Updated Covariance Processing Capabilities in the AMPX Code System*

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A concerted effort is in progress within the nuclear data community to provide new cross-section covariance data evaluations to support sensitivity/uncertainty analyses of fissionable systems. The objective of this work is to update processing capabilities of the AMPX library to process the latest Evaluated Nuclear Data File (ENDF)/B formats to generate covariance data libraries for radiation transport software such as SCALE. The module PUFF-IV was updated to allow processing of new ENDF covariance formats in the resolved resonance region. In the resolved resonance region, covariance matrices are given in terms of resonance parameters, which need to be processed into covariance matrices with respect to the group-averaged cross-section data. The parameter covariance matrix can be quite large if the evaluation has many resonances. The PUFF-IV code has recently been used to process an evaluation of ^{235}U, which was prepared in collaboration between Oak Ridge National Laboratory and Los Alamos National Laboratory.

I. INTRODUCTION

With the release of SCALE 5.1[1] the nuclear criticality safety analyst can use the Tools for Sensitivity and Uncertainty Analysis Methodology Implementation (TSUNAMI) sequences to perform sensitivity/uncertainty (S/U) analyses of fissionable systems. A concerted effort is in progress within the nuclear data community to provide new cross-section covariance data evaluations to support S/U analyses. The objective of this work is to update the cross-section processing methods used in the AMPX[2] library to process the latest Evaluated Nuclear Data File (ENDF)/B[3] formats to generate covariance data libraries for radiation transport software such as SCALE.

Since the release of Version IV of ENDF, standards and formats have been in place to permit communication of estimated uncertainties in evaluated cross-section data. With the release of ENDFB/VII.0 library[4], one new covariance format is supported. At the Oak Ridge National Laboratory, the module PUFF in the AMPX code system has traditionally been used to process covariance information from the ENDF library into group-averaged covariance matrices. We recently updated PUFF[5], now renamed PUFF-IV[6], to add support for the new ENDF formats. This includes full processing of R-Matrix resonance parameter covariance matrices in the resolved as well as in the unresolved resonance region. The new compact formats with variable number of digits are also supported.

II. GROUP-AVERAGED COVARIANCE DATA

File 31 contains $\bar{\nu}$ information (average total number of neutrons per fission and average total number of delayed neutrons), and File 33 contains 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 that 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 covariance 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 another material.

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

The covariance data in File 31 are typically self-contained and do not need to be combined with any other data. However, the covariance data calculated from File 32 and 33 may 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 1.

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TABLE I. Energy grid structures used in PUFF-IV

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

In most cases, group-averaged covariance matrices are calculated on the "Super-grid", that is, grid 5 in Table 1. 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 Ref. 6 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 considerably. In the remainder of this paper, "union grid" will refer to the grid on which calculation is done and as such refers to either grid 5 or grid 6, depending on File 31 and File 33 content.

The weighting φ_g^u function 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. Because 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:

$$\begin{aligned}\varphi_I &= \sum \begin{cases} \varphi_g^u \dfrac{E_{I+1}-E_I}{E_{g+1}^u - E_g^u} & E_g^u \le E_I < E_{I+1} \le E_{g+1}^u \\ 0 & \text{otherwise} \end{cases} \\ x_I^m &= \frac{1}{\varphi_I} \sum \begin{cases} x_g^{m,u} \varphi_g^u \dfrac{E_{I+1}-E_I}{E_{g+1}^u - E_g^u} & E_g^u \le E_I < E_{I+1} \le E_{g+1}^u \\ 0 & \text{otherwise} \end{cases} \end{aligned} \quad (1)$$

where the index *I* refers to union group $\left[E_I, E_{I+1}\right]$ and *g* to the user group $\left[E_g^u, E_{g+1}^u\right]$ [*]. The covariance matrices calculated on the union grid need to be collapsed to the user grid. Assume that $\left\langle \delta x_I^m \delta x_J^n \right\rangle$ is the covariance matrix element on the union grid; then the covariance matrix element on the user grid is

$$\left\langle \delta x_g^{m,u} \delta x_{g'}^{n,u} \right\rangle = \frac{1}{\varphi_g^u \varphi_{g'}^u} \sum\sum \varphi_I \varphi_J \left\langle \delta x_I^m \delta x_J^n \right\rangle \quad \text{for} \begin{cases} E_g^u \le E_I & < E_{I+1} \le E_{g+1}^u \\ E_{g'}^u \le E_J & < E_{J+1} \le E_{g'+1}^u \end{cases} \quad (2)$$

