Working Party on International Nuclear Data Evaluation Cooperation, Subgroup 28

# Processing Covariance Data for the Resonance Region: Status Report for Activities in 2006—2007

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M. E. Dunn (SG Chairman), R. Arcilla, G. Chiba, I. Kodeli, S. Kahler, T. Kawano, L. C. Leal

**Abstract**

The primary goal of Subgroup (SG) 28 is to build upon the work of WPEC/SG20 for developing new methods for cross-section covariance evaluation. Specifically, SG28 is tasked with developing the requisite processing methods needed to process resonance parameter covariance data, generate cross-section covariance data files and demonstrate the use of covariance data in radiation transport analyses. The following is a report of the technical accomplishments completed between May 2006 and March 2007.

## 1. Introduction

In WPEC/SG20 the evaluation and format issues were addressed for preparing new cross-section evaluations with resonance-parameter covariance data. However, the corresponding covariance processing methods have not been sufficiently developed and publicly disseminated for producing covariance data files for use in transport applications. Prototypic versions of the cross-section processing software have been developed to process the latest covariance formats, but additional work is needed to finalize the processing methods for distribution to the user community. At the completion of SG20, cross-section covariance evaluations were produced for Gd, Rh, and Fe isotopes, and this work provided much of the ground work needed to facilitate the work of SG28; however, covariance evaluations for important uranium and plutonium isotopes were not prepared as part of the SG20 effort. As a result, the work scope for SG28 is organized into three campaigns or phases.

1. The first phase of the project will be performed concurrently with the second phase. Specifically, new evaluations will be prepared with resonance-parameter covariance data for $^{235}$U which is the most difficult isotope to process in terms of the number of resonances and resulting covariance matrix size. This phase will follow directly from the work of WPEC/SG20, and the new evaluation will be generated using the new methods and formats that were developed in WPEC/SG20.

2. The second phase of the project will focus on the development of the needed covariance processing methods and the implementation of the new processing methodology in widely used cross-section processing systems (e.g., NJOY, AMPX, etc.). In addition, the cross-section checking codes will be updated to support the efforts of the nuclear data centers to check covariance data files for dissemination by the different data projects.

3. The third phase will focus on the generation of covariance data files for use in radiation transport analyses. As part of the third phase, sensitivity/uncertainty (S/U)

analysis tools will be used to demonstrate the propagation of the covariance data in specific radiation transport applications.

Membership

| | |
|---|---|
| Chairman | M. E. Dunn, ENDF (ORNL) |
| Monitor | R. Jacqmin, JEFF (CEA Cadarache) |
| ENDF | L. C. Leal (ORNL), S. Kahler (LANL), T. Kawano (LANL), R. Arcilla (BNL), S. Oh (KAERI) |
| JEFF | I. Kodeli (OECD/NEA) |
| JENDL | G. Chiba (JAEA), K. Shibata (JAEA), M. Ishikawa (JAEA) |
| BROND | M. Nikolaev (IPPE) |

## 2. Activities in 2006 and 2007

### 2.1 Resonance parameter covariance evaluation for $^{235}$U

The initial subgroup activity focused on the development of a resonance parameter covariance evaluation for $^{235}$U using the SAMMY R-matrix computer code. SAMMY calculates various cross sections via R-matrix theory (Reich-Moore approximation), includes corrections for experimental conditions (Doppler and resolution broadening, multiple scattering corrections, backgrounds, etc.) and determines the best fit of the theoretical calculation to experimental data by means of the generalized least-squares fitting procedure. Experimental uncertainties are incorporated directly into the evaluation process in order to propagate those uncertainties into the resonance parameter results. $^{235}$U is an evaluation for which resonance parameters were prepared with ENDF/B-VI Release 5. The objective of the current evaluation work is to preserve the existing resonance parameters but provide a resonance parameter covariance data file that corresponds to the existing resonance parameters. In the traditional resonance evaluation approach, the evaluator prepares the resonance parameter covariance matrix (RPCM) as part of the resonance analysis. Historically, the RPCM was discarded once the resonance parameters were prepared for the cross-section evaluation. For $^{235}$U, the resonance evaluation was prepared in the mid 1990s; however, the RPCM was not preserved. With the advent of robust sensitivity/uncertainty analysis methods in recent years, there is a demand for cross-section uncertainty data. In an effort to avoid a complete re-evaluation of existing cross-section data files, ORNL has developed a "retroactive" covariance analysis method to prepare covariance matrices while preserving the existing resonance parameters. In the case for $^{235}$U, SAMMY was used to retroactively generate the resonance parameter covariance data. Details about the retroactive analysis methodology and the generation of covariance data for $^{235}$U were published by Arbanas et. al. at the PHYSOR 2006 meeting in Vancouver, Canada September 2006 [1].

