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PROCESSING COVARIANCE DATA FOR THE RESONANCE REGION

A report by the Working Party
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FOREWORD

A Working Party on International Evaluation Co-operation (WPEC) was established under the sponsorship of the OECD/NEA Nuclear Science Committee (NSC) to promote the exchange of information on nuclear data evaluations, validation, and related topics. Its aim is also to provide a framework for co-operative activities between members of the major nuclear data evaluation projects. This includes the possible exchange of scientists in order to encourage co-operation. Requirements for experimental data resulting from this activity are compiled. The working party determines common criteria for evaluated nuclear data files with a view to assessing and improving the quality and completeness of evaluated data.

The parties to the project are ENDF (United States), JEF/EFF (NEA Data Bank member countries), and JENDL (Japan). Cooperation with evaluation projects of non-OECD countries is organized through the Nuclear Data Section of the International Atomic Energy Agency (IAEA).

The following report is issued by Subgroup (SG) 28, which builds 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 opinions expressed in this report are those of the authors only and do not represent the position of any member country or international organization. This report is published on the responsibility of the Secretary-General of the OECD.

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SUMMARY

This report summarizes the work performed by WPEC Subgroup 28 (SG28) on issues pertinent to the methodology used to process covariance data in the resonance region. Specifically, SG28 has developed 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 work performed by SG28 and documented in this report addresses the following tasks:

- Produce resonance parameter covariance evaluation for ^{235}U
- Develop resonance parameter covariance processing methods in widely used processing systems (e.g., NJOY, AMPX, etc.)
- Use the updated cross-section processing systems to generate covariance data files for use in radiation transport analyses. In addition, use sensitivity/uncertainty (S/U) analyses to demonstrate the propagation of the covariance data in specific radiation transport applications

PROCESSING COVARIANCE DATA FOR THE RESONANCE REGION

1. INTRODUCTION

In WPEC/SG20 the evaluation and format issues were addressed for preparing new cross-section evaluations with resonance-parameter covariance data. However, prior to SG28, the corresponding covariance processing methods had 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 has been performed concurrently with the second phase. Specifically, a new evaluation has been prepared with resonance-parameter covariance data for ^{235}U that is the most difficult isotope to process in terms of the number of resonances and resulting covariance matrix size. This phase followed directly from the work of WPEC/SG20, and the new evaluation has been generated using the new methods and formats that were developed in WPEC/SG20.

2. The second phase of the project focused on the development of the needed covariance processing methods and the implementation of the new processing methodology in widely used cross-section processing systems (i.e., NJOY and AMPX). At the outset of the project, SG28 planned to update the cross-section checking codes to support the efforts of the nuclear data centers to check covariance data files for dissemination by the different data projects. Due to limited resources, the checking codes could not be updated as part of the SG28 work effort. The decision has been made at the nuclear data centers to utilize the two independently developed cross-section processing systems with covariance processing capabilities (i.e., NJOY and AMPX). Because AMPX and NJOY are independently developed, covariance evaluation checking can be performed through independent verifications between AMPX and NJOY until the checking codes can be updated to test covariance evaluation files.

3. The third phase of the work has focused 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 have been used to demonstrate the propagation of the covariance data in specific radiation transport applications.

In the following subsections, additional details are provided for each of the SG28 work activities.

2. 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].

In a SAMMY evaluation, the uncertainties in the data, such as statistical and systematic uncertainties, are incorporated in the evaluation procedure. Various sources of experimental uncertainties must be included; among these are normalization, background, neutron time-of-flight, sample thickness, and temperature. Uncertainties in all of these are included in the evaluation process in order to properly determine the resonance-parameter covariance matrix. A Reich-Moore resonance evaluation (ENDF/B-VI) for ^{235}U was performed from 1.0-e5 to 2250 eV using the computer code SAMMY. A total of 3193 resonances, including the external levels, were used. At the time the evaluation was performed, the resonance-parameter covariance matrix was generated; however, this matrix is no longer available. Therefore, an approach was developed within SAMMY to retroactively generate approximate covariance matrices for resonance parameters. This procedure has been used to generate the covariance matrix for the ^{235}U parameters. Each resonance of ^{235}U in the Reich-Moore formalism is described by five parameters (the resonance energy E_r, the gamma width Γ_g, the neutron width Γ_n, and the two fission widths Γ_{f1} and Γ_{f2}), for a total of 15965 parameters. The large number of resonance