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:

$$x_I^m = \frac{1}{\int \varphi(E) dE} \int \varphi(E) \sigma^m(E) dE \quad (3)$$

and 0 otherwise.

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

$$\left\langle \delta x_I^m \delta x_J^n \right\rangle = \frac{1}{\varphi_I \varphi_J} \int\int \varphi(E) \varphi(E') \left\langle \delta\sigma^m(E) \delta\sigma^n(E') \right\rangle dE dE' \quad (4)$$

[*] 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.

III. RESONANCE REGION

In the resonance region the covariance data are commonly given as a function of the resonance parameters. To obtain the associated 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

$$\sigma_m(E) = \sigma_m(E, P_i) \tag{5}$$

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

$$\begin{aligned} \langle \delta\sigma_m(E)\delta\sigma_l(E') \rangle &= \left\langle \sum \frac{\partial \sigma_m(E)}{\partial P_k} \delta P_k \sum \frac{\partial \sigma_l(E')}{\partial P_n} \delta P_n \right\rangle \\ &= \sum \frac{\partial \sigma_m(E)}{\partial P_k} \langle \delta P_k \delta P_n \rangle \frac{\partial \sigma_l(E')}{\partial P_n} \end{aligned} \tag{6}$$

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

$$\begin{aligned} \langle \delta x_I^m \delta x_J^l \rangle &= \frac{1}{\varphi_I \varphi_J} \iint \varphi(E)\varphi(E') \langle \delta\sigma_m(E)\delta\sigma_l(E') \rangle dE dE' \\ &= \frac{1}{\varphi_I \varphi_J} \sum \iint \varphi(E)\varphi(E') \frac{\partial \sigma_m(E)}{\partial P_k} \langle \delta P_k \delta P_n \rangle \frac{\partial \sigma_l(E')}{\partial P_n} dE dE' \\ &= \frac{1}{\varphi_I \varphi_J} \sum \langle \delta P_k \delta P_n \rangle \left(\int \varphi(E) \frac{\partial \sigma_m(E)}{\partial P_k} dE \right) \left(\int \varphi(E') \frac{\partial \sigma_l(E)}{\partial P_n} dE' \right) \end{aligned} \tag{7}$$

If we define

$$D_{Ik}^m = \frac{1}{\varphi_I} \int \varphi(E) \frac{\partial \sigma_m(E)}{\partial P_k} dE \tag{8}$$

then Eq. (7) can be rewritten as

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

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 Ref. 6. The integrals defined in Eq. (8) are converted into a system of coupled partial differential equations that are solved numerically using a fourth-order Runge-Kutta algorithm with adaptive step-size.[7] This procedure allows one to easily adapt the step size to any fast-changing structures in the partial derivatives. The system of coupled differential equations is constructed from one integral each per resonance parameters. Ideally, only one systems of coupled partial differential equations should be solved. However, in the case of evaluations like ^{235}U[8], which has 15,947 resonance parameters, the system is broken up into several smaller systems. The program has an internal parameter controlling the maximal number of integrals calculated in one step. The integral is calculated over each group of the union grid. If the group extends over a large energy range or contains many resonances the step size limit may be exceeded. In these cases the program automatically breaks the integral into two or more steps until the integration succeeds.

