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EXTENDED COVARIANCE DATA FORMATS FOR THE ENDF/B-VI DIFFERENTIAL DATA EVALUATION*

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ABSTRACT

The ENDF/B-V included cross section covariance data, but covariances could not be encoded for all the important data types. New ENDF-6 covariance formats are outlined including those for cross-file (MF) covariances, resonance parameters over the whole range, and secondary energy and angle distributions. One "late entry" format encodes covariance data for cross sections that are output from model or fitting codes in terms of the model parameter covariance matrix and the tabulated derivatives of cross sections with respect to the model parameters. Another new format yields multigroup cross section variances that increase as the group width decreases. When evaluators use the new formats, the files can be processed and used for improved uncertainty propagation and data combination.

INTRODUCTION

The formal methods of data adjustment require representation of the variance-covariance matrix of all data used. If this requirement is not met in a realistic way, the results are not likely to have the value expected by the analyst. All workers in the field have found substantial challenge in satisfying this criterion for integral as well as differential data.

For the ENDF/B-V differential data evaluation,[1] much effort was expended in the development of formats to permit the inclusion of covariance data,[2] and the evaluators for many of the most important cross sections made serious efforts to use these formats. The main goal was to allow propagation of the differential data uncertainties to yield responsible uncertainty estimates for parameters calculated from the data base.

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Formally, this information is the same as that required for data adjustment,[3] though the level of detail required may be less demanding for simple uncertainty propagation.

The evaluation of covariance data for ENDF/B-V was difficult in part because of the lack of complete uncertainty estimates in the experiments and model calculations that underpin evaluations. In addition, provision was not included in ENDF/B-V formats to encode all the types of covariance data expected to be of importance to applications.

Since the release of ENDF/B-V, techniques for data evaluation that include covariance information have been more fully developed and tested at several installations, and a greater number of experimenters and model code users have taken pains to include covariance information with their results.[4]

Even when covariance data have been treated fully in a differential data evaluation, significant problems can occur in the development of the corresponding ENDF-format covariance files. For example, in the recent evaluation of standards and other important energy-dependent cross sections for ENDF/B-VI, the total of 800-odd output cross section values for ten reactions are correlated, but inclusion of 300,000 covariance elements in the evaluated file would be unsupportable. Our knowledge about such a variance-covariance matrix must be representable with a small fraction of this many parameters, particularly since the whole analysis is based on about 10,000 experimental data points.[5] The originally planned approach was to collapse the matrix strongly except near the diagonal; the method is untested as of this writing.

The approved ENDF-6 formats contain many options for easing and making more complete the representation of covariance data. Some are quite new in concept. Since one of the striking inadequacies was the inability to represent covariances of energy or angle distributions, the new formats include two general approaches to solving these problems.

The covariance representations outlined in this paper are new since publication of the format manual for ENDF/B-V.[6] The text below draws heavily on material prepared for the preliminary ENDF-6 format and procedure manual.[7]

COVARIANCES FOR THE PRODUCTION OF RADIOACTIVE NUCLEI

A new MF=40 file is provided in ENDF-6 formats to contain covariance data for the neutron activation cross section information that is in File 10. The formats and procedures are based on a proposal by F. Mann.[8] The formats and procedures are very similar to those for smooth cross sections in File 33, except that there is an additional level of indexing corresponding to the index LFS, the identifier of the final state of the activation reaction.

EXTENSIONS TO SOME EXISTING COVARIANCE FORMATS

Some relatively minor extensions have been included in the ENDF-6 formats to strengthen capabilities and avoid conflicts that arose in the development of uncertainty files for ENDF/B-V.

In the previous formats there were no provisions for encoding covariances between cross sections represented in ENDF files having different values of MF. One conflict arose concerning the thermal cross section parameters, for which tabulated covariances between neutron multiplicity

The Unresolved Resonance Region

There was no provision for uncertainties for the unresolved resonance region in ENDF/6 formats, except that relative uncertainties in File 33 for such energy regions refer to the sum of the smooth cross sections given in File 3 and the cross sections reconstructed from the resonance parameters in File 2. Such an approach for the unresolved resonance region is sufficient for applications in which the nuclide in question has a low enough concentration that uncertainties in self-shielding factors are small compared to those in the average cross sections at infinite dilution.