parameters leads to major issues regarding data storage for the covariance file. The required storage for the ^{235}U RPCM in the ENDF/B format is 1.76 Gigabytes [1]. The computer code PUFF-IV (Wiarda and Dunn, 2006) was used to process the ^{235}U evaluation in the ENDF/B format. Changes were made to the PUFF-IV code to reduce the processing time of the covariance data. A great reduction in processing time was achieved. Computation of the cross-section covariance matrices (CSCM) was optimized by utilizing the Basic Linear Algebra Subprograms (BLAS) to perform matrix multiplications. This optimization was crucial for computation of CSCM for actinides on energy grids with many points, since multiplication of very large matrices is required in this case. The CPU time used to compute CSCM for ^{235}U on 238-group energy grid decreased from more than a month to only 16 hours of CPU time after the optimization. While the resonance parameters are converted to the evaluated nuclear data file (ENDF) format in the so-called FILE2 representations, the RPCM is converted to the ENDF FILE32 representation. One major drawback for the RPCM is the computer's disk space required to store the data. In the ENDF format the ^{235}U RPCM representation requires 1.76 Gigabytes of computer storage. The size of the whole ^{235}U cross-section library in the ENDF format is about 3 MB. Therefore it is worthwhile to look for an alternative to represent the covariance data in the ENDF format that can still capture all the features inherent in the FILE32 representation with reduced computer storage. A procedure was developed and implemented in the code PUFF-IV to convert the RPCM representation into the ENDF FILE33 representation. The FILE33 CSCM representation is intended to characterize the variances of the cross sections within a specified energy region, and the correlation between cross sections of adjacent energy regions. The choice of CSCM over the RPCM is expected to lead to a reduction in computer storage. The size of the ENDF library using the FILE33 representation is reduced to about 30 Megabytes, that is, 57 times smaller than that using FILE32. The computer time needed to process the FILE33 covariance information is about 750 times smaller than that using FILE32. While computer speed and storage have constantly been improving, it is worthwhile to have small sized data evaluations. The evaluations are stored in nuclear data banks and are retrieved by users worldwide who may have limited network and processing capabilities to download and process the data.

Concurrent to the RPCM work at ORNL, LANL completed a "high-energy" (i.e., above the resonance region) covariance data analysis for ^{235}U. 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.

The capture cross-section covariance data processed with PUFF-IV code in the 44-group structure are shown in Figure 1. The average uncertainty in the capture cross section as displayed in Figure 1 is about 1% in the resolved resonance energy region (energies smaller than 2250 eV) and 10% above the resonance region.

