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New Capabilities for Processing Covariance Data in Resonance Region

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Abstract

The AMPX [1] code system is a modular system of FORTRAN computer programs that relate to nuclear analysis with a primary emphasis on tasks associated with the production and use of multi group and continuous energy cross sections. The module PUFF-III within this code system handles the creation of multi group covariance data from ENDF information. The resulting covariances are saved in COVERX format [2].

We recently expanded the capabilities of PUFF-III to include full handling of covariance data in the resonance region (resolved as well as unresolved). The new program handles all resonance covariance formats in File 32 except for the long-range covariance sub sections. The new program has been named PUFF-IV. To our knowledge, PUFF-IV is the first processing code that can address both the new ENDF format for resolved resonance parameters and the new ENDF "compact" covariance format. The existing code base was rewritten in Fortran 90 to allow for a more modular design. Results are identical between the new and old versions within rounding errors, where applicable. Automatic test cases have been added to ensure that consistent results are generated across computer systems.

KEYWORDS: AMPX, covariance data, resonance region

1. Introduction

Since the release of Version IV of the Evaluated Nuclear Data File (ENDF) [3], standards and formats have been in place to permit the communication of estimated uncertainties in the evaluated cross section data. By including the uncertainty or covariance information, the analyst can propagate cross section data uncertainties through sensitivity studies to the final calculated quantities of interest in nuclear applications. The covariance data files provide the estimated variance for the individual data as well as any correlations that may exist. Table 1 contains a summary of the ENDF covariance information and the corresponding file number location within the ENDF system that can be processed by PUFF-IV.

	Table 1. File information in ENDF the processed by POFF-IV
<u>File</u>	Covariance information
31	Average number of neutrons per fission
32	Resonance parameters (Additional information from File 2 containing the resonance parameters is needed to process the covariance information.)
33	Neutron cross sections

Table 1: File Information in ENDF file processed by PUFF-IV

ENDF formatted files may include covariance information for angular and energy distributions of secondary particles and production yield and cross sections of radioactive nuclei. However, this information is not processed by PUFF-IV at this time. Also, to our knowledge, no other processing codes process this information.

The covariance information in the ENDF formatted files is given with respect to point-wise cross section data in the case of File 31 and 33 and with respect to resonance parameters in File 32. Prior to

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using the covariance information in applications, a processing code must be used to convert the energydependent covariance information in the ENDF library to a multi group form. At the Oak Ridge National Laboratory (ORNL), PUFF-III has 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 do limited sensitivity analysis for selected File 32 formats. PUFF-IV can now do full processing of all File 32 formats except for long-range covariance information. 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. The amount of covariance information that can be processed by PUFF-IV is limited only by available computer memory.

Processing of File 31 and File 33 point-wise covariance data into group-averaged data is discussed in detail in the PUFF manual [4], summary information is provided as needed. The focus of this paper is processing of resonance parameter covariance data, that is, File 32 covariance information.

2. Group-averaged covariance data

File 31 and File 33 contain covariance information for point-wise cross section data as a function of energy. ENDF formats for the two files are identical. An ENDF file 31 or 33 consists of different subsections, each describing a covariance matrix. The subsections in turn contain sub-subsections which can be of "NI" or "NC" type. The "NI" sub-subsections give relative or absolute point-wise covariance data over an evaluator-defined energy range and energy grid. The "NC" sub-subsections define covariances matrices that are derived from "NI" sub-subsection covariance data over an evaluator-defined energy range. The "NI" sections referred to by an "NC" section may be in the material processed or refer to a standard material.

Formats for File 32 closely follow formats for File 2. Resonance parameter covariance matrices may be given for different isotopes and different energy ranges.

The covariance data calculated from the different sources in File 31, 32, and 33 need to be combined to form the full covariance matrix data. To facilitate that combination, the covariance data are calculated on a union grid. The various grids used by PUFF-IV are summarized in Table 2.