Concurrent to the RPCM work at ORNL, LANL completed a "high-energy" (i.e., above the resonance region) covariance data analysis for $^{235}$U. In late 2006, ORNL worked with LANL to merge the $^{235}$U RPCM with the high-energy covariance evaluation. As a result, a complete covariance evaluation has been prepared for $^{235}$U thereby satisfying the first SG28 objective. The complete $^{235}$U covariance file is available for processing and testing. Moreover, the covariance file will be distributed to all SG28 members in 2007 for processing and testing.

**2.2 Processing and checking Codes**

ORNL: AMPX Covariance Processing Developments

A summary of the ENDF/B Formats for File 2 and File 32 information is provided in Table 1 [2].

Table 1: Parameters characterizing the content of ENDF/B File 2 and 32

| | | | |
|---|---|---|---|
| LRU | = | 1 | Resolved resonance data |
| | | 2 | Unresolved resonance data |
| LRF | = | 1 | Single-level Breit-Wigner (SLBW) resonance parameters |
| | | 2 | Multi-level Breit-Wigner (MLBW) resonance parameters |
| | | 3 | Reich-Moore resonance parameters; no competitive reactions allowed |
| | | 4 | Adler-Adler resonance parameters |
| | | 7 | Reich-Moore resonance parameters containing all the generality of LRF=3 plus unlimited numbers and types of channels |
| LCOMP | = | 0 | Only diagonal elements provided |
| | | 1 | Entire covariance matrix is given for one or more blocks of resonances |
| | | 2 | Covariance matrices are given in a Compact Covariance Format (CCF) that allows a compromise between the amount of data given and accuracy of the covariance data. |

Prior to the start of SG 28, the AMPX covariance processing module PUFF-III was used at ORNL for processing covariance information in ENDF Files 31, 32, and 33. During the reporting period, a new version of the PUFF module was developed (PUFF-IV) with expanded File 32 resonance parameter covariance processing capabilities. PUFF-III had been used to process ENDF uncertainty information and to generate the desired multigroup correlation matrix for the application of interest. The processing code PUFF-IV is based on PUFF-III, but the original Fortran 77 code was rewritten in Fortran 90 to allow for a more modular design. PUFF-III had the capability to perform limited sensitivity analysis for select File 32 formats (i.e., restricted to SLBW). PUFF-IV can now do full processing of all formats noted in Table 1. Note that PUFF-IV does not process long-range covariance information as defined by the ENDF-102 manual. The user input for PUFF-IV is identical except for additional processing options. Test cases verify that PUFF-IV produces the same results as PUFF-III for File 31 and 33 processing and for File 32 processing where supported in PUFF-III. Additional comparisons have been performed with SAMMY to verify the processing results from PUFF-IV. The amount of covariance information that can be processed by PUFF-IV is limited only by available computer memory. Additional details concerning the PUFF-IV processing capabilities were published in a full paper at the PHYSOR2006 meeting in Vancouver, Canada September 2006 [3].

Although PUFF-IV is part of the AMPX cross-section processing system, a standalone PUFF-IV package has been developed and is available for distribution from the Radiation Safety Information Computational Center (RSICC) as software package P00534 [4]. PUFF is designed to function with the AMPX code system that provides nuclear data libraries to the SCALE radiation transport code system [5]; however, the standalone PUFF-IV package also includes utility modules to facilitate the data interface with the NJOY code system [6].

To verify that the new PUFF-IV capabilities in the resonance region give the expected results, covariance matrices have been compared with calculations performed with SAMMY [7] and ERRORJ [8]. The R-Matrix fitting program SAMMY is primarily used to determine resonance

parameters from experimental data but has the capability to generate group-averaged cross section data and covariance matrices from ENDF formatted data files. However, SAMMY cannot process ENDF data in the unresolved-resonance region. The program ERRORJ is an independently developed processing code for covariance matrices similar to PUFF-IV. More details about the recent ERRORJ developments is provided in the subsequent discussion. Note that PUFF-IV uses an analytic approach to obtain cross-section sensitivity parameters as a function of the underlying resonance parameters whereas ERRORJ uses a numerical approach to calculate the cross-section sensitivities to the resonance parameters. All three programs should therefore yield similar results given the same ENDF data file. This is indeed the case for all data files that were compared during the testing. Comparison with results from SAMMY was performed for all supported ENDF File 32 formats.

With regard to the SG28 objectives, PUFF-IV has been used to process the full (LCOMP=1) $^{235}$U covariance matrix that is documented in Section 2.1. Although it is beyond the work scope of SG28, PUFF-IV has been used to process full covariance matrices for full covariance matrices for $^{233}$U, $^{238}$U, and $^{239}$Pu. Therefore, processing full covariance matrices for key uranium and plutonium isotopes has been demonstrated with the latest PUFF software. Additional work will be performed to test the processing capabilities for covariance matrices in the Compact Covariance Format.

