

Covariance QA Document: Suggested Update

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Quality Assurance Requirements

- The QA requirements in effect for ENDF/B-VII.1 should be updated for future ENDF/B releases.
- The revised requirements should reflect a “raising of the bar” (to quote Mike Herman), consistent with what is feasible and reasonable.
- These updated requirements should be widely publicized within the nuclear data community, to guide evaluators as work progresses toward the next release of the ENDF/B library.

Details and Comments

- The existing **Covariance QA Document** is currently **posted** on the NNDC/CSEWG website at:
<http://www.nndc.bnl.gov/csewg/covdocs.jsp>
- The **motivations** for having this **QA document** at all were discussed in the **preceding presentation**.
- Most **existing provisions** of the ENDF/B-VII.1 QA document are **retained** in the **suggested revision**.
- The **recommended additions** are **consistent** with points mentioned in the **preceding presentation**.
- The next several slides show the **entire QA document** with the **recommended changes** indicated in **red**.
Deleted items are shown with **double strikethroughs**.

Quality Assurance Requirements for ENDF/B-~~VII.1~~ Covariances

Approved by the Cross Section Evaluation Working Group (CSEWG) for ENDF/B-VII.1
November 1, 2010

Recommended Revisions to the QA Requirements for Future Releases of ENDF/B

Note: The following requirements should apply to components of the neutron sub-library for all new evaluations (or evaluations that have undergone major revisions since the last release of ENDF/B) that are submitted after the date when this document is approved by CSEWG.

1. Basic Mathematical Requirements

*1.1 The numerical data and recipes provided in an evaluated full covariance file must enable complete (square and symmetric) positive **semi-definite** matrices that yield correlations as well as standard deviations (uncertainties) to be generated from the included values by the most widely used contemporary processing codes.*

1.2 Correlation matrices derived from the evaluated covariance data should have unity values along the matrix diagonal, and off-diagonal elements with magnitudes less than unity, to the extent allowed by the numerical precision of the file and consistent with the limitations of the ENDF formats.

1.3 Covariance matrices for evaluated normalized neutron-emission spectra (MF = 35) should satisfy the mathematically mandatory "sum-to-zero" property for rows and columns of the matrix to the extent allowed by the numerical precision of the applicable file and consistent with the limitations of the ENDF formats.

2. Matrix Eigenvalues Requirement

2.1 Full covariance matrices generated from information provided by the evaluator must be positive **semi-definite** (i.e., involve only **non-negative** ~~positive~~ eigenvalues) on the evaluator's original energy grid, to the extent allowed by the numerical precision of the file and consistent with the limitations of the ENDF formats. ~~unless the~~ **The presence** ~~occurrence~~ of zero eigenvalues **should only occur when it** is mandated mathematically by certain physical constraints such as normalization or consistency of partial reaction channel data and those for sums or differences of data for these reaction channels.

3. Requirement of "Realistic" Covariances

3.1 *Covariance data uncertainties and correlations should be consistent in magnitude with the contemporary expectations of experienced nuclear data evaluators as well as addressing the needs of users of these nuclear data for applications.*

3.2 *For evaluated **energy-dependent** cross sections that exceed 1% of the total cross section in magnitude, uncertainties greater than 50% predicted by the provided covariance data should be treated by reviewers as potentially unrealistic and flagged for possible rejection unless they can be amply substantiated by the evaluator. However, for cross sections smaller than 1% of the total cross section, a specified uncertainty that is greater than 50% (but always less than 100%) can be considered as representing a flag signifying that the evaluator believes that the evaluated data should be viewed as qualitatively very uncertain. Reviewers should then treat such large assigned uncertainties as acceptable under the circumstances.*

3.3 *Uncertainties which are very small, e.g., smaller than those assigned to neutron reaction cross section standards for the same process types, should be treated by reviewers as potentially unrealistic and flagged for possible rejection unless they can be amply substantiated by the evaluator. Reviewers should refer to the following table for general guidance in making these judgments, with the understanding that there will be some exceptions based on physical considerations.*

Reaction	Minimum Uncertainty
<i>(n,tot)</i>	1%
<i>(n,el)</i>	2%
<i>(n,γ)</i>	2%
<i>(n,inel)</i>	3%
<i>(n,f)</i>	0.7%
<i>(n,p)</i>	3%
<i>(n,α)</i>	2%
<i>nu-bar</i>	0.7%
<i>Other</i>	3%

4. Covariance Evaluation Consistency, **Completeness, and Methodology** Requirements

4.1 Consistency: *The provided uncertainties for an evaluation must be reasonably consistent in magnitude with the uncertainties in all relevant experimental data, as well as with the evaluator's estimates of the uncertainties associated with nuclear modeling practices employed in the present evaluation (see also Section 3).*

4.2 Completeness: *Covariance data must be provided for each evaluated physical process that is included in the ENDF/B library.*

4.3 Methodology: *The covariance data for each physical process must be generated along with (and as a direct consequence of) the evaluation procedures that produce the central values.*

5. Covariance Format Requirement

5.1 Covariance information must be specified using only approved formats as defined in the contemporary ENDF Formats Manual.

6. Documentation Requirement

6.1 A textual section must be provided within the evaluated file in the category "Descriptive Comments" (MF = 1; MT = 451) that describes how the provided covariance information was generated and also gives a justification for any uncertainty values which appear to be unrealistic (i.e., either unusually small or large as defined in Section 3). If references are available to more detailed descriptions of the procedures used to generate the provided covariance information, including links to information available from the Internet, then they must also be provided in this section.

7. Checking **Procedure Code** and Visual Inspection Requirements

*7.1 The evaluated covariance files must pass all the numerical **and physical consistency** tests that can be performed by the contemporary ~~suite of ENDF/B library checking codes~~ **procedures that are applied** ~~provided~~ by the NNDC **upon receipt of an evaluation that is to be considered for inclusion in the ENDF/B library.***

*7.2 An evaluated covariance file must pass a visual inspection of plots of uncertainties and correlations **matrices** by at least one independent reviewer in order to weed out obvious errors and nonsensical values, and to identify situations where the results appear to be otherwise unrealistic, so that they can be examined further and the issues resolved before the file is accepted (see Section 3).*

8. Processing Requirements

8.1 *The covariance data included in ENDF/B-VII.1 evaluations must be capable of being processed by the most widely used contemporary data processing codes, i.e., by NJOY and PUFF, for typical group structures that are employed in contemporary nuclear applications.*

8.2 *The covariance data generated from processing of ENDF files by NJOY and PUFF in comparable situations should agree numerically to within reasonable precision, consistent with the limitations associated with the ENDF formats and differences in the computational methodologies of these codes.*

Covariance QA “Step-by-Step” Forward

- The recommended changes to the ENDF/B-VII.1 covariance QA document represent an **incremental sharpening** of the **quality requirements** with **no backtracking** needed.
- They are **consistent** with the **capabilities** and **experience** gained by the **data evaluation** and **data applications communities** during the time that has elapsed **since** the release of **ENDF/B-VII.0**.
- The spirit of “**guiding**” and **not “micro-managing”** the **evaluation process**, as **reflected** in the **ENDF/B-VII.1 version** of **QA document**, is preserved.

- Questions?
- Discussion?