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# **MERGER OF NUCLEAR DATA WITH CRITICALITY SAFETY CALCULATIONS**

**N. M. Larson, L. C. Leal, H. Derrien (423)574-4659**

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## **MERGER OF NUCLEAR DATA WITH CRITICALITY SAFETY CALCULATIONS**

N. M. Larson, L. C. Leal, H. Derrien  
Oak Ridge National Laboratory<sup>1</sup>

### **Abstract**

In this paper we report on current activities related to the merger of differential/integral data (especially in the resolved-resonance region) with nuclear criticality safety computations. Techniques are outlined for closer coupling of many processes — measurement, data reduction, differential-data analysis, integral-data analysis, generating multigroup cross sections, data-testing, criticality computations — which in the past have been treated independently.

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## Introduction

Until recently, the evaluation of nuclear data and the use of those evaluated results in criticality safety calculations have been separate and distinct activities. Energy-differential nuclear data were measured, reduced, and analyzed by nuclear physicists, with little (if any) thought given to their eventual use for criticality computations. Although the computer codes which calculated  $k_{eff}$  and other quantities of relevance to criticality safety required differential nuclear data as input, those input numbers either were treated as exact or were modified to provide better agreement with integral quantities, without regard to the differential data from which they were originally derived.

This strategy of separate treatments for two strongly coupled operations is now challenged on both fronts. On the data analysis front, at least in the resolved-resonance region, certain integral quantities can be fitted directly within the analysis process.<sup>1</sup> The resulting values for resonance parameters are valid both for the differential data and for those integral data which were included in the fitting process. Preliminary evidence suggests that these parameter values also provide better agreement with other integral quantities than do values extracted from differential data alone.

On the criticality-calculation front, parameter covariance information is being incorporated into the integral calculations, first, in order to provide better determinations for the uncertainties on the integral calculations and, second, to assist in refining the values of the parameters obtained from the differential fit. In the past, haphazard revision of differential data was occasionally used to provide agreement with individual criticality-related integral quantities; this process significantly degrades the predictive power for other criticality computations. With the advent of new procedures based on the proper propagation of covariance information, use of such ad-hoc revisions should no longer be necessary. Instead, the resonance parameter values can be revised within the confines of the parameter covariance matrix, thus maintaining the quality of the fit to the differential data while simultaneously fitting the criticality data; this is possible because the values for the resonance parameters obtained during the analysis process are *not* unique, but instead are merely confined within limits specified by the covariance matrix and thus can be adjusted (within those limits) to fit additional data.

The covariance matrix provides the bridge between the analysis of differential data and the calculation of integral quantities. Communicating and utilizing the covariance matrix are daunting tasks, because (1) the resonance-parameter covariance matrix consists of a square array whose dimensions may number in the thousands, and hence is awkward to store and (2) use of the covariance matrix requires knowledge of sensitivity matrices (partial derivatives) for the quantities being calculated.

To address the first issue, techniques have been devised and are being tested for compacting this large array into concise formats which can be stored and transmitted more efficiently. To address the second issue, various options for calculation of sensitivity matrices are being explored.

## Differential Data

In order for criticality safety computations to be accurate, they must be based on reliable input. To this end, careful *measurement* of differential cross sections in the resolved-resonance region is necessary, because model calculations cannot predict resonance behavior. Details of the measurement must be extensively documented. Ideally, experimentalists will report all sources of uncertainty relevant to the measurement, and generate the data covariance matrix which incorporates those uncertainties.

Methodologies for generating the data covariance matrix have been described by several authors; see Ref. 2,3,4 for example. The computer code ALEX<sup>4</sup> was designed to be used by experimentalists for generating this matrix.

In addition to measurement, data *evaluation* in the resolved-resonance region is needed. Measurement alone cannot provide all cross sections at all energies and all temperatures, as needed in the calculations. The data evaluation/analysis process effectively removes features relevant to a particular measurement, and uncovers the underlying “true” cross section.