Grid	Grid Title	Description
1	Cross section	Multi group cross section energy grid provided as user input or from an AMPX master library
2	User	Final multi group structure provided as user input for the calculated covariance matrices
3	Uncertainty ranges	Energy grid values provided by evaluator in ENDF as energy boundaries in the uncertainty file(s). These include "NC" section boundaries from File 31 and File 33 and energy range boundaries from File 2 and File 32.
4	Uncertainty grid	Union of all the energy grids provided by "NI" sub-sections in File 31 and File 33, that is, the evaluator-provided energy grids.
5	Super-grid	Union of the user grid 2 and the uncertainty energy grid 3. In most cases, calculations are done on this grid.
6	Super-user	Union of the Super grid 5 and uncertainty grid 4. If File 31 or File 33 contains reference to, or is, a standard covariance matrix, calculations are done on this grid.

 Table 2: Energy grid structures used in PUFF-IV

In most cases, group-averaged covariances matrices are calculated on the "Super-grid", that is, grid 5 in Table 2. In some cases, calculation is done on the "Super-user" grid. The latter is necessary if covariance information is given as a ratio to a standard material covariance matrix or is itself a standard material; see [4] for more detail. Performing the calculation on the appropriate union grid ensures that energy range boundaries will always coincide with group boundaries, which eases calculation is done and as such refers to either grid 5 or grid 6, depending on File 31 and File 33 content.

The weighting function ϕ_g^u and group averaged cross section data $x_g^{m,u}$ for reaction *m* are supplied on the user grid but are needed on the union grid, where the subscript *g* refers to a user group and the superscript to the reaction. Since the union grid is always equal to or finer than the user grid, the flux ϕ_I and the cross section x_I^m on the union grid can be written as:

$$\phi_{I} = \sum_{g=1}^{NG} \begin{cases} \phi_{g}^{u} \frac{E_{I+1} - E_{I}}{E_{g+1}^{u} - E_{g}^{u}} & E_{g}^{u} \le E_{I} < E_{I+1} \le E_{g+1}^{u} \\ 0 & \text{otherwise} \end{cases} \\
x_{I}^{m} = \frac{1}{\phi_{I}} \sum_{g=1}^{NG} \begin{cases} x_{g}^{m,u} \phi_{g}^{u} \frac{E_{I+1} - E_{I}}{E_{g+1}^{u} - E_{g}^{u}} & E_{g}^{u} \le E_{I} < E_{I+1} \le E_{g+1}^{u} \\ 0 & \text{otherwise} \end{cases}$$
(1)

where the index *I* refers to union group $[E_I, E_{I+1}]$ and *g* to the user group $[E_g^u, E_{g+1}^u]^2$. The covariance matrices calculated on the union grid need to be collapsed to the user grid. Assume

 $\langle \delta x_I^m \delta x_J^n \rangle$ is the covariance matrix element on the union grid; then the covariance matrix element on the user grid is:

$$\langle \delta x_g^{m,u} \delta x_{g'}^{n,u} \rangle = \frac{1}{\phi_g^u \phi_{g'}^u} \sum_I \sum_J \phi_I \phi_J \langle \delta x_I^m \delta x_J^n \rangle \quad \text{for} \quad \begin{cases} E_g^u \leq E_I & \langle E_{I+1} \leq E_{g+1}^u \\ E_{g'}^u \leq E_J & \langle E_{J+1} \leq E_{g'+1}^u \end{cases}$$
(2)

and 0 otherwise.