IV. FLUX OPTION

The integral in Eq. (8) contains flux information that needs to be taken into account if calculating the integral. In reality the flux spectrum depends on resonance parameters due to self-shielding. In the SCALE Sensitivity and Uncertainty system, resonance self-shielding effects are treated in the sensitivity coefficients, and not included in the covariance values. The PUFF-IV module allows three methods to supply the flux:

1. A flux is given for each user group. As far as Eq. (8) is concerned, this is the same as assuming a constant flux over the length of a given union grid energy group. The correct user group flux will be used when collapsing the covariance matrix from the union grid to the user grid using Eq. (2). In most cases, the union grid and the user grid are almost identical in the resolved resonance region. Thus, this option is almost identical to using a constant flux.
2. A flux of 1/E is desired. In this case Eq. (8) is calculated with 1/E as a flux because 1/E can be easily evaluated for each energy needed during the evaluation of the integral.
3. A file containing flux information as a function of energy is given. The flux data are assumed to be given in a binary ENDF TAB1 format[3]. This format allows specification of the law (linear-linear, log-linear, etc.) to be used to interpolate the flux at energy points not given in the file. The integral is then calculated by interpolating the flux as prescribed by the interpolation law at energy points needed during the evaluation of the integral.

In Fig. 1 the relative standard deviations for fission are compared for ^{233}U[9] at a constant flux and thermal-1/E-fission flux. In the case of the 44-group structure, no large differences are found. In this group structure the lower groups represent higher energies and the higher groups lower energies.

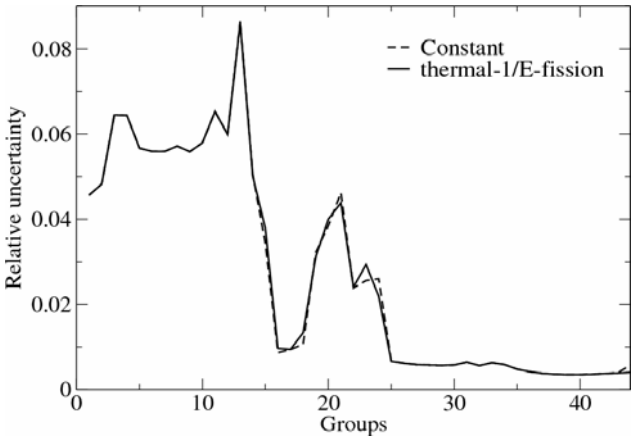

Fig. 1. Comparison between the relative uncertainty for the fission cross section for ^{233}U[9] calculated with a thermal-1/E-fission flux and a constant flux.

V. LARGE COVARIANCE MATRICES

The PUFF-IV module has been designed to handle large matrices if necessary. As an example we present the covariance matrix for ^{235}U for which the covariance matrix was determined via retroactive methods.[8] The number of resonance parameters is 15,947, which are stored in an ENDF formatted file with a size of 1.6 Gb. The program needs to be able to allocate sufficient array space to read the ENDF formatted data and to calculate the parameter covariance matrix itself. All internal calculations are done in double precision. In the case of ^{235}U, the required array size exceeds 2 Gb. These requirements dictate that the covariance matrix can only be evaluated on a 64 bit machine that allows addressing more than 2 Gb of memory. We used a 64 bit AMD Opteron Processor on which the processing took about 27 h. Figs. 2 and 3 show the correlation matrices for different reactions for ^{235}U.

The R-Matrix fitting program SAMMY[10] 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 in the resolved resonance region. If using a constant flux, the results between SAMMY and PUFF-IV can be directly compared. If the same energy grid is used, SAMMY and PUFF-IV do indeed give the same results. Note that this consistency check confirms what the evaluator intended

