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Processing Covariance Data for the Resonance Region

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Foreword

Nuclear energy applications require knowledge of fundamental nuclear physics in order to design and operate facilities. These data must be complemented by uncertainty information that quantifies the accuracy with which the data is known. In recent years, a considerable effort has been made to provide complete uncertainty information in nuclear data evaluations including all incident particle energy ranges.

The Nuclear Energy Agency (NEA) Working Party on International Nuclear Data Evaluation Co-operation (WPEC) was established under the NEA Nuclear Science Committee (NSC) in 1989 to promote the exchange of information on nuclear data. Following the recommendations of WPEC Subgroup 20 on Covariance Matrix Evaluation and Processing in the Resolved and Unresolved Resonance Regions, WPEC launched Subgroup 28 on Processing of Covariance Data in the Resonance Region to continue the efforts in resonance covariance processing.

The following report is issued by WPEC Subgroup 28, which builds upon the work of the previous Subgroup 20 for developing new methods for cross-section covariance evaluation. Subgroup 28 was 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.

Acknowledgements

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List of abbreviations and acronyms

AMPX	Nuclear data processing code (ORNL, United States)
BLAS	Basic Linear Algebra Subprogram
BNL	Brookhaven National Laboratory (United States)
CCF	Compact covariance format
C/E	Calculation and experimental values
CEA	French Alternative Energies and Atomic Energy Commission
COVCOMP	Nuclear data covariance comparison code (ORNL, United States)
COVERX	Nuclear data covariance format
CPU	Central processing unit
CSCM	Cross-section covariance matrices
ENDF	Evaluated Nuclear Data File (United States)
ERRORJ	Nuclear data covariance processing code (Japan)
ERRORR	Nuclear data covariance processing code (United States)
GB	Gigabytes
HST	Highly-enriched uranium, solution, thermalised benchmarks (ICSBEP)
IAEA	International Atomic Energy Agency
ICSBEP	International Criticality Safety Benchmark Evaluation Project (NEA)
IPPE	Institute of Physics and Power Engineering (Russia)
JAEA	Japan Atomic Energy Agency (Japan)
JEFF	Joint Evaluation Fission and Fusion File
JENDL	Japanese Evaluated Nuclear Data Library (Japan)
KAERI	Korea Atomic Energy Research Institute (KAERI)
KENO	Monte Carlo radiation transport code within the SCALE package
LANL	Los Alamos National Laboratory (United States)
LCOMP	Flag indicating resonance covariance compatibility in ENDF format
LRF	Flag indicating resonance parameter formalism in ENDF format
LRU	Flag indicating resolved or unresolved resonance parameters in ENDF format
MB	Megabytes
MF	File data block within ENDF format

MLBW	Multi-level Breit-Wigner
MT	Reaction data block within ENDF format
NEA	Nuclear Energy Agency (OECD)
NJOY	Nuclear data processing code (LANL, United States)
NNDC	National Nuclear Data Centre (United States)
NSC	Nuclear Science Committee (NEA)
OECD	Organisation for Economic Co-operation and Development
ORNL	Oak Ridge National Laboratory (United States)
PHYSOR	Physics of Reactors conference series
PUFF	Nuclear data processing code (ORNL, United States)
RPCM	Resonance parameter covariance matrix
RSICC	Radiation Safety Information Computational Centre (United States)
SAMMY	Nuclear resonance parameter analysis code (ORNL, United States)
SCALE	Modelling and simulation suite for nuclear analysis (ORNL, United States)
SLBW	Single-level Breit-Wigner
S/U	Sensitivity and uncertainty analysis
TSUNAMI	S/U analysis code within the SCALE package
WPEC	Working Party on International Nuclear Data Evaluation Co-operation

Executive summary

This report summarises the work performed by the Nuclear Energy Agency (NEA) Working Party on International Nuclear Data Evaluation Co-operation (WPEC) Subgroup 28 on Processing of Covariance Data in the Resonance Region. Subgroup 28 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 Subgroup 28 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 (NJOY, AMPX, etc.);
- use the updated cross-section processing systems to generate covariance data files for use in radiation transport analyses;
- use sensitivity/uncertainty (S/U) analyses to demonstrate the propagation of the covariance data in specific radiation transport applications.

