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The Simultaneous Evaluation of Interrelated Cross Sections by Generalized Least-Squares and Related Data File Requirements

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ABSTRACT

Though several cross sections have been designated as standards, they are not basic units and are interrelated by ratio measurements. Moreover, as such interactions as $^{6}Li + n$ and $^{10}B + n$ involve only two and three cross sections respectively, total cross section data become useful for the evaluation process. The problem can be resolved by a simultaneous evaluation of the available absolute and shape data for cross sections, ratios, sums, and average cross sections by generalized least-squares. A data file is required for such evaluation which contains the originally measured quantities and their uncertainty components. Establishing such a file is a substantial task because data were frequently reported as absolute cross sections where ratios were measured without sufficient information on which reference cross section and which normalization were utilized. Reporting of uncertainties is often missing or incomplete. The requirements for data reporting will be discussed.

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I. INTRODUCTION

It should be realized that the designation of some cross sections as "standards" is for convenience only. They are not basic units and not standards as they change with every new measurement. This situation can be compared with the problem faced a long time ago, when the meter was defined as 1/40000th of the circumference of the earth. Whereas the problem for the meter could be resolved because it is a basic unit, that for the cross section "standards" is a permanent feature of a derived quantity. It might be preferable to refer to them as reference cross sections instead of as standards. Any absolute cross section measured for a certain reaction, let us assume with an uncertainty of 1%, is completely equivalent to an absolutely measured cross section of a designated "standard", assumed again measured with 1% uncertainty. The moment a ratio between these two cross sections has been measured, the absolute value of the non-standard will, in part, redefine the value of the "standard". This is the consequence of an overdetermination: there are only two unknowns in this example, but three measured values are available.

The aforementioned basic problem with the definition of cross section "standards" becomes abvious with the fact that there is not one "standard" for the same type of quantity (a cross section which is a measure of an interaction probability in units of cm^2), but several. We may also note that we wish to evaluate these "standards" whereas a standard is defined. The desire for evaluating data is the result of overdetermination. The simplest degree of overdetermination is given by the multiple measurements of the same quantity. A "higher" degree of overdetermination is given by above example, e.g. if two different quantities are measured and a ratio or sum of these two quantities has also been obtained.

The question of how to combine multiple experimental observations is not a problem. It has been resolved ~200 years ago by Gauss and independently by Legendre. With improvements and additions we have today two approaches for the evaluation of data:

1. The generalized least-squares fit (GLSF), and

2. The Bayesian estimation.

If the same data base is used, then both techniques should give nearly identical results. We will consider here only the generalized least-squares fit which is being used for the ENDF/B-VI evaluation.

An APRIORI is required for the GLSF, however, in contrast to the Bayesian estimation, the APRIORI has only a secondary effect. It is used for the linearization of the non-linear problem, specifically for the application of the Taylor-series expansion. Adjustments to the APRIORI are obtained from

$$\delta = (A^T C^{-1} A)^{-1} A^T C^{-1} M$$

where C is the variance-covariance matrix of the measured data, A is the coefficient matrix determined by the Taylor series expansion, A^T its transpose, and M is the measurement vector. C becomes the correlation matrix after appropriate transformation. This has been discussed in more detail previously.[1]

Because several cross sections are involved we refer to this kind of evaluation as an simultaneous evaluation. In Section II we will consider the objects of the evaluation, types of experimental quantities to be used, and the need to reconstruct the originally measured quantities. The requirements for measurements and data reporting will be discussed in Section III. Some remarks on the evaluation of the standards and other principle cross sections will be made in Section IV.

II. THE PARAMETERS AND THE EXPERIMENTAL DATA

Realization of the interrelation of many cross sections has led to the approach of the simultaneous evaluation of the "standards and other principle cross sections" for ENDF/B-VI. The cross sections involved are called the "parameters" or "objects" of the evaluation.