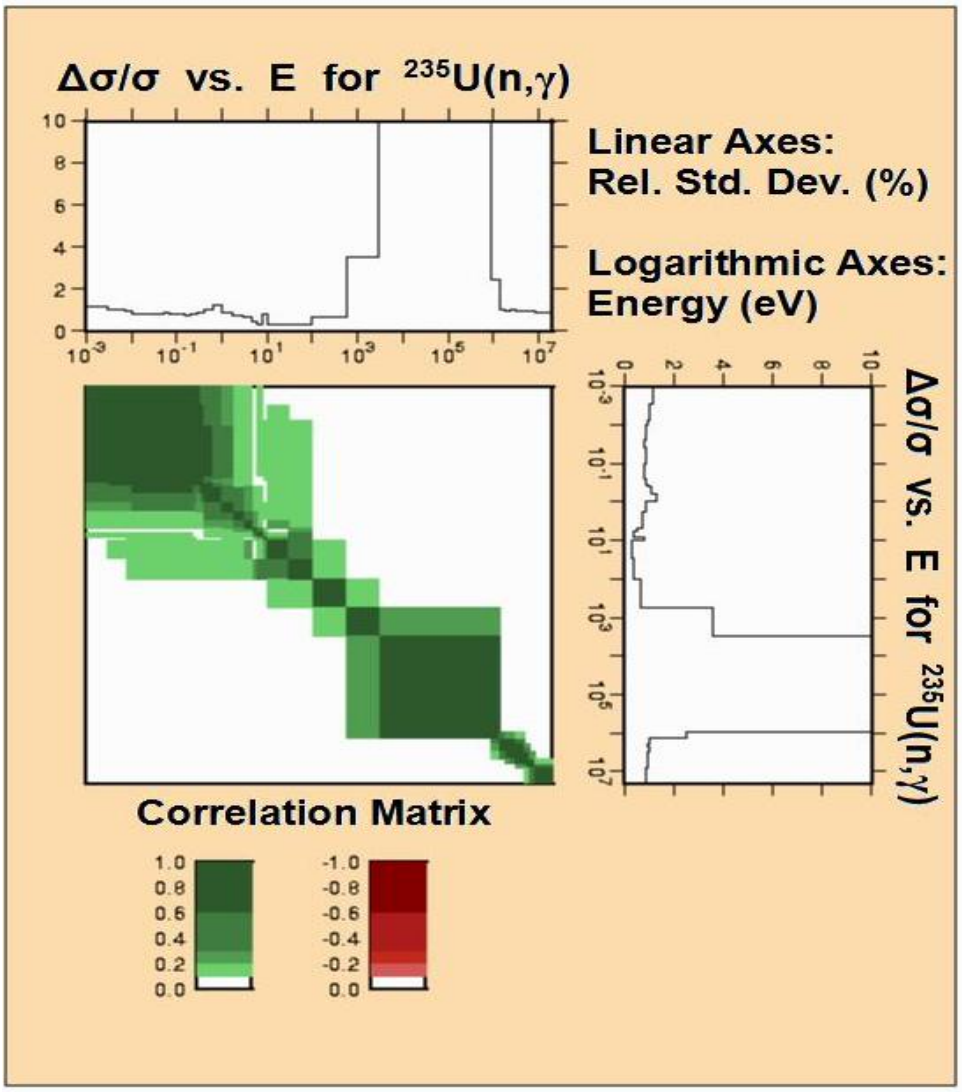

Figure 1. Correlation matrix for the ^{235}U capture cross-section in the 44-neutron energy group structure.

3. PROCESSING CODE DEVELOPMENT AND TESTING

3.1 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. As part of the SG28 work effort, a new version of the PUFF module has been 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 multi-group 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 are 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.

ENDF evaluations giving covariance information usually also contain point-wise covariance information in File 33. PUFF-IV processes this information using a pre-computed multi-group library. ERRORR default option is to compute the cross section on the evaluator-defined grid using point-wise cross section data. If comparing results between the two codes it is important to use the same option for calculating the cross section on the evaluator grid. PUFF-IV was updated to include both options available in ERRORR. The difference in results between the two options can be seen in Figure 2.