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 accessible to the user community.

1. Introduction

In the Nuclear Energy Agency (NEA) Working Party on International Nuclear Data Evaluation Co-operation (WPEC) Subgroup 20 on Covariance Matrix Evaluation and Processing in the Resolved and Unresolved Resonance Regions, the evaluation and format issues were addressed for preparing new cross-section evaluations with resonance parameter covariance data. However, prior to Subgroup 28 on Processing of Covariance Data in the Resonance Region, 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 finalise the processing methods for distribution to the user community. At the completion of Subgroup 20, 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 Subgroup 28; however, covariance evaluations for important uranium and plutonium isotopes were not prepared as part of the Subgroup 20 effort. As a result, the work scope for Subgroup 28 is organised 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 Subgroup 20, and the new evaluation has been generated using the new methods and formats that were developed in Subgroup 20.
2. The second phase of the project focused on the development of the necessary 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, Subgroup 28 planned to update the cross-section checking codes to support the efforts of the nuclear data centres 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 Subgroup 28 work effort. The decision has been made at the nuclear data centres to utilise 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 Subgroup 28 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 generalised 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 Evaluated Nuclear Data File (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, Oak Ridge National Laboratory (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 Physics of Reactors conference series (PHYSOR) 2006 meeting in Vancouver, Canada in September 2006 [1].

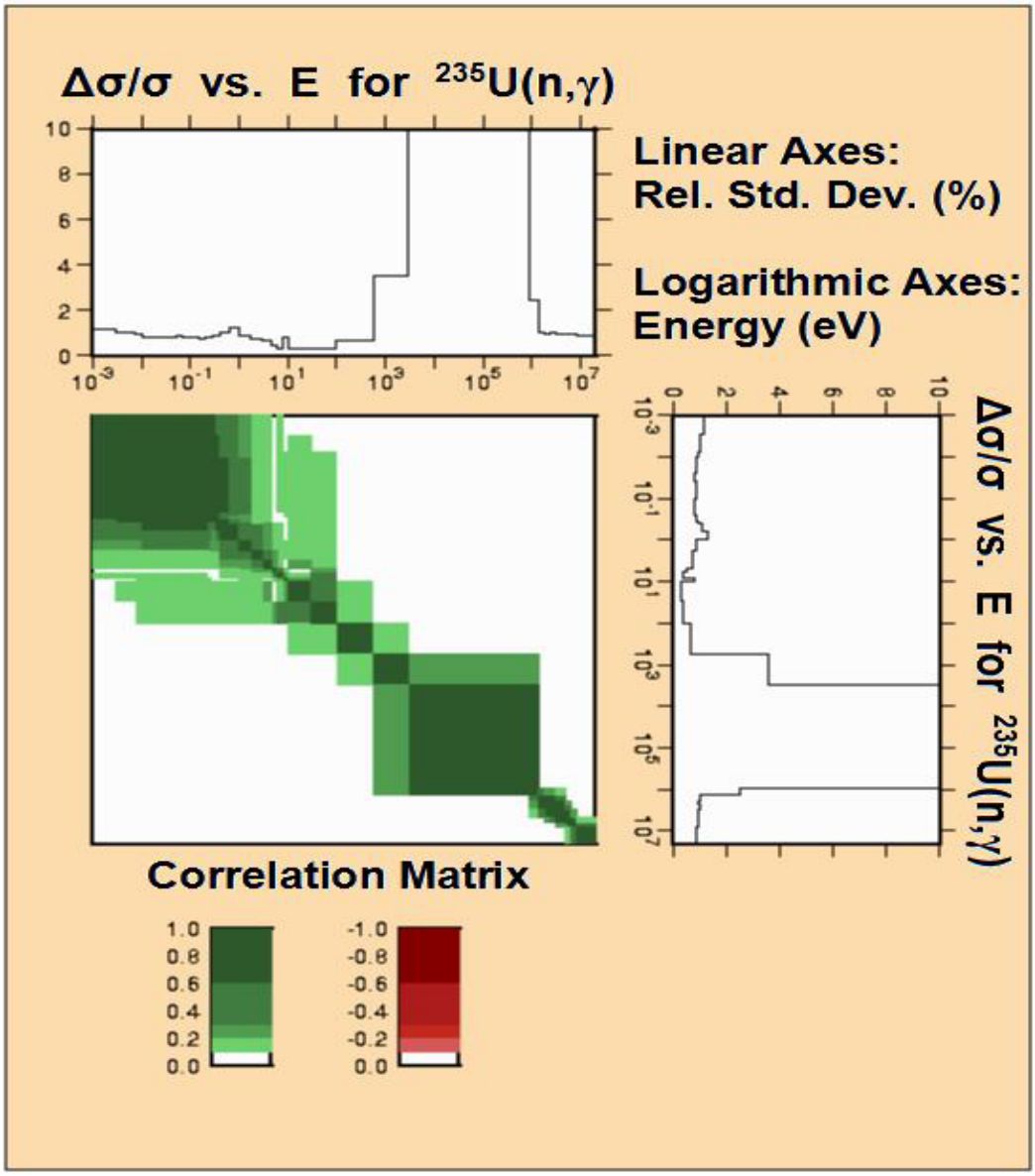
In a SAMMY evaluation, the uncertainties in the data, such as statistical and systematic uncertainties, are incorporated in the evaluation procedure. Various sources of experimental uncertainties must be included; among these are normalisation, background, neutron time-of-flight, sample thickness and 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 10 μeV to 2 250 eV using the computer code SAMMY. A total of 3 193 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 15 965 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 (GB) [1]. The computer code

