ~~a. Reactions (unitarity)~~
    b. Cross-isotope and when to neglect [Sobes/invite others]
    ~~c. Other types of data, distributions~~
    d. Fission yields [Sonzogni/Pigni/Fiorito/Serot/Rochman]
    ~~e. Space for storing evaluation/integral experiments correlation~~
    f. Fission spectra E_{in}/E_{out} Correlations

6. New computational benchmark

7. Formats and interpretation [Denise to reformat content from LANL report]
    a. Documentation of covariance evaluation technique

        i. Clear interpretation by evaluator
        ii. Model parameters and code
        iii. Reporting known unknowns vs estimating unknown unknowns
        iv. Clear interpretation by user
    b. Angular distribution covariance format and evaluation [Fiorito, Trkov]
    c. Verification: positive definite, robust, stable to numerical errors. How to deal with negative eigenvalues? [Write eigenvalue decomposition, Mattoon]
    d. ~~Multigroup cross section covariance group and weighting assumptions~~
    e. Thermal scatter law covariance methods [Sobes, Univ Mich]
8. Processing codes wish list – Collaboration with SG43
    a. Cross-correlations
    b. Prompt fission neutron spectra (PFNS) correlations to cross section [short note]
    c. Covariances of secondary distributions (e.g., inelastic) Legendre covariances [Trkov]
    d. Higher order angular distribution
    e. $S(\alpha,\beta)$ format [Sobes, Univ Mich]
    f. Random files cases where limitations of covariances are overcome via random files [Sjöstrand/Schnabel/others to invite]
9. Conclusion
10. References
11. Appendices