The SAMMY code<sup>5,6</sup> has been widely used for evaluation of energy-differential neutron cross section data: Values for resonance parameters are found by fitting to experimental fission, capture, transmission, and other data (angular distributions,  $\sigma$ , etc.). Data covariance information is included either explicitly (by inputting the complete covariance matrix) or implicitly (with SAMMY reproducing the effect of the data covariance matrix using information provided by the analyst). The calculated cross sections are modified by Doppler- and resolution-broadening, self-shielding, multiple-scattering, and other corrections as appropriate for the particular experiment, before fitting to the experimental data. Bayes’ method (generalized least squares) is used to determine both the best-fit values of the resonance parameters and the associated resonance-parameter covariance matrix. Independent data sets are analyzed sequentially, using the output resonance-parameter covariance matrix from one analysis as input to the next; the resonance-parameter values and covariances thus obtained provide a good fit to all the included data sets.

### **Including Integral Quantities within the Data Analysis**

Recently an option has been added to SAMMY,<sup>1</sup> to permit inclusion of selected integral quantities as an additional step within the analysis of the differential data. This option was first used for the evaluation of <sup>235</sup>U resonance parameters,<sup>7</sup> and the results of that evaluation are available as ENDF/B-VI Release 5.

Several integral quantities were available in SAMMY at the time of the <sup>235</sup>U evaluation. For absorption, fission, or capture: thermal cross sections, Maxwellian average at thermal energy, Westcott’s  $g$ -factor, resonance integral, and average integral. For fission only: Watt spectrum average,  $K1$ , and  $a$ . All these quantities are documented in detail in Ref. 1. Subsequently, to facilitate inter-code comparisons, the capability of calculating both the “thermal alpha integral” and the “thermal eta integral” was added to SAMMY, using the exact definitions (but independent programming) employed by the NJOY code.<sup>8</sup>

Data testing of this <sup>235</sup>U evaluation has been reported by several authors,<sup>9,10</sup> who noted improved agreement between calculation and experiment over that found with previous ENDF/B releases; these studies covered such quantities as buckling measurements,  $k_4$ , temperature-dependent Westcott  $g$ -factors, and spent-fuel analyses. Other tests by R.Q. Wright<sup>11</sup> specifically noted that inclusion of  $K1$  in the analysis process led to an increase in  $\beta$  of 0.12%; this change in  $\beta$  resulted in 0.1% increase in  $k_{eff}$  for highly enriched U systems. (Details of benchmark data testing of the <sup>235</sup>U ENDF/B-VI release 5 evaluation is discussed in a companion paper by R. Q. Wright and L. C. Leal.<sup>12</sup>)

### **Resonance-Parameter Covariance Matrix**

In order for criticality computations to properly utilize resonance parameter information, the resonance-parameter covariance matrix as well as the resonance parameter values must first be communicated from the originator code to the processing codes. SAMMY has several options designed for this purpose.

First, SAMMY provides resonance parameter values, uncertainties, and correlation matrices. These have always been reported in the SAMMY.LPT output file, so named because it was originally intended to be printed on a Line PrinTer for study by the analyst. The LPT file is not easily read by computers, but only by humans; other files provide computer-legible numbers: Parameter values are reported in the SAMMY.PAR output file, an ASCII file whose format is identical to the input parameter file. The covariance matrix, on the other hand, is provided in a *binary* file, which limits its usefulness to computers compatible with the particular computer on which the file was produced. To communicate the covariance information to other computers (and to future times), SAMMY now has an option to provide the uncertainties and an abbreviated form of the correlation matrix in a concise ASCII format. Preliminary studies to quantify the loss of information inherent in using such an abbreviated form were reported at the covariance conference held at Brookhaven National Laboratory in April, 1999<sup>13</sup>; a summary of that work is presented in the Appendix to this report.