PUFF-IV [4] 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 optimised by utilising the Basic Linear Algebra Subprograms (BLAS) to perform matrix multiplications. This optimisation 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 central processing unit (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 optimisation. While the resonance parameters are converted to the Evaluated Nuclear Data File (ENDF) format in the so-called "ENDF file 2" (MF2) representations, the RPCM is converted to the ENDF MF32 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 GB of computer storage. The size of the whole ^{235}U cross-section library in the ENDF format is about 3 megabytes (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 MF32 representation with reduced computer storage. A procedure was developed and implemented in the code PUFF-IV to convert the RPCM representation into the ENDF MF33 representation. The MF33 CSCM representation is intended to characterise 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 MF33 representation is reduced to about 30 Megabytes, that is, 57 times smaller than that using MF32. The computer time needed to process the MF33 covariance information is about 750 times smaller than that using MF32. 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, Los Alamos National Laboratory (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 Subgroup 28 objective. The complete ^{235}U covariance file is available for processing and testing.

Figure 1 shows the capture cross-section covariance data processed with PUFF-IV code in the 44-group 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 2 250 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



Source: ORNL, 2019.

3. Processing code development and testing

3.1. Oak Ridge National Laboratory: AMPX covariance processing developments

A summary of the ENDF/B Formats for Files 2 and 32 information is provided in Table 1 [2]. Prior to the start of Subgroup 28 on Processing of Covariance Data in the Resonance Region, 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 Subgroup 28 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. It should be noted 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 Files 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 in September 2006 [3].

Table 1. Parameters characterising the content of ENDF/B Files 2 and 32

ENDF parameter	Value	Definition
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.

Source: BNL, 1991 [2].

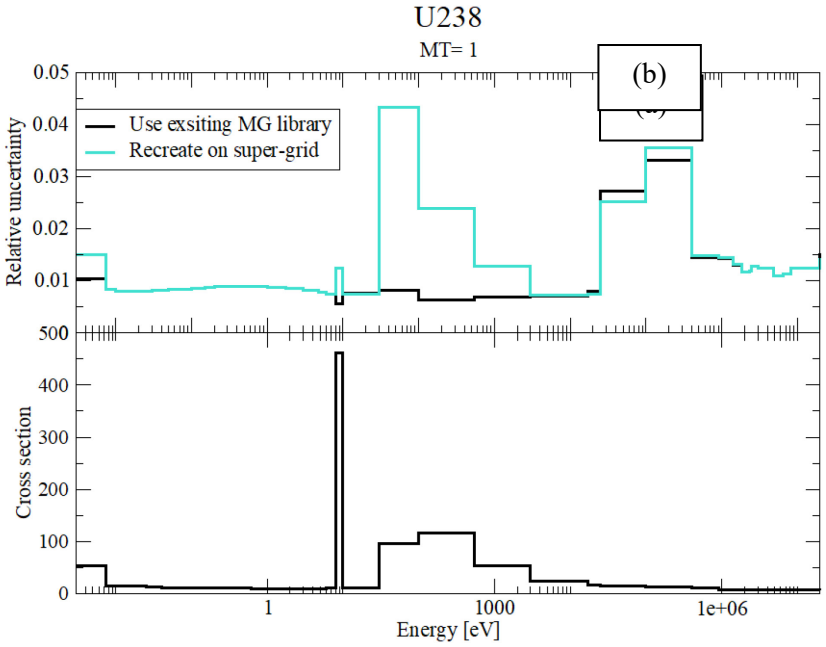
Although PUFF-IV is part of the AMPX cross-section processing system, a stand-alone PUFF-IV package has been developed and is available for distribution from the Radiation Safety Information Computational Centre (RSICC) as software package P00534 [4]. PUFF is designed to function with the AMPX code system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