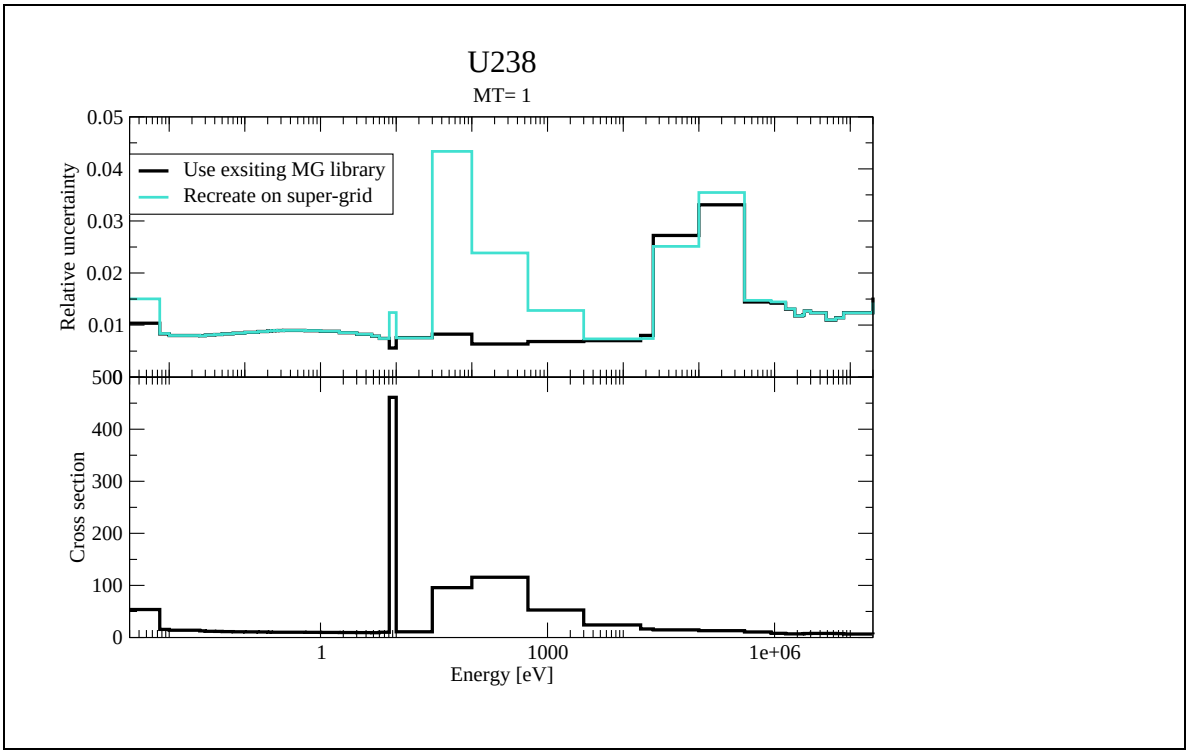

Figure 2. Difference for the two processing options implemented in PUFF-IV

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. In addition processing of the compact covariance format has also been tested for the available evaluations and compared with NJOY results.

3.2 LANL AND JAEA: NJOY Covariance Processing Developments

Skip Kahler input on NJOY resonance region covariance processing capabilities

3.3 U.S. National Nuclear Data Center (NNDC) Work Tasks

Dave Brown / Ramon input with regard to NNDC work activities to process and plot covariance data files

3.4 Processing Code Comparisons Between PUFF-IV and NJOY

Using AMPX and NJOY, covariance files were process for ^{235}U, ^{238}U, and ^{239}Pu. Comparison results between AMPX and NJOY for 239Pu is provided in Figure 3. Based on the results in Figure 3, both AMPX and NJOY give comparable results.