^{6}Li (n,α)	thermal - 3.0 MeV
^{6}Li (n,n)	thermal - 3.0 MeV
^{10}B (n,α_0)	thermal - 1.4 MeV
^{10}B (n,α_1)	thermal - 1.4 MeV
^{10}B (n,n)	thermal - 1.4 MeV
^{197}Au (n,γ)	thermal - 2.8 MeV
^{238}U (n,γ)	thermal - 2.2 MeV
^{235}U (n,f)	thermal - 20.0 MeV
^{239}Pu (n,f)	thermal - 20.0 MeV
^{238}U (n,f)	0.1 - 20.0 MeV

The parameters under consideration are the cross sections at "grid point" energies, however, the process does not put any restriction on the definition of these values other than that the definition must be consistent. For example, the "cross sections" for the light elements at all energies and for the heavy elements at higher neutron energies are indeed the cross sections at the given energies. At lower energies the "cross section" for the heavy elements are the decimal energy interval integrals.

The experimental quantities which are presently implemented in the generalized least-squares nuclear data evaluation code GMA[1] are:

1. Absolute measurements of cross sections.

2. Measurements of the shapes of cross sections.

3. Absolute measurements of the ratios of two cross sections.

4. Measurements of the shapes of the ratios of two cross sections.

5. Absolute measurements of the sums of cross sections (e.g. total cross sections).

6. Measurements of the shapes of the sums of cross sections (e.g. the shape of $\sigma(^{10}$B (n,$\alpha_0+\alpha_1$))).

7. Absolute measurements of the ratios of a cross section vs. the sum of cross sections (e.g. ^{235}U (n,f)/^{10}B (n,α_0 + α_1)).

8. The measurements of the shapes of the ratio of a cross section vs. the sum of cross sections.

9. The integral of a cross section over a (fission) neutron spectrum.

These quantities have been included in order to handle all data of importance for the evaluation of the standards and other principal cross sections for ENDF/B-VI. Other quantities could be accommodated as easily as it is only a matter of providing for the corresponding Taylor series expansions. The integral of a cross section over a neutron spectrum has been included, however, only values of the ^{235}U(n,f) and ^{239}Pu(n,f) reactions will be used in the evaluation because the averages of these cross sections over a fission neutron spectrum prove to be insensitive to the knowledge of the neutron spectrum.

It appears obvious that only original experimental information should be used in an evaluation. However, this requirement poses a large problem for the evaluation of a cross section data base. In most cases experimenters have presented their data in a "pre-evaluated" form. For example, if in an experiment the shape of the ^{235}U(n,f) cross section has been measured from thermal to 1 KeV and from 100 eV to 100 KeV, using the ^{10}B(n,α) reaction for the measurement of the neutron flux, then the experimenter will convert the measured ratios using some values for the ^{10}B(n,α) cross section, he will then normalize the high energy part of his data to the low energy part and he will finally normalize the data to some thermal cross section. There is no reason that the experimentor should not do so if he is interested in the outcome for the ^{235}U(n,f) cross section. However he should provide for the data files the unnormalized measurements of the ratio of ^{235}U(n,f)/^{20}B(n,α) for the two energy intervals in which they have been obtained. Only the latter should be used in an evaluation. It is the need to reconstruct the originally measured quantities which poses a substantial problem for the evaluator. All too often the reference cross sections are not specified and the separate pieces cannot be obtained.

There is also an unfortunate large amount of confusion about the currently valid data. Data from the same measurement may have been reported repeatedly and may have entered a data file prematurely. Also, errors in a measurement may have been recognized at a later time, but the data may not have been withdrawn from the data files.

III. THE REQUIREMENTS FOR MEASUREMENTS AND DATA REPORTING

Some of the cross sections involved in the simultaneous evaluation for ENDF/B-VI are now quite well known. An example is the ^{235}U(n,f) cross section. The uncertainties of the result are ~1% or lower at nearly all energies between thermal and 20 MeV neutron energy. It follows that any new measurement with an uncertainty of ~2% or larger will have only a minor impact. Still, it may be desirable to have some measurements at selected energies in order to check the accuracy with which the past measurements seem to establish this cross section. Such measurements might ease our discomfort with the evaluation result in areas where data discrepancies exist or where data with the low uncertainties suggested by the evaluation are not in the data base. It appears trivial to request that such new measurements should be of high quality. However, there are many newer measurements for which systematic effects were not recognized, or, if recognized, were not corrected but added to the uncertainties.