With regard to the objectives of Subgroup 28, 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 Subgroup 28, 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.

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



Source: ORNL, 2019.

3.2. Los Alamos National Laboratory (LANL) and Japan Atomic Energy Agency (JAEA): NJOY covariance processing developments

NJOY covariance processing is handled via the "ERRORR" module. As originally developed this module could handle covariance data found in ENDF's MF=31, MF=32 and MF=33. Over time, however, evaluated covariance data also became available in files MF=34 (scattering angular distributions), MF=35 (secondary emission spectra) and MF=40 (cross-sections).

In the absence of sponsor support NJOY's capabilities did not expand to handle these additional covariance data forms, but there was interest from the international community. With permission, the JAEA extracted NJOY's ERRORR module and created a stand-alone code, ERRORJ [8] that recognised these new data formats.

Subsequently, beginning in NJOY99.258 and with JAEA permission, the ERRORJ code was re-integrated into NJOY. The "ERRORR" module name was retained but the new JAEA developed capabilities were now embedded in NJOY. It should be noted however that the MF=34 and MF=35 processing capabilities have specific limitations. In particular MF=34 processing only works for the elastic scattering (MT=2) P1, i.e. mubar, moment. For MF=35 only the prompt fission neutron spectra (MT=18) has been processed. Finally, for MF=40 there is only one example in ENDF/B-VII (93Nb). The existing coding has been tailored to fit the data as presented in this evaluation and it is likely that further code updates will be necessary if and when the full MF=40 format is utilised.