LANL and JAEA: NJOY Covariance Processing Developments

During the reporting period, the ERRORJ module was updated to process the ENDF/B-VI resonance parameter covariance formats. The ERRORJ module is based on the ERRORR module that has been distributed with NJOY. Prior to SG28, ERRORJ was a stand-alone module that was not part of NJOY. Recently, work by Chiba (JAEA) and LANL has resulted in the development of a new ERRORJ module that can be used as part of the NJOY code system. In addition, covariance data can be processed at all energies that include the resonance region and high-energy region. ORNL and LANL have engaged in comparison studies to verify results from PUFF-IV and ERRORJ. The comparison studies have resulted in computational improvements in both code systems. As a result, versions of PUFF-IV and ERRORJ have been developed that will permit users to process existing ENDF/B covariance formats. Additional ERRORJ improvements have been made in the area of computational efficiency resulting in faster covariance calculations. In some cases, a factor of 2 to 3 speed-up has been observed with the updated version of ERRORJ.

U.S. National Nuclear Data Center (NNDC) Work Activities

Once the new covariance processing tools were in place, BNL performed the following covariance data processing activities at NNDC on the ENDF/B-VII.0 and JENDL-3.3 libraries between October 2006 and March 2007:

ENDF/B-VII.0

Twenty-four out of the 26 materials in the neutron reaction sublibrary were processed using the ERRORJ-2.3 module in NJOY-99.161. The remaining two materials ($^{23}$Na and $^{235}$U), which have incomplete covariance data in ENDF/B-VII, were processed with PUFF-IV 1.0.2 (See results at http://www.nndc.bnl.gov/exfor7/4web/covarplots.html). This was due to the inability of ERRORJ at that time to handle data files with missing MF=33. This desirable feature was communicated to Chiba (JAEA), the primary

developer of ERRORJ, who devised an update for ERRORJ. Subsequently, NNDC was able to successfully process $^{23}$Na and $^{235}$U using the upgraded version of ERRORJ.

Processing with PUFF-IV 1.0.2 revealed a couple of issues in the code: 1) the stepsize underflow problem, and 2) the value of **"0.0"** for the cross section in some of the energy groups which were not monotonically increasing. After subsequent investigation by ORNL, both problems appear to be attributed to a non-monotonic group structure provided to PUFF during the calculation. For nuclear applications, group structures are required to be monotonically constructed. Therefore, the issue of processing a non-monotonic group structure does not appear to be practical, and PUFF will be updated to check for monotonically increasing or decreasing group structure to alert users to this issue. In the meantime, L. Leal (ORNL) is also investigating another issue for some U isotopes where ERRORJ and PUFF-IV give slightly different answers.

JENDL-3.3

Twenty materials in the neutron reaction sublibrary were processed using the upgraded version of ERRORJ-2.3 module in NJOY-99.161 (See results at http://www.nndc.bnl.gov/exfor7/4web/covarplots_jendl33.html). As with ENDF/B-VII.0, the 44- and 187-group energy structures and the constant-flux weighting function were used. To successfully process isotopes which also belong to the standards sublibrary (e.g. $^{235}$U), some evaluated data from the same isotopes in the ENDF/B-VII.0 neutron cross section standards sublibrary were used.

OECD NEA Data Bank Activities

The NEA Data Bank has collected the following covariance processing and S/U analysis packages that have recently become available, and these packages are available for distribution to the international nuclear data community:

- NEA-1730: ZZ-COV-15GROUP-2006, 15-group cross section covariance matrix library: 15 energy group cross section covariance matrix library presenting a general overview of the presently available data. The codes for the transformation of the data to different energy group structure and for the verification of the mathematical properties of the matrices are also included.

- NEA-1264: ZZ VITAMIN J/COVA, Several covariance matrix data libraries for sensitivity and uncertainty analysis. The libraries are based on JEF-1, ENDF/B-IV and –V, EFF-2.3 and EFF-3 data

- PSR-0368: NJOY-99, General ENDF/B Processing System for Reactor Design Problems

- PSR-0534: PUFF-IV, Code System to Generate Multigroup Covariance Matrices from ENDF/B-VI Uncertainty Files

- NEA-1676: ERROR-J 2.3, Multigroup covariance matrices generation from ENDF-6 format

- NEA-1037: SAGEP, Sensitivity Analysis of Reactor Parameter to Cross-Sections Variation

- CCC-0732: SCALE 5.1/ORIGEN-ARP5.1: Modular system for criticality, shielding, source term, fuel depletion/decay, reactor physics (TSUNAMI code).