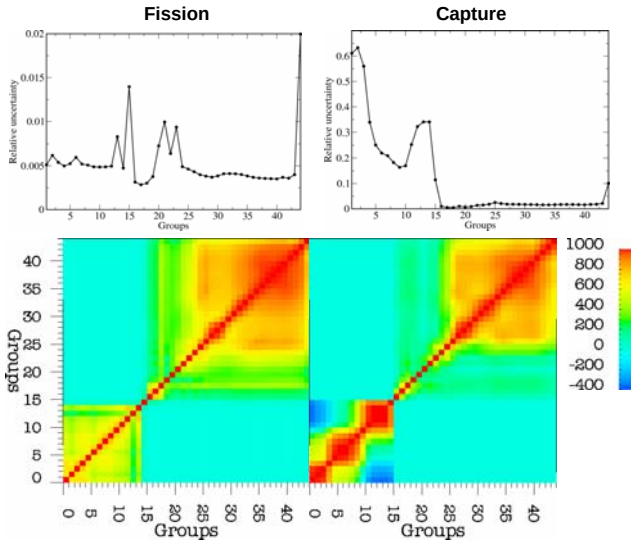

Fig. 2. Correlation matrix and relative uncertainties for ^{235}U[8] for fission and capture cross section on the 44 SCALE[1] group structure calculated with a 1/E flux.

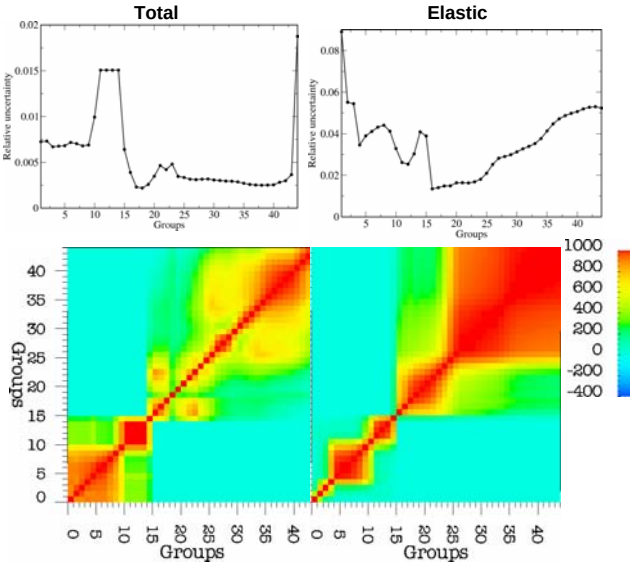

Fig. 3. Correlation matrix and relative uncertainties for ^{235}U[8] for total and elastic cross section on the 44 SCALE[1] group structure calculated with a 1/E flux.

because SAMMY was used to prepare all of the covariance data in the resolved resonance region discussed in this paper. For other choices of the energy grid the results are close, provided the energy grid is fine enough to describe the cross section structure. Typically the grid used by PUFF-IV to calculate the integral is very fine and in the case of ^{235}U includes 898,535 grid steps over the range of the resolved resonance region.

The program ERRORJ[11] is an independently-developed processing code used to calculate group averaged covariance matrices similar to PUFF-IV. In contrast to PUFF-IV the program ERRORJ uses numerical differentiation to calculate the group averaged covariance matrices from the resonance parameter covariance matrix. Because the programs use a different approach to calculate the group-averaged covariance data, the results are expected to be similar but not identical. In Fig. 4 we compare the relative uncertainties for elastic and capture cross sections as calculated by PUFF-IV and ERRORJ for ^{232}Th. The ^{232}Th data are taken from the ENDF-B/VII.0 release and give the resonance parameter covariance matrix in compact form.

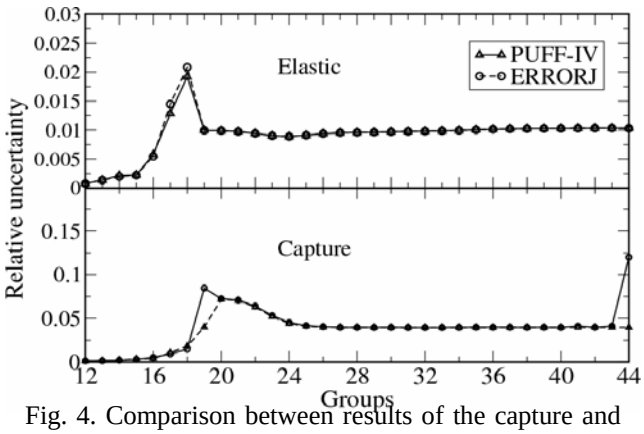

Fig. 4. Comparison between results of the capture and elastic cross section data from PUFF-IV and ERRORJ for ^{232}Th from the ENDF/VII library.