## **Sensitivity Matrix**

To make use of the covariance information provided by SAMMY, processing codes such as AMPX<sup>14</sup> or NJOY<sup>8</sup> must also have access to sensitivities (partial derivatives) of the point-wise cross sections with respect to the resonance parameters. This could be accomplished either by (1) programming the analytic expression for the derivatives, (2) making use of one of the “automatic derivatives” codes available for producing line-by-line derivatives of FORTRAN coding, or (3) calculating numerical differences to approximate the analytic derivatives. Use of the third technique is, however, discouraged, as numerical differences on rapidly-varying functions are easily miscalculated.

Alternatively, the processing codes could read sensitivities generated by SAMMY. One disadvantage of this is that the energy-grid must be pre-defined. However, if the level of accuracy required for the derivatives is not required to be as high as the level of accuracy for the cross sections, then perhaps interpolation can give reasonable approximations to the partial derivatives at energies not included in the pre-defined grid. If this method is to be used, ENDF formats will need to be defined for reporting the sensitivity matrix.

Yet another option would be to use SAMMY to generate the multigroup cross sections and the associated covariance matrix. This would permit using the full resonance-parameter covariance matrix (rather than an abbreviated matrix) in the calculations of the multigroup cross section covariance matrix, thus eliminating one possible source of error. Also, because the partial derivatives (sensitivity matrix) are already available in SAMMY, these would not need to be communicated across computers and across codes. The downside of this option is that the energy groups must be pre-defined. However, if archival information on resonance parameter values and covariance matrix is retained, then using SAMMY to generate the multigroup cross sections would be as straightforward as using AMPX or NJOY or other processing code for this purpose, and would eliminate the need for programming of the processing codes to generate the sensitivities.

## Multigroup Cross Sections

Calculations of the lowest-energy groups of the 199-group structure of the VITAMIN-B6 library<sup>15</sup> and of the 238-group structure of the LAW library<sup>16</sup> have been published in an ORNL report.<sup>17</sup> These calculations used an average cross section description of the multigroup average cross section; as of this writing, programming for the more general flux-weighted group cross section, and in particular for the Bondarenko narrow-resonance weighting scheme,<sup>18</sup> is being written and should be available in the next release of SAMMY.

## Prognosis

The work of incorporating resonance-parameter covariance matrices (and/or multigroup covariance matrices) into the final criticality safety computations is in its infancy. Authors of the data-analysis code SAMMY<sup>6</sup> and of the processing codes AMPX<sup>14</sup> and NJOY<sup>8</sup> are cooperating to develop methods for communicating resonance-parameter values, covariance matrices, and partial derivatives (sensitivities). The capability of generating certain types of multigroup cross sections and covariance matrices is available in SAMMY; plans are underway to extend this to more general definitions of multigroup cross sections. The processing codes will then have the option of either generating their own multigroup covariance matrices (using as input the resonance-parameter covariance matrices from SAMMY), or reading and using multigroup covariance matrices generated by SAMMY.

Inclusion of integral quantities as part of the analysis process has proven successful as a means of ensuring that results of the resonance-region analysis are compatible with both differential and integral measurements. Unfortunately, appropriate integral data are not available for all nuclides of interest; plans are being made for establishment of a data bank for integral data appropriate for use in SAMMY analyses.

Efforts are also underway to extend the analysis code SAMMY into the unresolved-resonance region and the high-energy region. Fröhner's FITACS code<sup>19</sup> has been incorporated in SAMMY as a first step in our treatment of the unresolved-resonance region, and Fu's TNG program<sup>20</sup> will form the basis for our treatment of the high-energy region. Ultimately, results (values and covariance matrices) from the resolved-resonance region will be combined with results from other sources (e.g., optical model calculations from the ECIS code<sup>21</sup>) to provide input for these higher-energy analyses, with the goal being to provide a consistent evaluation up to 20 MeV. Final parameter values, covariance matrix, and sensitivity information will be made available for use in criticality safety computations.