- NEA-1628: SUSD3D, 1-, 2-, 3-Dimensional Cross Section Sensitivity and Uncertainty Code

More information on these NEA software/data packages is available from: http://www.nea.fr/html/dbprog/.

**2.3 Demonstration of covariance data in sensitivity/uncertainty analyses**

During the review period, limited work has been performed by SG28 in the demonstration of the covariance data in S/U analyses. Therefore, future SG28 work activities will focus on the demonstration and testing of the new $^{235}$U covariance data in S/U analyses. Nonetheless, the following work activities were performed during the first year of SG28:

- ORNL has processed the complete $^{235}$U covariance evaluation using PUFF-IV and prepared 15-group covariance data for ANL nuclear R&D staff. In addition, ORNL prepared covariance data for $^{238}$U and $^{239}$Pu. In December 2006, the multi-group covariance data for $^{235}$U, $^{238}$U, and $^{239}$Pu were provided to ANL for testing in S/U analyses. ANL has performed testing calculations with the new covariance data, and results from the S/U calculations will be published at the ND2007 meeting in April 2007 [9]. Discussions with staff from ANL indicate that the $^{235}$U, $^{238}$U, and $^{239}$Pu covariance data appear to be too small when propagated to integral reactor quantities. ORNL will continue to work with ANL to investigate the covariance data issues.
- In addition, ORNL has prepared $^{235}$U 44-group covariance data for SCALE. In 2007, ORNL will perform S/U analyses with the new covariance data.
- I. Kodeli has already performed sensitivity/uncertainty analyses of fast and thermal reactor systems (KRITZ, SNEAK) using existing covariance data. Now that SG28 has successfully prepared a new $^{235}$U covariance file and the requisite processing tools, the NEA Data Bank plans to process the $^{235}$U covariance file and repeat the S/U analyses with the new covariance data.

**3. Future Work**

The following work activities will be performed by SG28 in the 2007—2008 timeframe:

- The new $^{235}$U covariance evaluation will be distributed to SG28 members for processing and testing.
- S/U analyses will be performed to demonstrate the use of the $^{235}$U covariance data.
- ORNL will continue to work with ANL to understand the impact of the $^{235}$U covariance data and revise the covariance evaluation as needed.
- Additional evaluation efforts will focus on the development of the $^{235}$U RPCM in the ENDF/B CCF.
- Once a new evaluation is prepared in the ENDF/B CCF, SG28 work activities will focus on the processing and testing with the compact $^{235}$U covariance file. S/U testing with the full $^{235}$U covariance evaluation will provide a baseline to compare results with the compact $^{235}$U covariance evaluation.

- Additional development efforts will focus on updates of the evaluation checking codes to permit testing of covariance evaluations by nuclear data centers.

**References**


1. Arbanas, G.; Leal, L. C.; Larson, N. M., and Derrien, H. *Retroactive Covariance Matrix for $^{235}U$ in the Resolved Resonance Region*, American Nuclear Society, PHYSOR-2006 Topical Meeting, Vancouver, BC, Canada, September 10-14, 2006.
2. ENDF-102 Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6", BNLNCS-44945, Rev. 10/91 (ENDF/B-VI), Brookhaven National Laboratory (October 1991).
3. D. Wiarda, M. E. Dunn, N. M. Greene, N. M. Larson, and L. C. Leal, "New Capabilities for Processing Covariance Data in the Resonance Region," PHYSOR-2006 ANS Topical Meeting on Reactor Physics, Vancouver, BC, Canada, September 10-14, 2006.
4. *PUFF-IV: Code System to Generate Multigroup Covariance Matrices from ENDF/B-VI Uncertainty Files*, August 2006. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as PSR-534.
5. *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluations*, ORNL/TM-2005/39, Version 5.1, Vols. I–III, November 2006. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-732.
6. *NJOY99.0: Code System for Producing Pointwise and Multigroup Neutron and Photon Cross Sections from ENDF/B Data*, March 2000. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as PSR-480.
7. N.M. Larson, "Updated User's Guide for SAMMY: Multilevel R-Matrix Fits to Neutron Data Using Bayes' Equations", ORNL/TM-9179/R7 (2006). Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as PSR-158.
8. G. Chiba, *ERRORJ : A code to Process Neutron-nuclide Reaction Cross-Section Covariance, Version 2.3*, JAEA-Data/Code 2007-007.
9. M. Salvatores, G. Aliberti, G.Palmiotti, D.Rochman, P.Oblozinsky, M.Hermann, P.Talou, T.Kawano, L.Leal, A.Koning, I.Kodeli, *Nuclear Data Needs for Advanced Reactor Systems. A NEA Nuclear Science Committee Initiative*, ND2007 International Nuclear Data Meeting, Nice, France, (to be published April 2007).