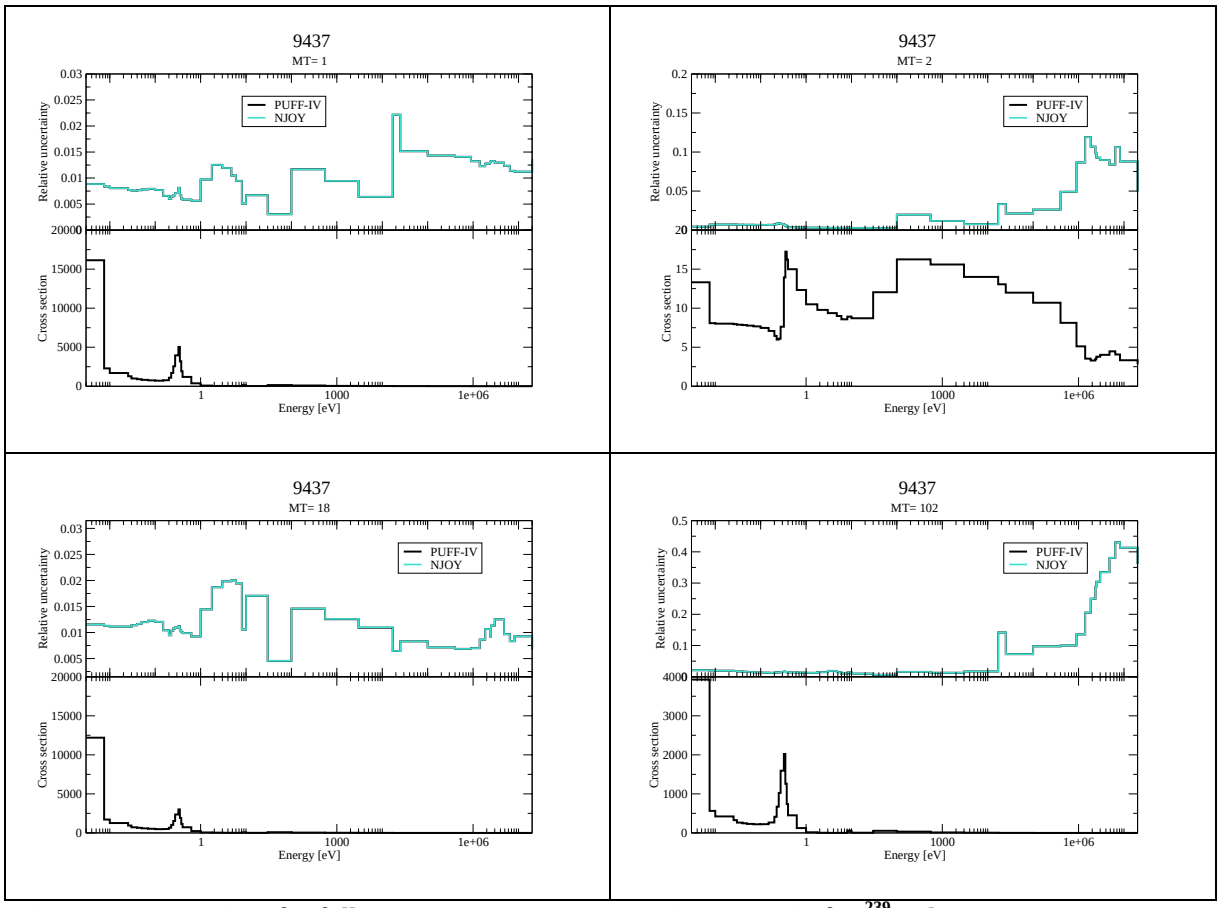

Figure 3: Comparison for full resonance parameter covariance matrix for ^{239}Pu between ERRORR and PUFF-IV

In addition, we processed covariance files containing covariance matrices, using both PUFF and NJOY. Point-wise data were generated with AMPX utilities and used for both PUFF-IV and ERRORR calculation. There are 185 evaluations from 418 that contain covariance information in ENDF/B-VII.0. Some of the evaluations only contain File 32 (resonance parameter covariance matrices). These evaluations (^{37}Cl, ^{39}K, and ^{41}K) can only be processed by PUFF-IV. Two evaluations (^{19}F and ^{35}Cl) use the LRF=7 Reich-Moore format, which cannot be processed by NJOY99 (99.364) and must be processed with NJOY2012. One evaluation (^{16}O) has a very large evaluator grid for the point-wise covariance matrices. PUFF-IV cannot process this evaluation without an increase in array space. The latest update to NJOY increases the array space to a size sufficient to process ^{16}O. Of the remaining evaluations 48 contain File 32 and File 33 data, whereas the rest only contain File 32 data. We generated the covariance matrices in COVERX format using both PUFF-IV and ERRORR. The resulting COVERX formatted files were

compared using the COVCOMP module. In most cases a good agreement was found between the results of ERRORR and NJOY. An example is shown in Figure 4 for ^{235}U. Please note that the ENDF data set contains the covariance matrices for ^{235}U in File 33 format. As described above the full resonance parameter covariance matrix was converted to point-wise format in order to conserve disc space.

