Recent Advances with the AMPX Covariance Processing Capabilities in PUFF-IV

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The program PUFF-IV is used to process resonance parameter covariance information given in ENDF/B File 32 and point-wise covariance matrices given in ENDF/B File 33 into group-averaged covariances matrices on a user-supplied group structure. For large resonance covariance matrices, found for example in ^{235}U, the execution time of PUFF-IV can be quite long. Recently the code was modified to take advandage of Basic Linear Algebra Subprograms (BLAS) routines for the most time-consuming matrix multiplications. This led to a substantial decrease in execution time. This faster processing capability allowed us to investigate the conversion of File 32 data into File 33 data using a larger number of user-defined groups. While conversion substantially reduces the ENDF/B file size requirements for evaluations with a large number of resonances, a trade-off is made between the number of groups used to represent the resonance parameter covariance as a point-wise covariance matrix and the file size. We are also investigating a hybrid version of the conversion, in which the low-energy part of the File 32 resonance parameter covariances matrix is retained and the correlations with higher energies as well as the high energy part are given in File 33.

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) analysis 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 analysis.

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.

II. GROUP-AVERAGED COVARIANCE DATA

The ENDF file format [3] allows to give covariance information. File 31 contains $\overline{\nu}$ covariances (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 contains 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.

File 32 gives covariance information for resonance parameters. As such the allowed formats loosely follow formats for File 2. Resonance parameter covariance matrices may be given for different isotopes and 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 Files 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 I.

In most cases, group-averaged covariance matrices are calculated on the "Super-grid", that is, grid 5 in Table I. 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 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 ENDF data in File 31, 32, and 33 yield point-wise covariance data. A problem-independent group-averaged cross section x_I^m for group I is calculated from the point-wise cross section, where the superscript denotes the reaction, via the formula

$$x_I^m = \frac{1}{\int w(E)\,\mathrm{d}E} \int w(E)\,\sigma^m(E)\,\mathrm{d}E, \qquad (1)$$

where $w(E)$ is a specified "generic" (e.g. infinite dilute) weight function. 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

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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

element via the following formula:

$$\langle \delta x_I^m \delta x_J^n \rangle = \frac{1}{w_I w_J} \int w(E)\, w(E') \langle \delta\sigma^m(E)\, \delta\sigma^n(E') \rangle \, \mathrm{d}E \mathrm{d}E'. \quad (2)$$

The resulting multigroup covariance is "generic", and can be used for variety of sensitivity/uncertainty applications with TSUNAMI or similar systems.

The weight function and group-averaged cross section data 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 weight function w_I and the cross section x_I^m on the union grid can be written as

$$\begin{aligned} w_I &= w_g^u \tfrac{E_{I+1}-E_I}{E_{g+1}^u - E_g^u} \\ x_I^m &= x_g^{u,m}, \end{aligned} \quad (3)$$

where the union group I energies are such that $E_g^u \leq E_I < E_{I+1} \leq E_{g+1}^u$. After the calculation is finished, the calculated matrices are collapsed to the user grid using the following formula:

$$\left\langle \delta x_g^{u,m} \delta x_{g'}^{u,n} \right\rangle = \frac{1}{w_g^u w_{g'}^u} \sum_I \sum_J w_I w_J \langle \delta x_I^m \delta x_J^n \rangle, \quad (4)$$

where the first sum extends over all union groups I contained in user group g and the second sum over all union groups J contained in user group g'.

In File 33 the covariance data are given as point-wise histogram data. If the energy grid on which the point-wise histogram data are given is coarser then the union grid, it is sometimes necessary to transfer the covariance element $\langle \delta x_c^m \delta x_{c'}^n \rangle$ from the coarse ENDF groups c and c' to the union groups I and J. This is done via

$$\langle \delta x_I^m \delta x_J^n \rangle = \frac{1}{w_I w_J} w_c w_{c'} \langle \delta x_c^m \delta x_{c'}^n \rangle . \quad (5)$$

File 32 gives resonance parameter covariance matrices that need to be converted to energy group-averaged covariance matrices. If we define

$$D_{Ik}^m = \int w(E) \frac{\delta\sigma_m(E)}{\delta P_k} \mathrm{d}E, \quad (6)$$

the energy group-averaged covariances are given by:

$$\left\langle \delta x_I^m \delta x_J^l \right\rangle = \frac{1}{w_I w_J} \sum_{kn} D_{Ik}^m \langle \delta P_k \delta P_n \rangle D_{Jn}^l \quad (7)$$

The derivatives in Eq. 6 are determined analytically, using the samrml library, which is part of the SAMMY package [5]. The integral in Eq. 6 is solved by converting the integrals to a system of differential equations and solving via a fourth-order Runge-Kutta method [6]. The total order of the system of differential equations is equal to the number of resonance parameters. However, since the differential equations are independent from one another, the system can be broken up into two or more systems. While the calculation speed can be influenced by the number of differential equations allowed in one system, the calculation time is relatively independent of the number of user groups.