The ENDF data in File 31, 32, and 33 yield point-wise covariance data. A group averaged cross section x_I^m is calculated from the point wise cross section $\sigma^m(E)$, where the superscript again denotes the reaction, via the formula:

$$x_{I}^{m} = \frac{1}{\int_{E_{I}}^{E_{I+1}} \phi(E) dE} \int_{E_{I}}^{E_{I+1}} \phi(E) \sigma^{m}(E) dE$$
(3)

Therefore the point-wise cross section covariance matrix element $\langle \delta \sigma^{m}(E) \delta \sigma^{n}(E') \rangle$ can be transformed into the group averaged covariance matrix element via the following formula:

$$\langle \delta x_I^m \delta x_J^n \rangle = \frac{1}{\phi_I \phi_J} \int_I \int_J \phi(E) \phi(E') \langle \delta \sigma^m(E) \delta \sigma^n(E') \rangle dE dE'$$
(4)

2.1 Resonance region

In the resonance region the covariance data are given as a function of the resonance parameters. To get the covariance data for the group averaged cross section data, the parameter covariance values need to be propagated to the point-wise cross section data. For a given reaction m and a set of parameters

 $[P_i]$ the point-wise cross section at energy *E* is given as: $\sigma_{--}(E) = \sigma_{--}(E, P_i)$ (5)

Define the expectation value for a given parameter as
$$\langle P_i \rangle$$
 and the parameter covariance matrix

² While weighting over lethargy in the resonance region might be more appropriate, PUFF-III has used the weighting

outlined in Eq. (1), and thus the same behavior has been preserved in PUFF-IV.

element as $\langle \delta P_i \delta P_j \rangle$, where δP_i is a small increment in P_i . Then the covariance matrix element for point-wise cross section between reaction *m* and *l* is given by:

$$\langle \delta \sigma_m(E) \delta \sigma_l(E') \rangle = \langle \sum_k \frac{\partial \sigma_m(E)}{\partial P_k} \delta P_k \sum_n \frac{\partial \sigma_l(E')}{\partial P_n} \delta P_n \rangle$$

$$= \sum_{kn} \frac{\partial \sigma_m(E)}{\partial P_k} \langle \delta P_k \delta P_n \rangle \frac{\partial \sigma_l(E')}{\partial P_n}$$
(6)

To get the group averaged cross section covariance matrix element we insert Eq. (6) into Eq. (4) which gives:

$$\langle \delta x_{I}^{m} \delta x_{J}^{l} \rangle = \frac{1}{\phi_{I} \phi_{J}} \int_{I} \int_{J} \phi(E) \phi(E') \langle \delta \sigma_{m}(E) \delta \sigma_{l}(E') \rangle dE dE' = \frac{1}{\phi_{I} \phi_{J}} \sum_{kn} \int_{I} \int_{J} \phi(E) \phi(E') \frac{\partial \sigma_{m}(E)}{\partial P_{k}} \langle \delta P_{k} \delta P_{n} \rangle \frac{\partial \sigma_{l}(E')}{\partial P_{n}} dE dE' = \frac{1}{\phi_{I} \phi_{J}} \sum_{k,n} \langle \delta P_{k} \delta P_{n} \rangle \left(\int_{I} \phi(E) \frac{\partial \sigma_{m}(E)}{\partial P_{k}} dE \right) \left(\int_{J} \phi(E') \frac{\partial \sigma_{l}(E)}{\partial P_{n}} dE' \right)$$

$$(7)$$

If we define

$$D_{Ik}^{m} = \frac{1}{\phi_{I}} \int_{I} \phi(E) \frac{\partial \sigma_{m}(E)}{\partial P_{k}} dE$$
(8)

then Eq (7) can be rewritten as

$$\langle \delta x_I^m \delta x_J^l \rangle = \sum_{kn} D_{Ik}^m \langle \delta P_k \delta P_n \rangle D_{Jn}^l \quad , \tag{9}$$

which gives the desired covariance information for the group-averaged cross sections as a function of energy. Calculation of the partial derivatives is done analytically as outlined in Sect. 2.1.1 and 2.1.2. The integrals defined in Eq. (8) are converted into a system of coupled partial differential equations. This set is solved numerically using a fourth-order Runge-Kutta algorithm with adaptive step-size [5]. This procedure allows one to easily adapt the step size to any fast-changing structures in the partial derivatives. The step size required may be finer than the step size required to calculate the group averages of the cross section itself. If the number of resonance parameters is large, the system is broken into separate systems of up to 1000 coupled differential equations.

