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

Donald L. Smith

Argonne National Laboratory

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INTRODUCTION

Objective

Formulate and adopt a set of minimal Quality Assurance (QA) requirements that should be satisfied for covariance information to be included in the ENDF/B-VII.1 library

Motivation

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 encourage its widespread use in nuclear applications that require evaluated uncertainty information

Discussions and Opinions

- Various e-mails and draft QA documents have been circulating on this topic for nearly a year with the intent of collecting ideas and airing opinions on how to approach this issue.
- Discussion contributors: Doug Muir, Andrej Trkov, Pavel Oblozinsky, Mike Herman, Pat Griffin, Don Smith, Caleb Mattoon, Roberto Capote, … and others.
- Mattoon & Oblozinsky paper (ND2010).
- Lessons learned: 1) The QA document should initially be as simple as possible! 2) The QA document should provide guidelines rather than attempt to micro-managing the technical details.

Practical Considerations

- The initial document should include only QA requirements that can be realistically satisfied prior to the release date for ENDF/B-VII.1.
- The file checking procedures and software must be either currently available or easily produced.
- The evaluator community should agree with the QA requirements and be willing to cooperate by insuring that the submitted evaluations comply.
- The QA requirements must be written so they can be easily modified (without backtracking) for implementation in future releases of ENDF/B libraries, consistent with evolving evaluation methodology and user covariance data needs.

A Suggested Timetable

- Discuss the various issues (mini-CSEWG Mtg).
- Agree upon the essential elements of the QA requirement document (mini-CSEWG Mtg).
- Draft the final QA document (July to October).
- Approve document (November CSEWG Mtg.).
- Adopt and post document on CSEWG website.
- Establish the enforcement procedures (e.g., NNDC reviews, independent visual reviews, ...).

Covariances QA Issues to Discuss

- Technical / mathematical requirements.
- Covariances scope.
- Covariance evaluation procedures.
- Covariance formats.
- Covariance evaluation documentation.
- Checking code testing and visual reviews of the submitted files.
- Processing requirements.
- What constitutes “realistic” evaluated data uncertainties and correlations.

Notation

- To avoid confusion, in the following slides all the recommended inclusions for this QA document will be indicated in red font and italics, and they will be preceded by the symbol “ ”.

TECHNICAL

Basic Mathematical Requirements

The numerical information and recipes provided in an evaluated covariance file must allow complete (square and symmetric) matrices that yield correlations as well as standard deviations (uncertainties) to be generated by the processing codes from the included data.

Correlation matrices derived from the evaluated covariance data should have unity values on the diagonal, and off-diagonal elements with magnitudes less than one, to the extent allowed by the numerical precision of the file, i.e., to less than 1 10^{-6}.

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, i.e., to less than 1 10^{-6} for each row and column.

Matrix Eigenvalues

Covariance matrices generated from information provided by the evaluator must be positive definite (i.e., positive eigenvalues) on the original evaluator's energy grid to the extent allowed by the numerical precision of the file (i.e., to less than 1 10^{-6}) unless the occurrence of zero eigenvalues is mandated mathematically by constraints such as normalization or consistency of partial reaction channel data and those for sums of reaction channels (as, e.g. the total cross section).

Note: It has been pointed out that any requirement of mandatory positive-definiteness (P.D.), while desirable in principle, may be too stringent in many instances, since this is not needed for those applications where matrix inversions are not performed. Also, processing to finer grid structures than intended by the original evaluator will almost always lead to non-positive definite matrices. However, failure to require from the evaluator the minimal P.D. requirement stated above debases the quality that is expected by users of ENDF/B-VII.1 given its traditional and clearly defined role as a general-purpose library that is serviceable for a wide variety of nuclear science applications.

EVALUATION PROCEDURES

Background Comments

- The adopted QA requirements for ENDF/B-VII.1 covariances should not dictate the methodology to be used by evaluators in providing these data. However, more restrictive requirements may need to be incorporated in future covariances QA documents as the quality demanded by users grows and evaluation procedures used to satisfy these needs mature.
- There is a wide disparity of views between idealism and realism regarding consistency of evaluation procedures. At this point, it appears that the best that can be done is to insist that evaluators document the procedures they have actually used in preparing the files submitted for inclusion in ENDF/B-VII.1.

Covariance Evaluation Consistency

It is desirable that covariances be consistent with the evaluation of central values. Ideally they should emerge directly from the evaluation process. However, as a practical consideration the present QA requirement is that the provided uncertainties for an evaluation must at least be reasonably consistent with the uncertainties suggested by the evaluated experimental data as well as with the evaluator's estimates of the anticipated uncertainties associated with contemporary nuclear modeling practice.

Note: Reviewers should flag cases of gross inconsistency leading to direct interaction with the evaluators and initiation of steps to eliminate them to the extent possible in the time available.

FORMATS

Covariance Format Requirement

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

DOCUMENTATION

Documentation Requirement

A brief 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). If references are available to more detailed descriptions of the procedures used to generate covariance information then they should also be listed in this section.

FILE TESTS

Checking Code and Visual Tests

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 as well as visual inspections by reviewers to weed out obvious errors and nonsensical values, and to identify situations where the results appear to be unrealistic so that they can be examined further before approving the file for inclusion in ENDF/B-VII.1.

PROCESSING

Processing Requirements

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

The evaluated covariance data processed by NJOY and PUFF should agree numerically to within reasonable precision.

“REALISTIC” UNCERTAINTIES

Background Comments

- It is vital that the uncertainties and correlations provided in the ENDF/B-VII.1 Library be viewed by potential data users as being “realistic” or they will be ignored to the Library’s determent.
- The term “realistic”, as applied to ENDF/B-VII.1 covariances, most likely will have to be defined in terms of what can be expected at this point in time in the way of contemporary uncertainties in measured and model calculated data used for evaluations rather than in terms of more specific quantitative values or statistical tests.

Requirement of “Realistic” Covariances

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

Uncertainties which are deemed by reviewers to be smaller than those assigned to neutron reaction cross section standards for the same process types should be viewed as “unrealistic” and therefore flagged as such and rejected for ENDF/B-VII.1 unless they can be justified by the evaluators in a convincing manner.

Further Thoughts, Discussion …?

- Additional comments and suggestions from the audience?
- Consensus on essential elements of a QA requirement document for ENDF/B-VII.1 covariance data?
- Agreement on suggested timetable?

The End