An ENDF-6 format is defined for covariances in the unresolved resonance region. It may be used when self shielding can be important in this energy range. In File 32 the covariance matrix of one set of average Breit-Wigner resonance parameters is given for the whole region, and in File 33 are found the covariance data for the infinite dilution average cross section. The cross section processor obtains the covariance matrix of the shielded or effective cross sections by combining these two types of information. (Note that the File 32 average parameters themselves do not need to reproduce the self-shielding factors.) A means for this combination in a slightly less restricted case has been demonstrated by de Saussure and Marable.[10] In one test case using their results, Broadhead and Dodds found that the covariances of effective cross sections were only weakly affected by uncertainties in the average cross sections.[11] While it is unclear what the quantitative outcome will be for other cases, it is clear that no better approach has been identified. The idea is similar to the new ENDF-6 unresolved resonance region representation for the cross sections themselves, in which infinite dilution cross sections are given in the necessary detail, but average parameters are given at only a few energy points and are used only for the calculation of self shielding.

SECONDARY ENERGY AND ANGLE DISTRIBUTIONS

Simplified representations are now provided for covariances of secondary angle and energy distributions that are contained in Files 4 and 5. These files are being replaced by File 6 in many evaluations for ENDF/B-VI because Files 4 and 5 do not permit the secondary energy variation of the angular distributions of outgoing particles that is usually observed for incident and secondary energies above a few MeV.

Covariance data for angular distributions of secondary particles can be encoded in File 34 in terms of covariances among Legendre coefficients. Energy-dependent correlations of the magnitude of the cross section with the angular dependence can be recognized using covariances of the a_0 coefficient even though its nominal value is unity in the ENDF formats. Covariances are expected to be encoded for only one or two Legendre moments. The original expectation was that this format would be used at least for the scattering of neutrons on hydrogen, but the formulation of the next Section should permit more direct evaluation.

Based on a proposal by Perey,[12] a simplified covariance format is provided in File 35 for energy distributions of secondary neutrons. Covariance matrices for secondary neutron energy distributions may be tabulated for a few large primary neutron energy bands. It is assumed (not realistic) that there is full correlation for a given secondary energy within each primary energy band. The secondary energy distributions are however assumed to be completely uncorrelated between the various primary

energy bands (equally unrealistic). No covariances linking different materials or reaction types are allowed. Furthermore, no covariances with information in other files are allowed, for example smooth cross sections in File 3 or fission neutron multiplicities in File 1. The usefulness of this new format will depend on the evaluator judiciously balancing the effects of the incorrect assumptions. Note that the ENDF/B-V assumption of zero uncertainty in File 5 energy distributions is even more incorrect.

COVARIANCES OF QUANTITIES FROM MODEL CODES

Covariance data for cross sections and angular distributions that are output from any model or fitting code can in principle be represented by the model parameter covariance matrix and tabulated derivatives (sensitivities) of cross sections etc. with respect to key model parameters.[5] In favorable cases where relatively few parameters represent some cross sections over broad energy ranges, the representation can be quite compact as well as general. The details of the formulation and even the meaning of the parameters need not appear in the evaluated file. An advantage of such generality is that the results of a wide variety of evaluation methodologies can be described.

The idea of a covariance file structure based on this idea was explored by Muir,[13] who observed that multigroup averages of sensitivities are identical to the parameter sensitivities of the corresponding multigroup data; the latter are needed for most applications. To take full advantage of this equivalence, the sensitivities must be represented in a format as close as possible to that for the data itself, so that the sensitivities can be retrieved and integrated by processing codes that have received minimum modification. A proposal for such a format was presented by Muir at the May, 1988 CSEWG meeting.[14] Subsequently an ENDF-6 format modification was proposed[15] and accepted by the CSEWG Methods and Formats Committee for allowing the needed information to be placed in File 30.[16] The new approach may mitigate the considerable difficulty otherwise experienced in representing covariances for correlated energy-angle distributions and multiplicities, and should simplify covariance evaluation whenever the evaluated cross sections etc. have been derived from a theoretical formula using parameters among which the covariance matrix is known.

The potential value of a covariance format of this type became especially clear in connection with the R-matrix analysis of the light-element reaction systems for ENDF/B-VI,[17] in particular for the evaluation of the light-element neutron standards.[18] The parameters in this example describe levels (resonances) in the relevant compound systems. Where all resonances can be enumerated, the formulation can be considered exact and, if the relevant experimental data are consistent, the parameter covariance matrix can be trustworthy.