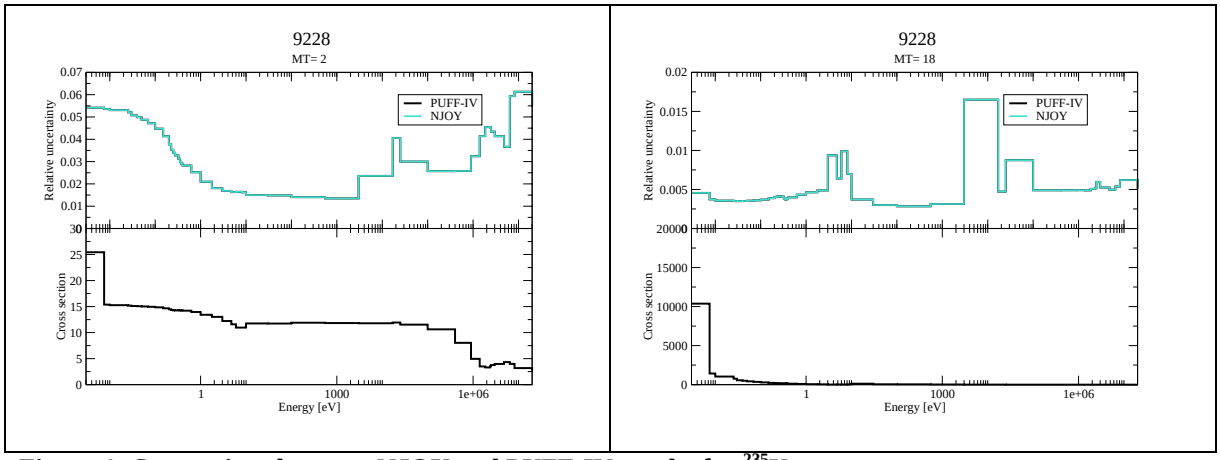

Figure 4: Comparison between NJOY and PUFF-IV results for ^{235}U.

Good agreement is also found in most cases where File 32 resonance parameters are given. As an example see the results for ^{239}Pu with the full resolved resonance parameter matrix in Figure 2. If resolved resonance parameters are given in Single-Level or Multi-Level Breit-Wigner format, PUFF-IV converts to Reich-Moore format prior to calculating the analytical derivatives. This can sometimes lead to differences between NJOY and PUFF especially for fission. An example is shown for ^{241}Am in Figure 5.

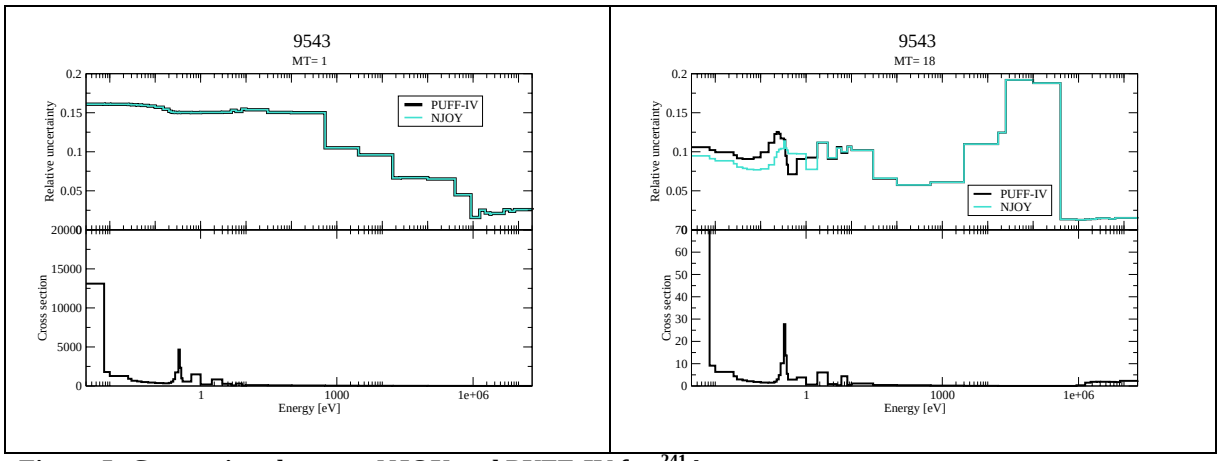

Figure 5: Comparison between NJOY and PUFF-IV for ^{241}Am

4. DEMONSTRATION OF COVARIANCE DATA IN SENSITIVITY/UNCERTAINTY ANALYSES

The impact of data uncertainty in calculations for benchmark systems for which ^{235}U isotope is a major component has been investigated. The ^{235}U covariance data were processed with the PUFF-IV code in the COVERX format for use in the calculations with the TSUNAMI code [5]. The covariance data were processed into the SCALE 44-group neutron structure. The average uncertainty in the capture cross section as displayed in Figure 1 is about 1% in the resolved resonance energy region (energies smaller than 2250 eV) and 10% above the resonance region.