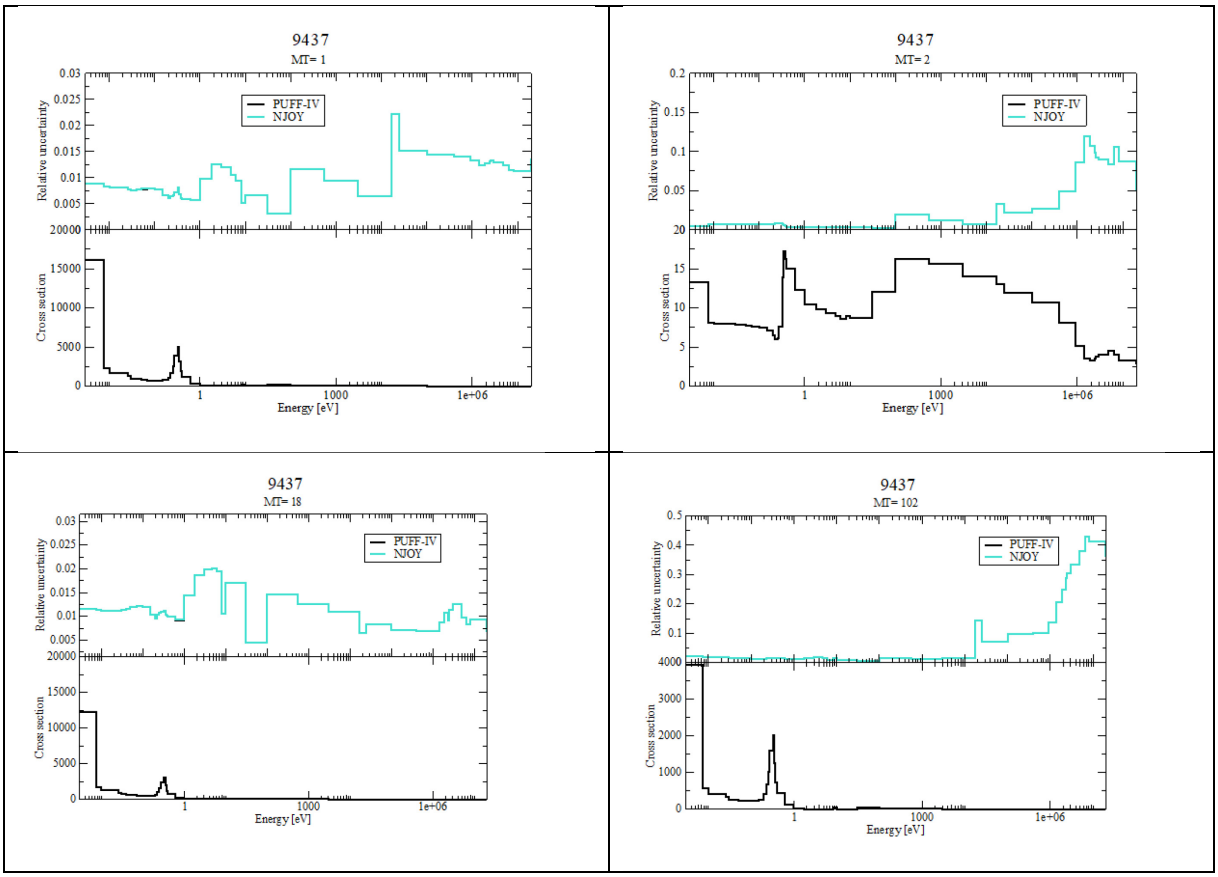
3.3. US National Nuclear Data Centre activities (NNDC)

Following the release of ENDF/B-VII.0 and in preparation for ENDF/B-VII.1, the US National Nuclear Data Centre (NNDC) processed all of the covariance data available in the ENDF/B neutron sub-library using NJOY99. The covariances were placed in the ORNL 44 group structure and the LANL 187 group structure. In addition, covariances from Joint Evaluation Fission and Fusion File (JEFF)-3.1 and Japanese Evaluated Nuclear Data Library (JENDL)-3.3 were processed using the same system. The results are posted on the NNDC website[1]. This comparison illustrated that the JENDL-3.3 suite of covariances is by far the most complete as of 2008. More modern libraries such as ENDF/B-VII.1, ENDF/B-VIII.0 and JENDL-4 far exceed the JENDL-3.3 covariance inventory.

3.4. Processing code comparisons between PUFF-IV and NJOY

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

Figure 3. Comparisons between resonance parameter covariance matrices for ^{239}Pu processed with ERRORR and PUFF-IV