Much of the angle-energy dependent data being encoded in File 6 for the 1-20 MeV region is derived from optical and statistical-preequilibrium theoretical models. Relevant parameters for this case include the optical and level-density parameters, preequilibrium matrix elements, and gamma-ray strength functions. Parameter covariance matrices for similar models have been demonstrated in a few cases based on the experimental data used to define the parameters.[19] While such model parameter covariance data are not available for current U. S. evaluations of this type, developments elsewhere suggest that the general model parameter covariance propagation technique will be applicable to a broad range of cross sections in the

future. This prospect places certain difficulties in our path, since the resulting propagated uncertainties in individual differential cross sections would doubtless be smaller than systematic discrepancies observed in some angle and energy ranges.

Since the idea of the new ENDF File 30 is somewhat new, it seems worthwhile to outline the approach. In the context of File 30 the term "sensitivity" is defined as the derivative σ' of an evaluated quantity, say σ', with respect to the logarithm of one of the model parameters α_i, i.e.,

$$\sigma'_i = \alpha_i \, \partial\sigma/\partial\alpha_i \quad .$$

An advantage of employing such derivatives in File 30 is that the σ'_i are expressed in exactly the same units as σ whether it be an actual cross section or a distribution quantity. This means that integrations over energy and angle can be performed with minimal changes in multigroup processing codes. Therefore, an ENDF/B processing program that calculates multigroup cross sections can be used with few modifications to obtain the parameter sensitivities of the multigroup constants using data encoded in File 30. The use of derivatives with respect to the logarithms of the parameters also meshes nicely with the use of relative parameter covariance matrices. It is understood that the data fields normally used to store information on cross sections etc. are used in File 30 to record the corresponding sensitivity information, but that other quantities have have standard (MF≠30) ENDF-6 definitions.

The first section, MT=1, of File 30 contains of a directory that displays the contents and ordering of information that is recorded in other sections of the file. (Note that in File 30 the MT-values do not correspond to reaction types.) It also contains an optional cross-material and cross-library correspondence table that may be utilized if the same parameter values are important for covariance data outside the library/material in which a particular File 30 is placed. The directory serves as a guide for the processing codes and provides also an eye-readable list of the files and sections elsewhere in the current evaluation that are significantly sensitive to the parameters under consideration. A series of pointers for each parameter indicate the sections (MFSEN, MTSEN) of data in the main body of the evaluation that are sensitive to that parameter. MFSEN and MTSEN also determine the formats to be used to represent the dependence of the sensitivities on the applicable independent variables such as energy, angle, etc.

The second section of File 30, MT=2, contains the relative covariance matrix of the model parameters. The upper half of the symmetric matrix is encoded by rows in a way that saves space if the last elements in a row are null.

Sections MT=3 through MT=10 are set aside for possible future assignment, and those from 11 to 999 are used for the sensitivities. A single section in this range of MT values is the collection of all the sensitivities relevant to a given model parameter MP. The section number is determined by the parameter index, using the relation MT=MP +10. Each subsection corresponds to a record in the MT=1 directory, and contains the derivatives of the cross section etc. quantities in the referenced section (MFSEN, MTSEN) of the main file to the model parameter identified in that record.

The information in File 30 is considered to describe sources of uncertainty that are independent of those described in Files 31-40. Therefore, for a given set of multigroup cross sections, the multigroup

covariance matrix obtained from File 30 should be added to any such matrix derived from the other files.

In addition to the utility of File 30 that is directly apparent, some possibilities exist that are less obvious. (a) To permit covariance data for a smooth cross section evaluated from experiments to appear in File 30, an evaluator could set up an ad hoc "nuclear model" in which the model parameters are just the cross section values at particular grid points; for linear interpolation the sensitivity functions would be triangles centered on each grid point and reaching zero at the next adjacent grid points. (b) To seek more compact storage for any nuclear model, one could diagonalize the parameter covariance matrix and compute linear combinations of the original sensitivities using the resulting transformation matrix. If the transformed sensitivities interpolate as well as the original ones, at least for the important eigenvalues, the result would be useful and elegant. However, adjustment of parameters might become more complicated. (c) Another idea is for a processing code to store only the multigroup sensitivities and the original parameter covariance matrix rather than expand this information into the full multigroup covariance matrix which can be very large. For a particular applied problem, matrix products might be computed and stored that are the sensitivities of integral parameters (e.g. Doppler coefficients) to the nuclear model parameters. The same point is valid here as has been recognized for resonance parameters:[20] whenever practicable, formal adjustment can better proceed using the model parameters as variables rather than the intervening group cross sections.