The integral in Eq. (8) contains flux information. If the flux is known as a function of energy it can easily be incorporated into the numerical integration. This is the case if the user specifies 1/E weighting. If the flux is known only on the union grid, that is, the flux is not known as a function of energy but only as a function of the user grid, as is the case for all the other weighting options in PUFF-IV, the best we can assume is that the flux ϕ' as a function of energy is constant over the range of a given union group:

$$\phi_{I} = \int_{I} \phi' dE = (E_{I+1} - E_{I}) \phi' \text{ therefore } \phi' = \frac{\phi_{I}}{(E_{I+1} - E_{I})}$$
(10)

Thus Eq. (8) becomes:

$$D_{Ik}^{m} = \frac{1}{\phi_{I}} \int_{I} \phi' \frac{\partial \sigma_{m}(E)}{\partial P_{k}} dE = \frac{1}{\phi_{I}} \int_{I} \frac{\phi_{I}}{E_{I+1} - E_{I}} \frac{\partial \sigma_{m}(E)}{\partial P_{k}} dE = \frac{1}{E_{I+1} - E_{I}} \int_{I} \frac{\partial \sigma_{m}(E)}{\partial P_{k}} dE$$
(11)

This is equivalent to assuming constant flux as far as the calculation of the integral is concerned. Collapsing the covariance matrix from the union grid to the user-grid is still done using the user supplied weighting function, that is, Eq. (2). The procedure outlined in Eq. (10) and Eq. (11) is only used if a weighting option other than 1/E is chosen.

File 2 and File 32 information is divided into isotope sections, each specifying the relative abundance of the isotope. Each isotope section is further divided into energy ranges. Each energy range is characterized by the parameters given in Table 3, where LCOMP is only used for resolved-resonance

covariances in File 32. Not all possible combinations of LRU, LRF, and LCOMP are allowed by the ENDF formats. In the unresolved-resonance region, only one format is defined.

LRU	=	1	Resolved resonance data
2		2	Unresolved resonance data
LRF = 1 Single-level Breit-Wigner (SLBW) r 2 Multilevel Breit-Wigner (MLBW) r 3 Reich-Moore resonance parameters; allowed			Single-level Breit-Wigner (SLBW) resonance parameters
			Multilevel Breit-Wigner (MLBW) resonance parameters
			Reich-Moore resonance parameters; no competitive reactions allowed
		4	Adler-Adler resonance parameters (not implemented in PUFF-IV)
		7	Reich-Moore resonance parameters. It contains all the generality of LRF=3 plus unlimited numbers and types of channels
LCOMP	=	0	Only diagonal elements are given.
		1	The entire covariance matrix is given for one or more blocks of resonances.
		2	Covariances are given in a compact format that allows a compromise between amount of data given and accuracy of the covariance data.

Table 3. Parameters	characterizing	the content	in	File 2	and File 32
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PUFF-IV assumes that there is no correlation between data in different isotope and energy range blocks, therefore the covariance matrices calculated for the different energy ranges and isotopes can simply be added together. Suppose one isotope is described by parameter set $[P_i]$ and has a relative abundance of *a*. Let the second isotope be described by parameter set $[Q_i]$ and a relative abundance of *b*. The point-wise cross section is given by:

$$\sigma^{m}(E) = a \sigma_{1}^{m} \left(E, \left[P_{i} \right] \right) + b \sigma_{2}^{m} \left(E, \left[Q_{i} \right] \right)$$

$$\tag{12}$$

The group-averaged cross section covariance matrix element is then:

$$\langle \delta x_{I}^{m} \delta x_{J}^{l} \rangle = \frac{a^{2}}{\phi_{I} \phi_{J}} \sum_{kn} \int_{I} \int_{J} \phi(E) \phi(E') \frac{\partial \sigma_{1}^{m}[E, [P_{k}]]}{\partial P_{k}} \langle \delta P_{k} \delta P_{n} \rangle \frac{\partial \sigma_{1}^{l}[E', [P_{n}]]}{\partial P_{n}} dE dE$$

$$= \frac{b^{2}}{\phi_{I} \phi_{J}} \sum_{ij} \int_{I} \int_{J} \phi(E) \phi(E') \frac{\partial \sigma_{2}^{m}[E, [Q_{i}]]}{\partial Q_{i}} \langle \delta Q_{i} \delta Q_{j} \rangle \frac{\partial \sigma_{2}^{l}[E', [Q_{j}]]}{\partial Q_{j}} dE dE'$$

$$= \frac{ab}{\phi_{I} \phi_{J}} \sum_{kn} \int_{I} \int_{J} \phi(E) \phi(E') \frac{\partial \sigma_{2}^{m}[E, [P_{k}]]}{\partial P_{k}} \langle \delta P_{k} \delta Q_{j} \rangle \frac{\partial \sigma_{2}^{l}[E', [P_{k}]]}{\partial Q_{j}} dE dE'$$

$$= \frac{a^{2}}{\phi_{I} \phi_{J}} \sum_{k,n} \langle \delta P_{k} \delta P_{n} \rangle D_{lk}^{m,1} D_{Jn}^{l,1} + \frac{b^{2}}{\phi_{I} \phi_{J}} \sum_{i,j} \langle \delta Q_{i} \delta Q_{j} \rangle D_{li}^{m,2} D_{Jj}^{l,2}$$

Formulae for adding energy-range covariance matrices are similar, since group boundaries coincide with energy-range boundaries. Covariance matrices are added first for the different energy ranges for a given isotope. The isotopic covariance matrices are added next, taking into account the relative abundance information. The processing of covariance information is depicted in Fig. 1.





2.1.1 Resolved resonance region

In the resolved resonance region the derivatives are calculated using only data provided in File 2 using a library (*samrml*) developed by N. M. Larson, the author of the R-Matrix fitting program SAMMY [6]. The library analytically calculates derivatives of point-wise cross sections for Reich-Moore parameters. Even if the resonance data are given in terms of Single- or Multi-Level Breit-Wigner formalism, the Reich-Moore formulae are used to calculate the derivatives. Although this is an approximation, nevertheless it should be quite good. For situations in which the Breit-Wigner approximations are adequate, they give nearly the same cross sections and derivatives as does the Reich-Moore approximation. However, problems may arise for older evaluations that provide an averaged value for the total angular momentum of the resonances. The Reich-Moore formalism cannot handle this situation, which is allowed if using Single- or Multi-Level Breit-Wigner formalism. If a

case like this is encountered, PUFF-IV aborts the calculation. It is suggested to fall back to the PUFF-III type sensitivity analysis. This option can be selected via user input.

The *samrml* library provides derivatives for elastic scattering (ENDF reaction number 2), absorption (radiative capture - ENDF reaction number 102-, plus all remaining reactions), and for the remaining reactions, if applicable. The remaining channels are fission (ENDF reaction number 18) if LRF = 1,2,3 and material is fissionable, or the reaction number specified by the particle pair information if LRF = 7. PUFF-IV translates these channels into ENDF reaction numbers and calculates the derivative for the total cross section as a sum over all the other derivatives.