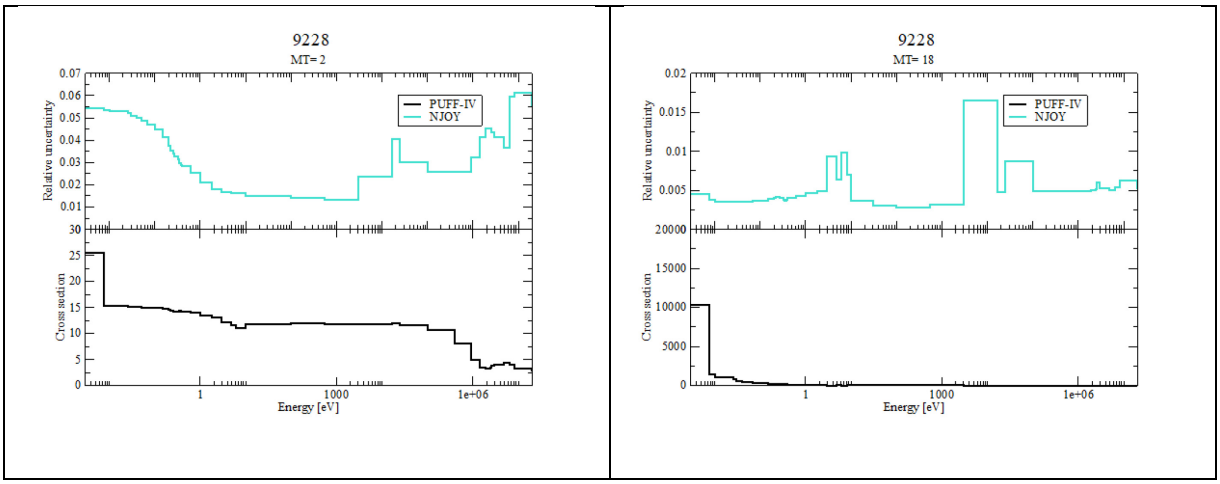


Source: ORNL, 2019.

1. Available for direct download at www.nndc.bnl.gov/endf/b7.1/covariances.html.

In addition, covariance files containing covariance matrices were processed 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. Covariance matrices were generated 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. It should be noted 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.

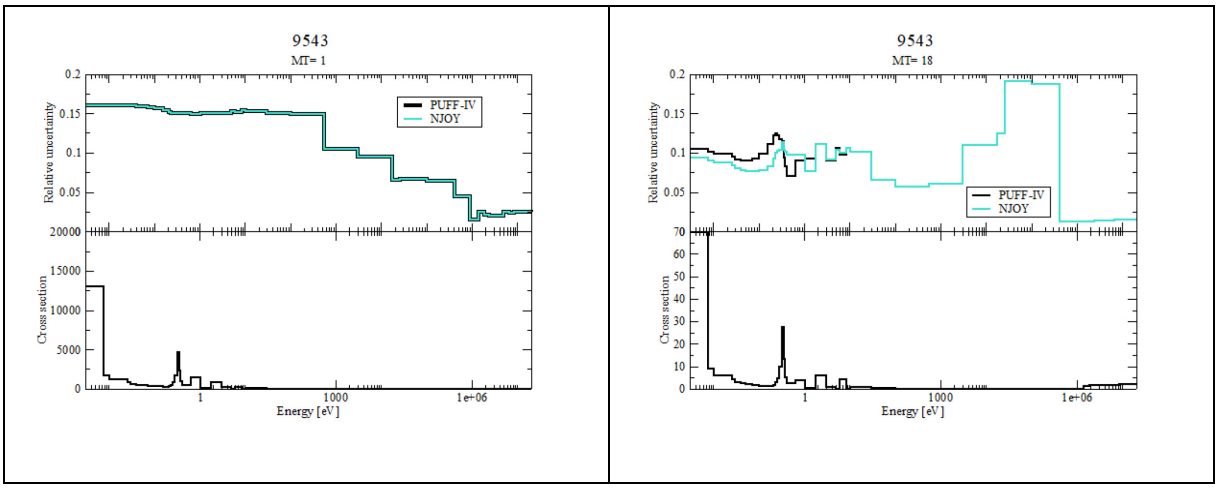
Figure 4. Comparisons between resonance parameter covariance matrices for ^{235}U processed with ERRORR and PUFF-IV



Source: ORNL, 2019.

Good agreement is also found in most cases where File 32 resonance parameters are given. As an example, Figure 2 shows the results for ^{239}Pu with the full resolved resonance parameter matrix. 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. Comparisons between resonance parameter covariance matrices for ^{241}Am processed with ERRORR and PUFF-IV



Source: ORNL, 2019.

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 2 250 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 multi-group cross-section data are produced with adjoint-based perturbation theory.