There are other cross sections involved in the simultaneous evaluation for which the available data base is unfortunately poor. Examples are the $^{10}B(n,\alpha_1)$ and $^{10}B(n,\alpha)$ cross sections for which very few absolute measurements are available. It is clear that measurements of these quantities are needed. However, any new measurement should be of a "standard type quality", that is:

1. All systematic effects should be considered.

2. All required corrections should be applied and not merely added to the uncertainties.

3. The reproducebility should be proven.

4. The experimental result should be compared with an additional measurement in which as many components are independent (e.g. uncorrelated, see Youden[2]) as possible from the first experiment.

5. Resolution unfolding should be applied.

There are requirements for the reporting of data from any new measurement:

1. The originally measured quantities should be reported.

2. All constants used to derive the reported quantities should be reported. If a constant is not involved as a straightforward factor, then the sensitivity of the result to this constant should also be given (e.g. the half-life in an activation experiment).

3. All corrections applied to the measured data should be given. This permits the later updating with improved secondary data.

4. The statistical uncertainties and estimates of the systematic uncertainties should be given. The latter should be given for each contributing component. The separation of the statistical uncertainties of the reaction rate measurement and the flux measurement is required if two cross sections are measured at the same time.

5. Some estimate on how the systematic uncertainty components are correlated as a function of energy should be given.

6. Correlations with prior experiments should be stated and an estimate of the degree to which such correlation exist should be given.

7. The energy uncertainty and the resolution should be given.

Table I gives as an example the listing of a data set used for the ENDF/B-VI evaluation.

IV. SOME COMMENTS ON THE ENDF/B-VI EVALUATION OF THE STANDARDS AND OTHER PRINCIPAL CROSS SECTIONS

The number of cross section parameters of this evaluation is at present 861. Each data set of a shape measurement adds one parameter. There are currently ~100 shape measurements among the ~300 data sets. The measured quantities reduce to ~4800 values at the grid-point energies. It is clear that the correlation matrix of the experimental data, C, could not be constructed as it would require $\sim 2.10^7$ bytes of memory. However, it has been demonstrated[1] that the grouping of the data sets into "data blocks", which contain the correlated data sets, permits the immediate construction of the matrix $T_A\ C^{-1}A$ which is of size N x N where N is the number of parameters. C is in this case the correlation matrix of the data block. With $N \sim 10^3$ this matrix requires $\sim 4.10^6$ bytes of prompt memory which is available. (The total required memory approximately doubles due to the storage requirements for A, C, M, etc.)

The correlation matrix is constructed in GMA based on the given uncertainty components and correlation factors which are calculated based on the parameters given in the data file. The cross correlations with prior data sets are calculated based on the correlated uncertainty component pairs which are given in the file and a simple factor, also given in the file. The correlations within one data set are calculated based on the totally correlated normalization uncertainties and the systematic uncertainty components which are assumed to be correlated between the energies E_1, E_2 by a function which consists of a constant, a, and a triangle of height b and width c with $a + b \leq 1$.

Though all the correlation matrices of the presently involved ~300 data sets were found to be positive-definite (a requirement to obtain the inverse matrix), a few data blocks were not. It is known that if C is a symmetric matrix a constant p exists such that $C^{\sim} = C + pI$ is positve definite. If C is the variance-covariance matrix of an experimental data block, than this operation implies the addition of a constant statistical uncertainty of $\sqrt{p}$. This reduces the overall weight of the data of the specific data block which might not be acceptable. However, in the present evaluation a transformation has been made such that C is the correlation matrix and $C^{\sim}$ is transformed again to become a correlation matrix. Thus the addition of pI results in a reduction of the correlation coefficients which appears more acceptable because the latter have much larger uncertinties than the uncertainties of the data have.

The resolution of the linear equation system required that at least one data value is available for each parameter. The energy grid has been selected to represent the gross structure of the cross sections. In an energy region were one cross section requires a dense energy grid (e.g. the $^6Li + n$ cross sections over the 240 keV resonance) data may not be available for all other cross section parameters. This problem has been resolved by introducing artificial data sets for each cross section with very large uncertainties.

V. DISCUSSION

It has been demonstrated that a simultaneous evaluation of many inter-related cross sections can be carried out with present computer technology. The major problem is the creation of the corresponding data file. It is near impossible to reanalyze ~300-400 data sets, specifically because much information about the measurements is missing. It is felt that it should be the responsibility of the experimenter to assure that his data, including their uncertainties and correlations, are properly included in the data files.