2.1.2 Unresolved resonance region

The covariance data given in File 32 for the unresolved resonance parameters assume that the parameters are energy independent. This is the case even if the corresponding resonance parameters given in File 2 are energy dependent. Therefore, the partial derivatives with respect to the resonance parameters cannot be calculated solely from the information given in File 2. Instead, the resonance parameters are read from File 32 and the degrees of freedom, needed to calculate the energy average of the width parameters (see [3]), are read from File 2 as they are not repeated in File 32. Evaluation of the energy-averaged width integral is done using a quadrature integration outlined in [7], with the weights and abscissa given in [8]. Since the partial derivatives are only needed at T = 0, no Doppler broadening or line shape functions are included. In this case, the analytical derivation of the partial derivatives, the same quadrature integration procedure can be used to do the numerical calculation of the integral.

3. Program Verification

To verify that the new capabilities in the resonance region give the expected results, covariance matrices have been compared with calculations done with SAMMY [6] and ERRORJ [9]. The R-Matrix fitting program SAMMY is primarily used to determine resonance parameters from experimental data but has the capabilities 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 a processing code for covariance matrices similar to PUFF-IV. All three programs should therefore yield similar results given the same ENDF data file. This is indeed the case for all data files that we compared. Comparison with results for SAMMY was done for all supported ENDF File 32 formats.

Here we present the comparison for 233 U [10]. The resolved-resonance region of 233 U has 770 resonances (or 3850 resonance parameters), which allows us to test whether the covariance information can be calculated in a timely manner. The CPU time required for the full resonance calculation of 233 U is around 3 h on a 3 GHz INTEL processor running Linux. Covariance information is provided in the resolved as well as in the unresolved region. The resolved-resonance information in File 32 is provided in LRF = 3, LCOMP = 1 format (see Table 3) and was generated using the R-Matrix fitting program SAMMY.

Both SAMMY and PUFF-IV offer various options for the weighting functions. However, the option allowing the most direct comparison is a constant flux as function of energy. This option was used for the data in Table 4, which compares the relative standard deviation for the total cross section calculated by SAMMY and PUFF-IV. Differences are to be expected as the numerical integration routines used are slightly different for the two codes. In addition the effective energy grid used in PUFF-IV contains about double the number of energy points compared to the grid supplied to SAMMY. Due to size and computer limitations SAMMY would not run using the same energy grid as PUFF-IV for the ²³³U ENDF. In regions with many resonances, the group uncertainties are very dependent on the energy grid used. The numerical integration with adaptive step-size used by PUFF-IV automatically selects the appropriate grid. The correlation matrices for the total cross section over the resolved resonance region

are compared in Fig. 2. As can be seen, no significant differences are found between the results of the two codes.

Table 4: SAMMY and PUFF-IV results for total cross section data and relative standard deviation for groups 16–44 of the 44-group structure of the SCALE [11] code system. This corresponds to the energy range [550 eV,0.00001 eV], which is the range for which resolved resonance covariance data exist in the ²³³U ENDF formatted file used. Group-averaged cross section data are taken from the SAMMY calculation