The TSUNAMI-3D sequence in SCALE uses the KENO V.a Monte Carlo neutron transport code to produce the sensitivity of multiplication factor (k_{eff}) to the cross-section data on an energy-dependent, nuclide-reaction-specific basis. In this calculation, the sensitivities of k_{eff} to the problem-dependent multigroup cross-section data are produced with adjoint-based perturbation theory.

The benchmarks used in the calculations are ten thermal benchmark systems. The k_{eff} KENO calculations were done with cross section data from the ENDF/B-VI release eight based on the 238-energy group structure of the SCALE system. The thermal benchmark systems for which the uncertainty in the k_{eff} was investigated consist of critical experiments involving a tank of highly enriched uranyl nitrate. This series of experiments was performed in the 1970s at the Rocky Flats Plant. These experiments are included in the International Criticality Safety Benchmark Evaluation Project (ICSBEP) (International, 2006) and are identified as HEU-SOL-THERM-001.

The sensitivities of the multiplication factor to the ^{235}U ν-bar, fission, and capture cross sections for the HEU-SOL-THERM-001-01 benchmark are shown in Figure 6, which indicates that k_{eff} is very sensitive to ν-bar. The KENO calculation of the k_{eff} for this system using the ENDF/B-VI Release 8 cross section-library is 0.9989 ± 0.0004. The quoted uncertainty is due to the stochastic aspect of the Monte Carlo calculation. As calculated by TSUNAMI, the uncertainty in k_{eff} due to the ^{235}U covariance data is 0.7213 ±0.0002 percent Δk/k. The contributions to the uncertainty in k_{eff} due to individual cross sections, ν-bar, and their correlations are shown in Table 2. The relative standard deviation (% Δk/k in k_{eff}) is computed from individual values by adding the square of the positive values, subtracting the square of the negative values, and taking the square root. As can be seen from Figure 6, the sensitivity in the k_{eff} is significant in the energy region below 2250 eV. Therefore the uncertainty in the k_{eff} is predominantly due to the uncertainty in the resonance region of the ^{235}U.

Table 2. Relative percent standard deviation of k_{eff} due to ^{235}U uncertainty data for the HEU-SOL-THERM-001-01 benchmark system.

	(n,γ)	(n,f)	(n,n)	(n,n')	(n,2n)	ν-bar
(n,γ)	2.0057×10^{-1} ± 6.7745×10^{-5}					
(n,f)	1.1572×10^{-1} ± 8.3693×10^{-5}	8.5765×10^{-2} ± 9.1514×10^{-5}				
(n,n)	1.4599×10^{-2} ± 3.8936×10^{-6}	-6.4656×10^{-3} ± 2.9765×10^{-6}	3.2326×10^{-3} ± 3.7405×10^{-6}			
(n,n')			6.1170×10^{-3} ± 1.0276×10^{-5}	1.0497×10^{-2} ± 1.2372×10^{-5}		
(n,2n)			6.4745×10^{-5} ± 1.1040×10^{-7}		5.6611×10^{-4} ± 5.2855×10^{-7}	
ν-bar						6.7756×10^{-1} ± 5.2886×10^{-5}