III. BASIC LINEAR ALGEBRA SUBPROGRAMS (BLAS)

If a large number of user groups and/or resonance parameters is involved, the processing time needed by PUFF-IV can be very long. This is especially true if File 32 covariance data are provided. The bulk of the processing time is spent in calculating the double sum in Eq. 7, since the sum extends over user groups as well as over resonance parameter if the whole covariance matrix is calculated. The evaluation for ^{235}U has 3193 resonance with 5 parameters each, for a total of 15965 resonance parameters [7]. Albeit the summation in Eq. 7 was optimized to account for zero values on parameters

or derivatives, the calculation for ^{235}U on the 44-group Scale group structure takes about 28 h.

In order to speed up this part, we changed the code to use Basic Linear Algebra Subprograms (BLAS) routines [8] for the matrix multiplications. The installation procedure has been updated to automatically detect whether a suitable BLAS implementation is available on the target system. If an implementation is available, it is used; otherwise, the code reverts back to the unoptimized code. This led to a substantial decrease in execution time. As an example, the execution time for ^{235}U on a 238-group energy grid decreased from over a month to only 16 hours after the optimization. Actual optimization varies with BLAS implementation used and the number of processors available. This new optimization allowed us to calculate the covariance matrix on a very fine grid. Figure 1 shows the covariance matrix for ^{235}U on a 562-group energy grid.

IV. CONVERSION TO FILE 33

The resonance parameter covariance matrix stored in File 32 can be quite large depending on the number of resonance parameters. In the case of ^{235}U, the file is almost 2 Gb. In order to allow for smaller file size, we investigated whether File 32 can be converted into a File 33 format, that is into point-wise covariance matrices, without sacrificing too much covariance information. The covariance information in File 33 is point-wise information given in a histogram format. In order to transform File 32 data to these histogram type point-wise data, we calculate group-averaged data using a constant weight function on a suitable energy grid. To achieve seamless integration with existing File 33 data, this energy grid has to include the energy at which File 32 data terminate. Recall that PUFF-IV calculates the covariance matrix on the union grid and collapses the result to user groups. For the File 32 to 33 conversion, the covariance matrix on the union grid is needed. Therefore, we added an option to PUFF-IV that allows the collapse to the user grid to be suppressed. The resulting COVERX file contains the covariance matrices in point-wise histogram format. The data need to be written in File 33 format and merged with an existing File 33. A program, COVCONV, was written to achieve this task. For all imported matrices, the LB=5 format [3] is used. This format allows to give the energy group structure and the upper triangular part of the covariance matrix if symmetric or the whole matrix otherwise. In this format, and in most of the File 33 formats, point-wise covariance information is given relative to the cross section.

In principle, the merging procedure can just assume that each covariance matrix generated by File 32 data can be added as a new "NI" sub-subsection to File 33, since the final matrix is defined as a sum of File 32 and File 33 data. This is indeed the case if File 33 does not contain any "NC" sub-subsections, or derived covariance matrices. The covariance information for elastic scattering (MT=2), is often given as a "NC" section defining elastic scattering as total cross section minus absorption. The energy range of this "NC" section often extends into the energy range of File 32. However, the processing codes PUFF-IV and ERRORJ [9] first process File 33 and determine all explicit and implicit covariance matrices and only then process File 32 covariance information. Thus, albeit defined over the whole energy range, the "NC" section does not take effect in the energy range covered by File 32. In converting the COVERX file into File 33 format, there are two options to deal with these implicit matrices:

- Let the derived section extend over the whole energy range and do not import any matrix defined by the "NC" section. If MT=2 is defined by an "NC" section as $\sigma_2 = \sigma_1 - \sigma_{102} - \sigma_{18}$, where MT=1 is total cross section, MT=102 capture, and MT=18 fission, the cross matrices $\langle\sigma_2, \sigma_1\rangle$, $\langle\sigma_2, \sigma_{102}\rangle$, and $\langle\sigma_2, \sigma_{102}\rangle$ are also defined implicitly. The merging procedure will therefore not import these matrices.

- Change the energy boundary of the "NC" to not extend into the File 32 energy range. In that case all converted covariance matrices are imported.

