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

… NARRATIVE …

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Introduction

Evaluated covariance data have become increasingly important in various nuclear applications owing to their roles in assessing the uncertainties of nuclear system operating parameters that are calculated using these data, in conjunction with sophisticated mathematical models of these systems. We can call this application "data assessment."

For many years, the quality of evaluated nuclear data libraries has been judged by their performance when utilized to compute the operating parameters of nuclear reactors and other nuclear systems. Good performance is equated to the occurrence of C/E comparisons close to unity for various system parameters, especially for the criticality constant k-eff, for key nuclear system benchmark facilities.

To achieve good data "quality" in this sense of the word, it has often been necessary to alter the data using ad hoc (non-statistical) methods. Unfortunately, the gains in accuracy produced by such ad hoc data alterations are not guaranteed to extend outside the immediate neighborhood of the systems explicitly considered.

Covariance data offer the ability to improve the accuracy of the differential data in a more general way, namely, through the introduction of accurate integral data using established statistical methods. Such a statistical "data adjustment" is best performed by the user community after the general release of the library, because such an adjustment vastly increases the extent of correlations among the data.

A brief consideration of the two main applications of covariance data discussed above, data assessment and data adjustment, provides a useful framework for performing a quality assurance (QA) examination of covariance data. For example, both of these front-line applications require that the covariance data be processed reliably into multigroup form. Furthermore, neutronics and sensitivity studies are normally done in a relative coarse energy-group environment, with say 33 or 44 energy groups. For this reason, tests to determine whether or not the data are (1) reasonable in magnitude and (2) mathematically well-behaved can be applied most profitably at the coarse-group level.

ENDF/B is a library which has evolved over several decades. At each stage the content, sophistication, and quality of this library has improved. ENDF/B-VII.1, scheduled for release in December 2011, is the latest version of this library, and one that contains more covariance information than any previous version of ENDF/B. It arrives on the scene at a time when the demand for covariance data is strongly on the rise.

Consequently, CSEWG has undertaken to formulate and adopt a set of minimal QA requirements that must be satisfied for covariance information to be included in the ENDF/B-VII.1 library. It is anticipated that the establishment and enforcement of QA requirements for the covariance data included in ENDF/B-VII.1 will enhance the stature of this library and further encourage its widespread use in nuclear applications that require evaluated uncertainty information.

The development of the QA requirements that appear in the following document involved a process extending over nearly two years. It included extensive exchanges of communications between interested and informed individuals from both the evaluator and nuclear data user communities. Crucial to this process was a session of intense face-to-face discussions that was held during at the summer mini-CSEWG meeting in June 2010. The draft document that was discussed at that time underwent further refinement during the following months prior to the Annual CSEWG meeting in November 2010 where the final version was adopted.

Philosophical Approach

The variety and structure of evaluated nuclear data files such as ENDF/B reflect the variety and complexity of fundamental nuclear processes. This applies for the representation of covariance data as well as for other evaluated nuclear parameters. For this reason it was decided adopt a flexible approach in specifying QA requirements for ENDF/B-VII.1 covariances, and to focus on providing guidelines rather than attempting to address specific issues in great detail. Another point that has been recognized by CSEWG is that insistence on establishing QA requirements which are overly stringent could lead to unnecessary delays in releasing this library and, quite possibly, to pressures on CSEWG by both data evaluators and data users to soften or even overlook the requirements in many instances. This, it is believed, would undermine the intent of the QA process.

Although it might appear to some that the current document is rather vague, it nevertheless establishes QA requirements that CSEWG considered to be reasonable as well as achievable in the time frame available prior to the release of ENDF/B-VII.1 in December 2011. At the same time, these requirements insure that the most glaring technical issues that could compromise the quality of this library are addressed and resolved to the benefit of the user community. It is understood that this QA document will be further revised prior to future releases of ENDF/B, hopefully without the need for significant backtracking, and consistent with evolving evaluation methodology and user covariance data needs.

Comments on the Document

The present QA document aims to address the following issues that impact upon the quality of an evaluated covariance file:

- Technical and mathematical requirements.
- Definition of "realistic" evaluated data uncertainties and correlations.
- Covariance formats.

- Covariance evaluation documentation.
- Checking code testing and independent visual reviews of the submitted files.
- Processing requirements.

Section 1 considers basic mathematical requirements that one expects to be satisfied for a covariance matrix. In this context, CSEWG acknowledges two important points. First, that the formats used for specifying covariance matrices, if properly adhered to, guarantee satisfaction of at least some of these requirements. Second, owing to limitations of the ENDF formats, as well as to related problems with numerical precision, one cannot always expect values that ought to be exactly zero or unity to be precisely zero or unity in the file. Allowance for the possible occurrence of small deviations from the ideal is evident from the wording of the QA document.