Relative standard deviation % $\Delta k/k$ in k_{eff}

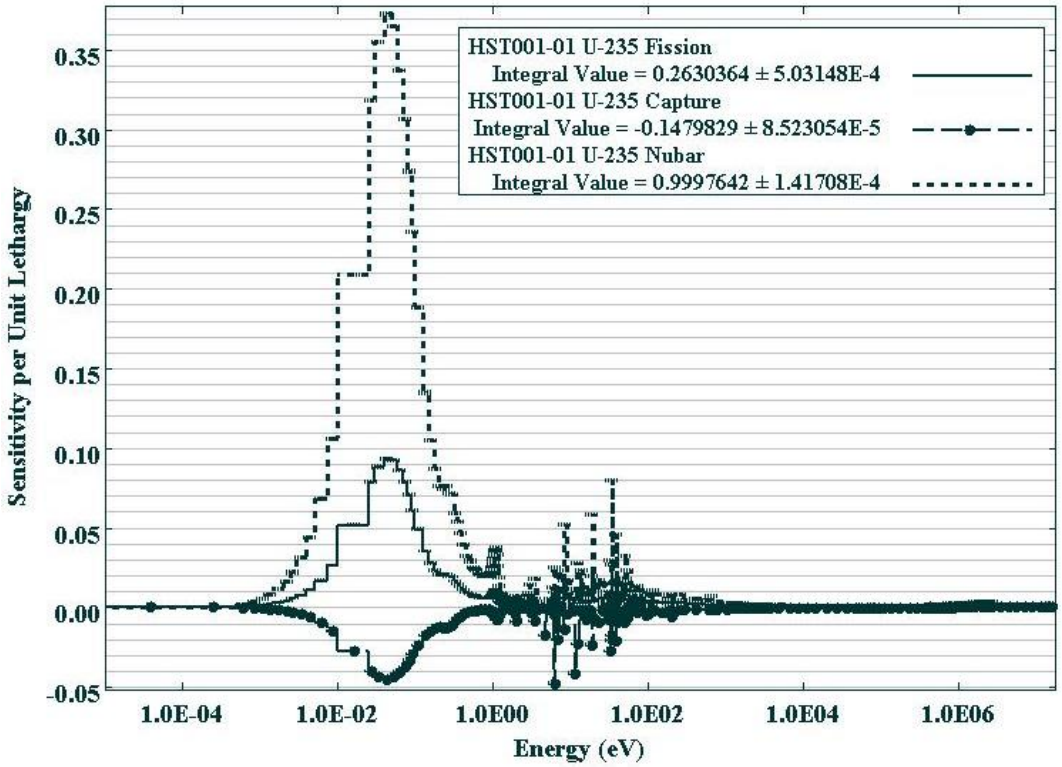

Figure 6. Sensitivity of the multiplication factor to ν-bar, fission, and capture cross section for ^{235}U for the HEU-SOL-THERM-001-01 benchmark system.

The k_{eff} results for the ten cases of the HEU-SOL-THERM-001 benchmark systems are presented in Table 3. The uncertainty in k_{eff} due to data uncertainty of ^{235}U is also listed. The average uncertainty in k_{eff} due to ^{235}U data is about 0.7%.

Table 3. Uncertainties in k_{eff} and % Δk/k due to ^{235}U covariance data for thermal systems.

Case	k_{eff}	% Δk/k due to ^{235}U covariance data
HST-001-01	0.9989 ± 0.0004	0.7213 ± 0.0002
HST-001-02	0.9952 ± 0.0003	0.6938 ± 0.0001
HST-001-03	1.0025 ± 0.0004	0.7219 ± 0.0002
HST-001-04	0.9987 ± 0.0004	0.6932 ± 0.0001
HST-001-05	0.9999 ± 0.0003	0.7415 ± 0.0002
HST-001-06	1.0033 ± 0.0003	0.7403 ± 0.0002
HST-001-07	0.9987 ± 0.0004	0.7229 ± 0.0002
HST-001-08	0.9998 ± 0.0003	0.7213 ± 0.0002
HST-001-09	0.9948 ± 0.0004	0.6930 ± 0.0001
HST-001-10	0.9939 ± 0.0003	0.7390 ± 0.0001

OECD NEA Data Bank Activities

Ivo Kodeli input on resonance parameter processing and use of covariance data files in S/U analyses

5. CONCLUSION

This report summarizes the work performed by WPEC Subgroup 28 (SG28) on issues pertinent to the methodology used to process covariance data in the resonance region. At the start of the work effort, SG28 planned to perform the following tasks: 1) Produce resonance parameter covariance evaluation for ^{235}U; 2) Develop resonance parameter covariance processing methods in widely used processing systems (e.g., NJOY, AMPX, etc.); and 3) With the processing capabilities in place, generate covariance data files and demonstrate the use of the covariance data files in sensitivity/uncertainty analyses. The subgroup has successfully completed each of the planned tasks, culminating in the demonstration of the use of covariance data files in sensitivity/uncertainty calculations for systems that are sensitive to the resonance region. In addition, the covariance resonance processing capabilities are now available in the cross-section processing systems that are available to the user community. Based on the successful completion of the SG28 work tasks, the work of SG28 is complete and the subgroup should be closed.

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