The program COVCONV allows the user to select either of these two methods. In most cases we opted to change the energy boundary of the "NC" section and to import all covariance matrices generated by File 2 into File 33. Of course the final results should be identical if the same cross section data and group structure is used to process the new File 33 data. However, we found that due to rounding better results are obtained by changing the energy boundary. The original COVERX file used for conversion of File 32 to 33 is written in single precision binary format. For ^{235}U we took these binary data and calculated the covariance matrix <MT=2;MT=2> according to the prescription given in the "NC" section and compared it with the matrix <MT=2;MT=2> actually given in the COVERX file. While the same results are achieved for many groups, there are some group-averaged cross section and covariance elements that do not agree even if the binary data are used. For these groups, the elastic cross section is small compared to the other cross section data, and it is numerically unstable to subtract numbers of equal size to determine the difference. Thus, we have choosen the numerical more stable method of storing all File 32 derived matrices explicitly in File 33.

A conversion of File 32 into File 33 necessitates a choice of a group structure on which a converted File 33 is defined. Of course information is lost due to the conversion process, especially if the group structure chosen for the conversion is coarser then the user-desired group structure. A given choice for such a

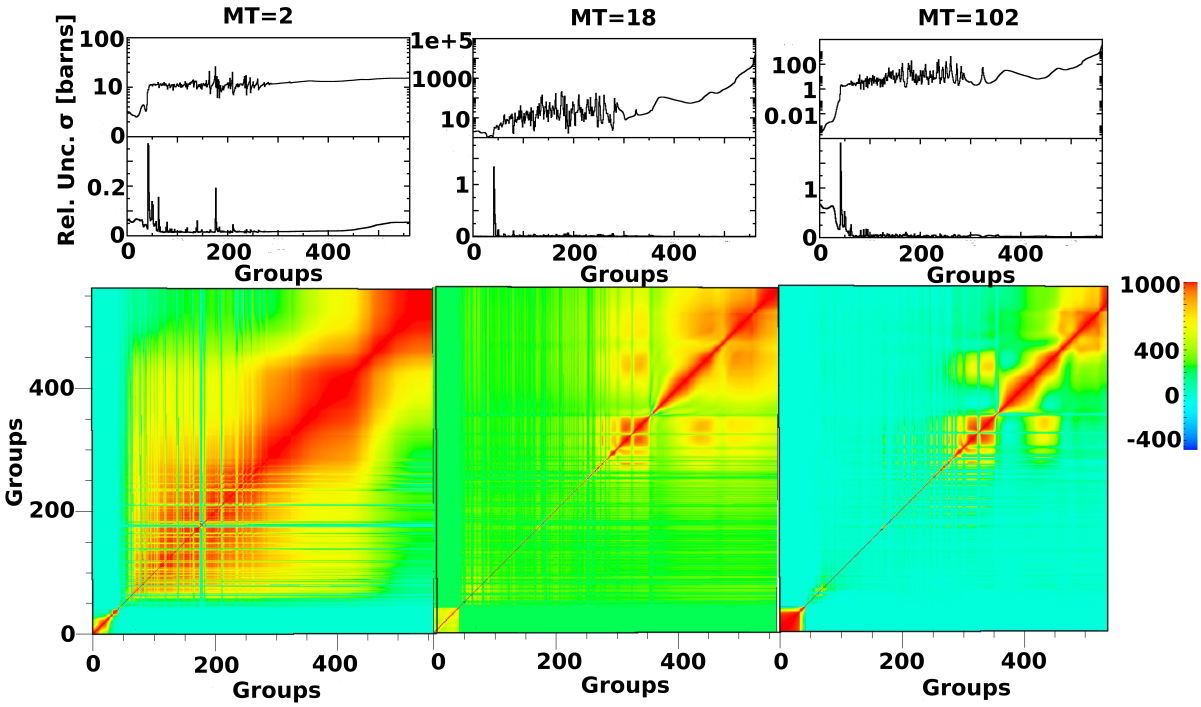

FIG. 1: ^{235}U correlation and group-averaged cross section data for 562 groups

group structure is unlikely to coincide with a group structure needed by a File 33 end user. Nevertheless, in the absence of a preferable File 32, a user is likely to proceed computing approximate uncertainties using a converted File 33. The improvements in the processing time due to BLAS allowed us to explore the effect of using different group structures in more detail [10]. The group structure chosen depends on the nuclide under consideration. Due to the details of the computation, such deviations are most likely to become significant for groups comparable to a width of a single resonance in the resolved resonance range [11]. If the group structure chosen for the conversion is coarser, then the user-desired group structure covariance elements would be approximated using Eq. 5, thus leading to a loss of precision. However, even if compatible group structures are used, we see some difference between the calculations done using File 32 and converted File 33. The reason is that covariance matrices in File 33 are given relative to the cross section. Assume the desired user grid is coarser than the grid used for the File 32 to 33 conversion, Then, because relative covariances are given, Eq. 4 becomes:

$$\left\langle \delta x_g^{u,m} \delta x_{g'}^{u,n} \right\rangle = \frac{1}{w_g^u w_{g'}^u} \sum_I \sum_J w_I w_J \frac{x_g^{u,m} x_{g'}^{u,n}}{x_J^m x_I^n} \left\langle \delta x_I^m \delta x_J^n \right\rangle , \tag{8}$$

which can lead to differences if the group-averaged cross section changes drastically between adjacent groups. If File 33 contains covariance matrices for point-wise cross section data given in File 3, we expect that the cross section data on the user grid are derived via methods similar to those given in 3. The evaluator would have chosen similar energy grids to produce File 3 and File 33 data and therefore we expect

$$\frac{x_g^{u,m} x_{g'}^{u,n}}{x_J^m x_I^n} \approx 1.0. \tag{9}$$

However, if the cross section data are cascaded from resonance parameters given in File 2, the cross section on the user grid may be quite different from the cross section data used to convert File 32 to File 33. This is especially true if the group boundaries straddle resonances.

A. Hybrid Method

Here we describe a method (schematically outlined in the Section 33 of ENDF-2 Manual [3]) that alleviates the deviations of uncertainties from those obtained from a full File 32 computation as described in the previous paragraph. We refer to this method as "hybrid" because it involves a complementary combination of File 32 and File 33: File 32 is used for the low-energy region where the energy groups are anticipated to be narrow relative to the widths of individual resonances, while File 33 is used everywhere else. Thus, File 33 includes energy groups that are more likely to span a large number of resonances, increasing its accuracy. The energy range covered in File 33 still extends into the low-energy region. This allows capture of correlation effects between the low- and high-energy region. Furthermore, a truncation of

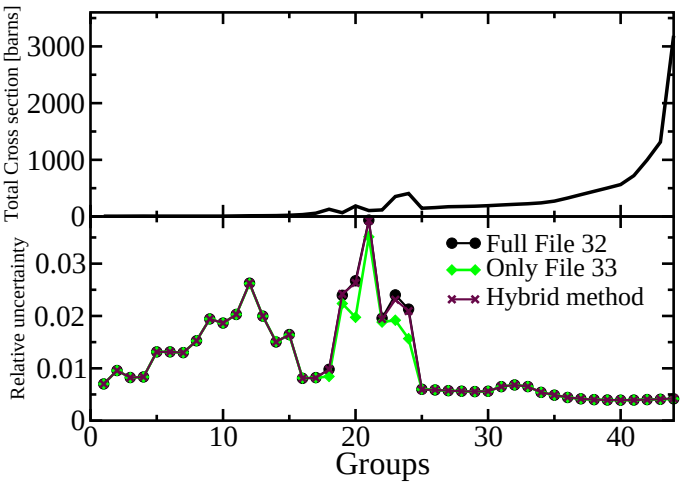

FIG. 2: Total cross section and relative standard deviation for ^{233}U calculated using different representations of the covariance information in the ENDF/B file

File 32 to just the lowest energy region yields the desired reduction in size relative to the full File 32.

We tested the hybrid method on ^{233}U. The orignal File 32 extends to 600 eV and contains resonance parameter covariance information for 770 resonances. The energy range of File 32 was restricted to below 30 eV, and covariance information was only given for resonance with resonance energies below 100 eV. This allows the correlation effects of higher energy resonances in the below 30 eV energy range (see Eqs. 6 and 7) to be taken into account. A complementary File 33 was found by subtracting covariance matrices computed from the truncated File 32 alone from the covariance matrices computed from the whole File 32. This procedure ensured self-consistency and completeness of the complementary File 32 and File 33. Each imported covariance matrix contains a block of zeros for groups with energies below 30 eV.

For ^{233}U the hybrid method reduced the deviation of uncertainties induced by using a 380-group File 33 on a 44-group structure, from approximately 26% down to 2% in the groups below 10 eV (Fig. 2).

V. CONCLUSION

The execution time of the program PUFF-IV used to process covariance information from the ENDF file into group-averaged covariances was substantially reduced by utilizing BLAS routines. This enabled us to use very fine group structures to convert File 32 information into File 33 information for evaluations with a large number of resonance parameters. This conversion reduces the file size substantially. A new program was created that aids in this conversion. We also investigated a hybrid method where some of the File 32 information is retained in File 32 format.

Acknowledgments

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