One of the major advantages of a simultaneous evaluation of many cross sections is that it "randomizes" the systematic errors. This can be expected because a much larger variety of measurement techniques is involved than there would be for a single cross section. The simultaneous evaluation also provides consistency of the results as well as cross-materials covariances.

The goal of the present simultaneous evaluation is to obtain "best" values for the involved cross sections based on the available data. Subjective selection of data sets is avoided. This approach should result in an objective evaluation result which is expected to be independent of the evaluator. Still, the evaluator has to estimate (systematic) or guess (statistical) uncertainty components where such information was not given by the experimentor. The possible effect of these estimates by the evaluator on the result will be investigated. For this purpose the uncertainty components have been tagged in the file to indicate their origin.

It is believed that the present simultaneous evaluation, combined with R-matrix fits f r the light elements and nuclear model fits for the heavy elements will pr de improved evaluated cross sections for ENDF/B-VI.

ACKNOLWEDGMENT

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REFERENCES

1. W.P. Poenitz, "Data Interpretation, Objective Evaluation Procedures and Mathematical Techniques for the Evaluation of Energy-dependent Ratio, Shape and Cross Section Data", Proc. Conf. on Nuclear Data Evaluation Methods and Procedures, Brookhaven National Laboratory, Sept. 1980, BNL-NCS-51363, Vol. 1, 249 (1980).

2. W.J. Youden, Technometrics 14, 1 (1972).

TABLE I. Example of a Data Set Used for the ENDF/B-VI Evaluation

```
SET NR     YEAR    QUANTITY                         AUTHORS                                REFERENCE
  305      1976   AU(N,G)/B10(N,G)                  R.GWIN ET AL.                          NSE59,79(1976)   ****
TYPE OF QUANTITY   7
ID OF OBJECTS       6   3   4   0   0
DATA SET TAG          2
DATA POINTS           5
NO OF COMMENTS        9

NO OF CORR. MATR. ELEM.       0
NO OF CROSS CORR.             1
*

COMMENTS
C      1      UNCERTAINTIES
C      2      1 NORMALIZATION
C      3      3 STATISTICS
C      4      4 BACKGROUND
C      5      5 GAMMA DET EFF.
C      6      6 B DET EFF.
C      7      7 SELFSHIELDING AND ATTEN.
C      8
C      9      SET 304 IS THE COINC. DATA, 305 IS SUM MODE
*

NORMALIZATION UNCERTAINTIES
     3.0      .0      .0      .0      .0      .0      .0      .0      .0      .0
       2       0       0       0       0       0       0       0       0       0
*

ENERGY DEPENDENT UNCERTAINTY PARAMETERS
  3    9          .00          .00          .00
  4    2          .50          .50          .50
  5    2          .50          .50          .50
  6    2          .50          .50          .50
  7    2          .50          .50          .50
*

DATA
NO   ENERGY /MEV    QUANTITY    OF  RES     UNCERTAINTIES, PC
   *                                     13   14   15   16   17   18   19   20   21
   1   .1500E-01   .1967E 00   .0 33.3  2.0  3.0   .3   .2  2.9   .0   .0   .0   .0  5.5
   2   .2500E-01   .1922E 00   .0 20.0  2.0  3.0   .8   .4  2.6   .0   .0   .0   .0  5.4
   3   .3000E-01   .1895E 00   .0  3.0  2.0  3.0  1.0   .6  2.5   .0   .0   .0   .0  5.4
   4   .3500E-01   .1852E 00   .0 14.3  2.0  3.0  1.3   .7  2.4   .0   .0   .0   .0  5.5
   5   .4500E-01   .1762E 00   .0 11.1  2.0  3.0  1.8   .9  2.1   .0   .0   .0   .0  5.5
*

CROSS CORELATIONS WITH PRIOR DATA SETS
DATA SET  PRESENT UNC. COMP./ PRIOR UNC. COMP. PAIRS
  304        14  14  16  16  17  17   0   0   0   0   0   0   0   0   0   0   0   0   0   0
                1.0     1.0     1.0      .0      .0      .0      .0      .0      .0      .0
*

THIS IS THE END OF A DATA BLOCK

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