A new preliminary evaluation of ^{239}Pu[12] was recently completed in Oak Ridge National Laboratory, and the evaluation contains full covariance information in the resolved resonance range from [1 x 10^{-5}eV, 2500.0 eV]. As another example of processing covariance matrices with PUFF-IV, we present the relative uncertainties and correlation matrices in Figs. 5 and 6 for ^{239}Pu.

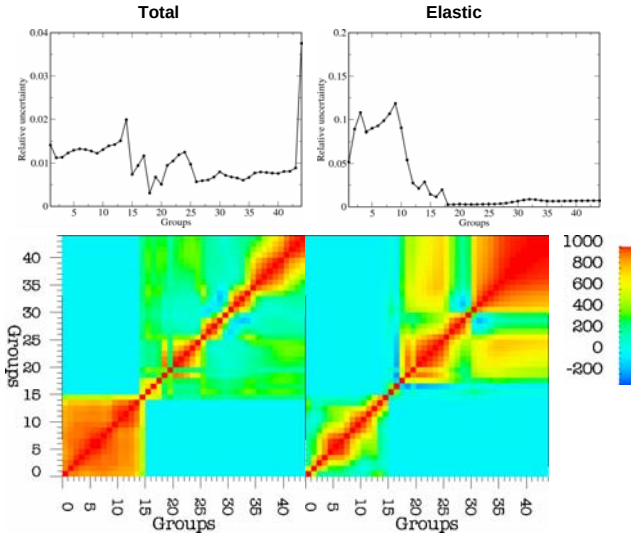

Fig. 5. Correlation matrix and relative uncertainties for ^{239}Pu[12] for total and elastic cross section on the 44 SCALE[1] group structure calculated with a 1/E flux.

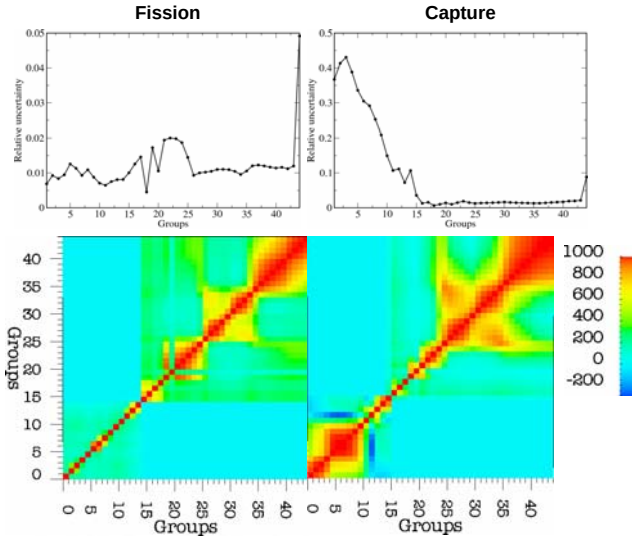

Fig. 6. Correlation matrix and relative uncertainties for ^{239}Pu[12] for fission and capture cross section on the 44 SCALE[1] group structure and 1/E flux.

VI. CONCLUSION

The PUFF-IV module can be used to generate the group-averaged covariance information based on the point-wise and resonance parameter covariance information given in the ENDF library. The sensitivities needed to calculate the group-averaged covariance matrices are calculated analytically. If using a constant flux the calculated group averaged uncertainties and correlation matrices are very similar to the values calculated by the R-Matrix fitting program SAMMY. Depending on the computing platform PUFF-IV can operate on very large covariance matrices like the one for the resolved resonance region for ^{235}U. The PUFF-IV package can be obtained from Radiation Safety Information Computational Center (RSICC) under code number P00534. The package contains modules that allow interfacing PUFF-IV with group-averaged cross section data produced by the NJOY[13] package.

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