Group	Lower energy [eV]	Upper energy [eV]	Total cross section [barns]	Relative std. dev. PUFF-IV	Relative std. dev. SAMMY
16	5.500x10 ⁺²	$1.000 \times 10^{+2}$	3.36286x10 ⁺¹	4.22060x10 ⁻³	4.22129x10 ⁻³
17	$1.000 \times 10^{+2}$	3.000x10 ⁺¹	5.83891x10 ⁺¹	4.26230x10 ⁻³	4.26128x10 ⁻³
18	3.000x10 ⁺¹	$1.000 \times 10^{+1}$	$1.28274 \mathrm{x10^{+2}}$	5.03140x10 ⁻³	5.03257x10 ⁻³
19	$1.000 \mathrm{x10^{+1}}$	8.100x10 ⁺⁰	6.74858x10 ⁺¹	1.21770x10 ⁻²	1.21375x10 ⁻²
20	8.100x10 ⁺⁰	6.000x10 ⁺⁰	1.86188x10 ⁺²	1.34800x10 ⁻²	1.34775x10 ⁻²
21	$6.000 \mathrm{x10}^{+0}$	4.750x10 ⁺⁰	1.04716x10 ⁺²	1.99130x10 ⁻²	1.99304x10 ⁻²
22	$4.750 \times 10^{+0}$	3.000x10 ⁺⁰	1.16561x10 ⁺²	9.91260x10 ⁻³	9.91448x10 ⁻³
23	3.000x10 ⁺⁰	1.770x10 ⁺⁰	3.52685x10 ⁺²	1.20930x10 ⁻²	1.21013x10 ⁻²
24	$1.770 \mathrm{x10^{+0}}$	$1.000 \mathrm{x10^{+0}}$	4.07034x10 ⁺²	1.07210x10 ⁻²	1.07173x10 ⁻²
25	$1.000 \mathrm{x} 10^{+0}$	6.250x10 ⁻¹	1.46331x10 ⁺²	3.12840x10 ⁻³	3.12664x10 ⁻³
26	6.250x10 ⁻¹	4.000x10 ⁻¹	1.57519x10 ⁺²	3.04960x10 ⁻³	3.05055x10 ⁻³
27	4.000x10 ⁻¹	3.750x10 ⁻¹	1.72806x10 ⁺²	3.01350x10 ⁻³	3.01704x10 ⁻³
28	3.750x10 ⁻¹	3.500x10 ⁻¹	$1.77170 \mathrm{x10^{+2}}$	2.94510x10 ⁻³	2.95030x10 ⁻³
29	3.500x10 ⁻¹	3.250x10 ⁻¹	1.82229x10 ⁺²	2.88930x10 ⁻³	2.89585x10 ⁻³
30	3.250x10 ⁻¹	2.750x10 ⁻¹	1.91714x10 ⁺²	2.89480x10 ⁻³	2.90025x10 ⁻³
31	2.750x10 ⁻¹	2.500x10 ⁻¹	2.04090x10 ⁺²	3.38000x10 ⁻³	3.37978x10 ⁻³
32	2.500x10 ⁻¹	2.250x10 ⁻¹	2.14953x10 ⁺²	3.36660x10 ⁻³	3.37133x10 ⁻³
33	2.250x10 ⁻¹	2.000x10 ⁻¹	2.25609x10 ⁺²	3.27540x10 ⁻³	3.28172x10 ⁻³
34	2.000x10 ⁻¹	1.500x10 ⁻¹	2.41047x10 ⁺²	2.67360x10 ⁻³	2.67571x10 ⁻³
35	1.500x10 ⁻¹	1.000x10 ⁻¹	2.71798x10 ⁺²	2.48750x10 ⁻³	2.49168x10 ⁻³
36	1.000x10 ⁻¹	7.000x10 ⁻²	3.25469x10 ⁺²	2.26820x10 ⁻³	2.27745x10 ⁻³
37	7.000x10 ⁻²	5.000x10 ⁻²	3.86043x10 ⁺²	2.10160x10 ⁻³	2.10917x10 ⁻³
38	5.000x10 ⁻²	4.000x10 ⁻²	4.43917x10 ⁺²	1.99450x10 ⁻³	1.99893x10 ⁻³
39	4.000x10 ⁻²	3.000x10 ⁻²	5.02889x10 ⁺²	1.93540x10 ⁻³	1.93746x10 ⁻³
40	3.000x10 ⁻²	2.530x10 ⁻²	5.63899x10 ⁺²	1.90960x10 ⁻³	1.90922x10 ⁻³
41	2.530x10 ⁻²	1.000x10 ⁻²	7.20819x10 ⁺²	1.90900x10 ⁻³	1.90408x10 ⁻³
42	1.000x10 ⁻²	7.500x10 ⁻³	9.97115x10 ⁺²	1.95240x10 ⁻³	1.94371x10 ⁻³
43	7.500x10 ⁻³	3.000x10 ⁻³	1.31286x10 ⁺³	1.98540x10 ⁻³	1.97474x10 ⁻³
44	3.000x10 ⁻³	1.000x10 ⁻⁵	3.17821x10 ⁺³	2.03580x10 ⁻³	2.02840x10 ⁻³

To compare results between ERRORJ and PUFF-IV, we used the 1/E weighting option. Results for the unresolved resonance region are listed in Table 5. The agreement between the relative uncertainties calculated by PUFF-IV and ERRORJ is not expected to be exact, as PUFF-IV uses analytical differentiation, whereas ERRORJ uses numerical differentiation of the cross section data with respect to the resonance parameters. In addition, the energy grids used to integrate the data are different for the two codes.