## Summary

The covariance matrix (in its several incarnations, from experimental-data to resonance-parameter to multigroup-cross-section covariance matrix) provides the link between the many processes which play a role in criticality safety computations. In this report we have explored various methods of generating, communicating, and using covariance matrices to increase accuracy in the final results.

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## Appendix. Abbreviating the Resonance-Parameter Covariance Matrix

In this appendix are summarized results first reported at *Workshop on Covariance Matrices: Generation, Formats, and Applications in Nuclear Energy Technologies*, held at Brookhaven National Laboratory April 22-23, 1999.<sup>13</sup>

If the resonance-parameter covariance matrix is written as uncertainties plus correlation matrix, then each element  $c$  of the correlation matrix is in the range  $-1 \leq c \leq +1$ . One easily-visualized and easily-programmed approximation has two elements: (1) Drop correlation coefficients with  $|c| \leq \text{small}$ , where *small* is a number whose value is to be determined empirically. (2) Map the remaining correlations from real numbers to  $N$ -digit integers, where  $N$  is also to be determined empirically. (In this study, the real-to-integer mapping was uniform from *small* to 1, but non-uniform mappings could also be considered.)

To test these abbreviated covariance matrices, group cross sections were calculated by SAMMY, using the average definition of group cross section,

$$\bar{s}_{x,i} = \frac{\int_{E_i}^{E_{i+1}} s_x(E) dE}{\int_{E_i}^{E_{i+1}} dE};$$

here the subscript  $x$  refers to the particular type of cross section (e.g. capture or fission). The associated covariance matrix was also generated using the chain rule

$$C_{i,j} = \sum_{k,kl} \frac{\partial \bar{s}_{x,i}}{\partial P_k} M_{kkl} \frac{\partial \bar{s}_{x,j}}{\partial P_{kl}}$$

where  $P$  represents the resonance parameters and  $M$  the resonance-parameter covariance matrix. The sums are over all resonance parameters.

Using  $^{235}\text{U}$  in the energy range 4.5 to 50 eV (590 resonance parameters) as a test case, the group-cross-section covariance matrix  $C$  was first generated using the “exact” resonance-parameter covariance matrix  $M$ , and then using a variety of approximations for  $M$ . Differences in the resulting group-cross-section covariance matrices were studied. Details are presented in the report<sup>13</sup>; the major conclusions from this study are these: Dropping correlations smaller than 1% produces noticeable but modest differences in  $C$ ; as *small* is increased, differences become larger. Using a 4-digit representation for  $M$  is virtually equivalent to using the exact representation; some differences are seen with a 3-digit representation. More differences are seen with a two-digit representation, but those differences are in general no larger than the differences found by dropping correlations smaller than 1%.

Table 1 shows the number of non-zero correlation coefficients which must be stored for the particular approximation (defined by values of *small* and  $N$ ). Note that the number of non-zero correlations is reduced dramatically by dropping correlations smaller than 1%, resulting in considerable savings in storage space.

Based on this study, the following preliminary recommendations are made: (1) Correlations smaller than 1% can be ignored. (2) Correlations can be represented by  $N$ -digit mappings, where  $N = 2$  may be adequate. Further study is needed with other nuclides before these conventions can be confidently adopted.

Table 1. Number of rows required in an ASCII file to report the abbreviated covariance matrix, when the abbreviation uses  $\lfloor \# \text{small} \rfloor$  and an  $N$ -digit mapping. The final row (labeled “#”) gives the number of non-zero correlation coefficients for each value of *small*.

$N \setminus \text{small}$	0	0.01	0.02	0.03	0.04	0.40	0.99
11	28960	8509	4724	3149	2362	214	0
4		4694	2786	1908	1462		
3		3765	2306	1600	1254		

<i>N \ small</i>	<b>0</b>	<b>0.01</b>	<b>0.02</b>	<b>0.03</b>	<b>0.04</b>	<b>0.40</b>	<b>0.99</b>
<b>2</b>		2890	1765	1345	1065		
<b>#</b>	173755	21231	10977	7173	5250	294	0