Section 2 addresses the issue of requiring positive-definiteness for covariance matrices. That is, full covariance matrices for sets of physical observables normally should not have any zero eigenvalues unless they represent uncertainties for physical quantities derived from other physical quantities, leading to the imposition of constraints, or if they represent uncertainties for normalized sets of physical quantities such as neutron spectra. Again, CSEWG recognizes that this requirement can be satisfied only to the extent allowed by the ENDF formats or related matters of numerical precision as well as file processing issues. Allowance for this is made in the wording of this document. It should be noted that covariance matrices used for uncertainty propagation alone need not be positive definite in order to be useful, although no harm is experienced if they are positive definite. However, matrices that need to be inverted, such as those employed in reactor dosimetry and certain other specialized applications, do need to be positive definite. CSEWG has included the requirement of positive definiteness in the QA document in keeping with the spirit that the ENDF/B library should be a "general purpose" nuclear database.

Sections 3 and 4 address the issue of what is "reasonable" and "consistent" and what is not regarding the uncertainties that are indicated in the evaluated covariances. These QA requirements are unavoidably vague since the concepts are arbitrary. Therefore, considerable expert judgment must be exercised in deciding what is and is not "reasonable" and/or "consistent". CSEWG does not consider it to be appropriate at this time to dictate to evaluators what methods they should employ to generate evaluated covariances. There are a variety of methods in current use and new approaches are under development. Rather, it is the view of CSEWG that a satisfactory resolution of this complicated issue can be had through adherence to the guidelines suggested in the QA document as well as from interactions between experienced evaluators and reviewers on the details, if and when controversies arise, prior to final acceptance the files for inclusion in ENDF/B-VII.1.

Section 5 specifies that all provided evaluated covariance data for ENDF/B-VII.1 should comply with the contemporary format requirements specified in the ENDF Formats Manual. This requirement is non-controversial, and its enforcement will be achieved through application of the NNDC checking codes.

Section 6 establishes a requirement for documentation of the covariance evaluations to be provided within the library itself in the category "Descriptive Comments" (MF = 1; MT = 451). Evaluators are allowed considerable leeway as to the content of the provided documentation, but that content should satisfy the scrutiny of independent reviewers, and certainly it should provide sufficient descriptive information to justify unusually large or small uncertainties. CSEWG believes that this requirement of documentation is extremely important because it adds the element of transparency to the ENDF/B library which is an essential ingredient of quality.

Enforcement of the covariance QA requirements is defined by Section 7 of the document (see below). Basically, it is stated that the submitted evaluated covariance data must satisfy the NNDC checking codes and also convince independent reviewers that the information is reasonable based on their examinations of visual plots of uncertainties and correlation patterns as well as perusal of the provided textual documentation.

Finally, Section 8 establishes the important requirement that the evaluated covariance data in ENDF/B-VII.1 must be processable by NJOY and PUFF, the two most widely used data processing codes. This is a very important requirement since evaluated data almost universally need to be processed into forms appropriate for the applications codes before they can be used. Furthermore, when processed on typical group structures, these two codes should yield essentially the same answer, at least within the precision allowed by the formats and processing algorithms. CSEWG assumes, in requiring this to be the case, that there are no "bugs" in either NJOY or PUFF that could lead to non-processability or significant numerical differences for a proper ENDF covariance file, and therefore that any problems encountered could automatically be attributed to defects in the evaluated covariance file in question.

Enforcement

No set of QA requirements can be effective without establishing a mechanism for their consistent enforcement. Enforcement will be effective provided that the requirements are reasonable, considering the contemporary circumstances, and that the enforcement procedures can be pursued effectively by the nuclear data community with the resources available to it. Enforcement of the present QA requirements is comprised of the two aspects mentioned in the QA document and discussed as follows:

First, evaluated covariance data submitted for inclusion in ENDF/B-VII.1 must pass all the tests that are performed by the suite of checking codes developed by the NNDC. It is assumed that these codes incorporate the tests needed to assess compliance with the requirements specified in the QA document. These codes are readily available to all evaluators, and they are encouraged to perform these tests before their evaluations are submitted to the NNDC. The NNDC will also run these checking codes upon receipt of any submitted evaluation. Any encountered failures to satisfy these checking codes will trigger a process aimed at resolving the issues in question through interactions between the NNDC and the individual evaluators.

Second, the NNDC will prepare a visual review package that consists of plots of uncertainties (in percent) as well as plots of correlation patterns. This can be accomplished using codes available at the NNDC. At least one independent reviewer will be assigned to review these plots for each submitted evaluation, along with the written material within the file in the category "Descriptive Comments" (MF = 1; MT = 451), and asked to submit a report to the NNDC on the findings. Any reasonable concerns of these reviewers will be referred to the evaluators for discussion and resolution. While this process relies heavily on the experience of the reviewers, and their willingness to devote some time and effort to the task, it nevertheless represents the best hope for insuring that a particular evaluation possesses decent quality.

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

Approved by the Cross Section Evaluation Working Group (CSEWG)

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1. Basic Mathematical Requirements

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.*

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

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. 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.*