Quality Assurance for ENDF/B-VII.1 Covariances

Donald Smith

Argonne National Laboratory

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Introduction

- Work has been in progress for over a year to develop a reasonable set of QA requirements for ENDF/B-VI.1 covariances

- Extensive discussions were held during a mini-CSEWG meeting in June 2010

- The document presented in the next slides reflects a number of compromises that had to be made to gain adequate acceptance

- Improvements can be made to these QA requirements in future releases of ENDF/B as individual user needs evolve over time

1. <u>Basic Mathematical Requirements</u>

- *1.1 The numerical data and recipes provided in an evaluated full covariance file must enable complete (square and symmetric) 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 definite (i.e., involve only 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 occurrence of zero eigenvalues 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 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.*

Table of Minimum "Reasonable" Uncertainties *

Reaction	Minimum Uncertainty
(n,tot)	1%
(n,el)	2%
(n,γ)	2%
(n,inel)	3%
(n,f)	0.7%
nu-bar	0.7%
Other	3%

* Deviations encountered in a review should trigger examination of potential causes

4. Covariance Evaluation Consistency Requirement

- **4.1** *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).*

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 Code and Visual Inspection Requirements

- *7.1 The evaluated covariance files must pass all the numerical tests that can be performed by the contemporary suite of ENDF library checking codes provided by the NNDC.*

- *7.2   An evaluated covariance file must pass a visual inspection of plots of uncertainties and correlations 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. <u>Processing Requirements</u>

- **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.*

Closing Remarks

- A year remains until the planned release of ENDF/B-VII.1 … This should provide enough time to insure that these requirements are met

- It will add to the stature of ENDF/B-VII.1 to have such a set of QA requirements in place and enforced by CSEWG