Table 5: ERRORJ and PUFF-IV results for total cross section data and standard deviation for the groups 13-15 of the 44-group structure of the SCALE [11] code system. This corresponds to the energy range [100000 eV, 550 eV] which is the range for which unresolved resonance covariance data exist in the ²³³U ENDF formatted file used. Group-averaged cross section data are calculated using appropriate modules of the AMPX [1] library.

Group	Lower energy [eV]	Upper energy [eV]	Total cross section [barns]	Relative std. dev. PUFF-IV	Relative std. dev. ERRORJ
13	$1.700 \times 10^{+4}$	$2.500 \times 10^{+4}$	$1.4682 \times 10^{+1}$	2.1068x10 ⁻²	2.1036x10 ⁻²
14	3.000x10 ⁺³	1.700x10 ⁺⁴	1.6267 x10 ⁺¹	1.6113x10 ⁻²	1.5578x10 ⁻²
15	5.500x10 ⁺²	$3.000 \times 10^{+3}$	2.2387x10 ⁺¹	1.9942x10 ⁻²	1.8356x10 ⁻²

Figure 2: Comparison of the correlation matrix for total cross section between SAMMY and PUFF_IV ²³³ U. Groups 16–44 of the 44-group structure of the SCALE [11] code system are depicted. This corresponds to the energy range [550 eV,0.00001 eV], which is the range for which resolved resonance covariance data exist in the ²³³U ENDF formatted file used.



4. Test cases

To provide quality assurance of the PUFF-IV package, a suite of automatic test cases has been created. This includes unit tests for various parts of the program as well as full covariance calculations for selected abbreviated ENDF data files. Unit test cases exist for the expansion of "NI" type subsubsections in File 31 and File 33, reading of the various ENDF record types, the numerical integration for group-averaged derivative data, the correct expansion of parameter covariance data from ENDF File 32 data, and adding of covariance matrices for range and isotope data. For all these cases, the test program generates fictitious data and assures that the program returns the expected results.

The test suite also includes full covariance calculations for selected material numbers and compares the resulting data with a standard COVERX [2] formatted file for the material under consideration. The AMPX [1] module COVCOMP is used to compare two COVERX formatted data files. The test includes most ENDF-6 materials that contain File 31 and/or File 33 information. The standard COVERX formatted data files were in most cases created with PUFF-III. Exceptions include materials where there are known issues in PUFF-III that have been corrected in PUFF-IV. In the case of File 32 processing, the COVERX formatted files were generated with PUFF-IV. However, the data were compared to group-averaged covariance data generated by the R-matrix fitting program SAMMY [6] before being used as a standard file.

5. Conclusion

The program PUFF-IV was designed to process covariance information from File 31, 32, and 33 in any of the formats defined in the ENDF manual [3] except for long-range parameter covariance data. To our knowledge, PUFF-IV is the first processing code that can address both the new ENDF format for resolved resonance parameters, and the new ENDF "compact" covariance format. The code is written in a modular fashion, which will allow future upgrades to support any new ENDF covariance formats. The program results in the resolved and unresolved resonance region were compared to results obtained using SAMMY and ERRORJ to ensure correct working of the program. Results were in all cases similar, accounting for the different energy grids and numerical integration used in the different code packages. The program package includes an automatic test suite containing unit tests and regression tests to ensure that future upgrades do not impact program results.

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