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

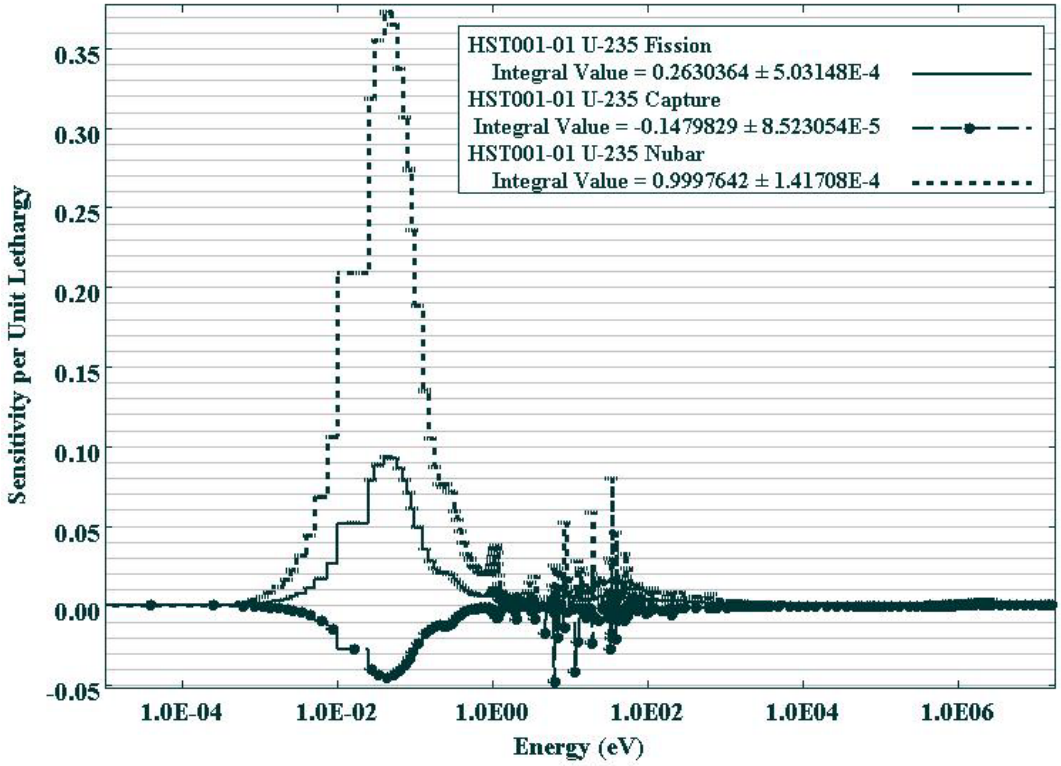
	(n,γ)	(n,f)	(n,n)	(n,n')	(n,2n)	v-bar
(n,γ)	2.0057×10^{-1} $\pm6.7745\times10^{-5}$					
(n,f)	1.1572×10^{-1} $\pm8.3693\times10^{-5}$	8.5765×10^{-2} $\pm9.1514\times10^{-5}$				
(n,n)	1.4599×10^{-2} $\pm3.8936\times10^{-6}$	-6.4656×10^{-3} $\pm2.9765\times10^{-6}$	3.2326×10^{-3} $\pm3.7405\times10^{-6}$			
(n,n')			6.1170×10^{-3} $\pm1.0276\times10^{-5}$	1.0497×10^{-2} $\pm1.2372\times10^{-5}$		
(n,2n)			6.4745×10^{-5} $\pm1.1040\times10^{-7}$		5.6611×10^{-4} $\pm5.2855\times10^{-7}$	
v-bar						6.7756×10^{-1} $\pm5.2886\times10^{-5}$

Note: Relative standard deviation is % $\Delta k/k$ in k_{eff}.

Source: ORNL, 2019.

The benchmarks used in the calculations are 10 thermal benchmark systems. The k_{eff} KENO calculations were performed 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 (United States). These experiments are included in the International Criticality Safety Benchmark Evaluation Project (ICSBEP) and are identified as HST-001.

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



Source: ORNL, 2019.

The sensitivities of the multiplication factor to the ^{235}U ν-bar, fission and capture cross-sections for the HST-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 2 250 eV. Therefore, the uncertainty in the k_{eff} is predominantly due to the uncertainty in the resonance region of the ^{235}U.

Table 3 presents the k_{eff} results for the 10 cases of the HST-001 benchmark systems. 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

Source: ORNL, 2019.

5. Conclusions

This report summarises the work performed by the Nuclear Energy Agency (NEA) Working Party on International Nuclear Data Evaluation Co-operation (WPEC) Subgroup 28 on Processing of Covariance Data in the Resonance Region. At the start of the work effort, Subgroup 28 planned to perform the following tasks:

- produce a resonance parameter covariance evaluation for ^{235}U;
- develop resonance parameter covariance processing methods in widely used processing systems (NJOY, AMPX, etc.);
- 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.

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