A SELF-SCALING MINIMUM VARIANCE FOR GROUP CROSS SECTIONS

Up to now, ENDF covariance files processed on a sufficiently fine energy mesh yielded physically unreasonable full correlation between adjacent group cross sections; these singular multigroup covariance matrices caused distress in some mathematical manipulations and were conceptually objectionable. A "minimum variance" format has now been approved[16] to assure that, if an evaluated covariance matrix on the evaluator's grid is positive definite, the multigroup cross section covariance matrix on any user's grid will also enjoy this property. A second goal is to allow the evaluator to represent the effect of the underlying unresolved resonance structure on the uncertainty in the cross section averaged over regions smaller than those otherwise considered in the evaluation. The new format does not address minimum uncorrelated variances for energy or angle distributions.

Under this new procedure, diagonal (variance) components are added to the overall multigroup covariance matrix. These components can be small enough to make no unwarranted change to a propagated uncertainty averaged over a broad spectrum, but large enough to assure that multigroup covariance matrices are positive definite even for fine energy groups.

The covariance evaluator specifies values of F_k for selected energy intervals ΔE_k in an LB=8 "NI-type" sub-subsection of e.g., File 33. The magnitude of the resulting variance component for a processed average cross section depends strongly on the size of the energy group as well as on the values of F_k in the sub-subsection. For the simplest case of a multigroup covariance matrix processed on the energy grid of this sub-subsection with a constant weighting function, the variance components VAR_{kk}

contributed by the LB=8 component are just F_k; the off-diagonal contributions are zero. LB=8 sub-subsections cannot be used to represent cross-reaction or cross-material covariances.

In general, each F_k characterizes a contribution to the absolute variance of the indicated cross section averaged over any energy interval (sub-group) ΔE_j that lies completely within the energy interval ΔE_k and that is narrow with respect to variations in the energy-dependent multigroup weight functions utilized in the intended applications. The variance contribution VAR_{jj} from an LB=8 sub-subsection to the processed group variance for the energy group (E_j, E_{j+1}) is inversely proportional to its width ΔE_j and is obtained from the relation

$$VAR_{jj} = F_k \, \Delta E_k / \Delta E_j \quad ,$$

where $E_k \leq E_j < E_{j+1} \leq E_{k+1}$. Note that the VAR_{jj} are variances in average cross sections. No contributions to off-diagonal elements of the multigroup covariance matrix are generated by LB=8 sub-subsections.

In contrast to other processing laws to date, the law for processing LB=8 sub-subsections directly references the variance of an average cross section rather than the variance of a pointwise cross section. If a fine-grid covariance matrix is developed and then collapsed to the evaluator's LB=8 E_k grid with constant weighting, the resulting variance components are just the F_k.

The values of F_k may be chosen by the evaluator to account for the statistical fluctuations in fine-group average cross sections that are induced by the width and spacing distributions of the underlying resonances. Values may also be chosen to represent the uncertainty inherent in estimating the average cross sections for small energy intervals where little or no experimental data exist and smoothness is not certain.

The LB=8 sub-subsections help prevent mathematical difficulties when multigroup covariance matrices are generated on an energy grid finer than that used by the evaluator, but F_k values must be chosen carefully to avoid accidental significant dilution of the evaluated covariance patterns represented in the other sub-subsections. If no physical basis is apparent for chosing the F_k values, they may be given values about 1% as large on the evaluator's grid as the combined variance from the other sub-subsections. Such values would be small enough not to degrade the remainder of the covariance evaluation, and large enough to assure that the multigroup covariance matrix will be positive definite for any energy grid if the matrix on the evaluator's energy grid is positive definite.

The requirement to include LB=8 sub-subsections should relieve numerical problems encountered by data adjusters whether the adjustments are based on integral data or on new differential data. However, even if F_k values are very carefully chosen, problems are inherent in covariance evaluations that utilize extremely coarse energy grids and thereby imply unphysical high correlations among cross sections for large energy regions. Some such evaluations were provided in ENDF/B-V because the main purpose of the covariance information was to permit the propagation of nuclear data uncertainties for applications with broad neutron spectra. However, some users who have employed the adjustment equations to update an existing evaluation by "adding" new data and their associated covariances have needed to modify certain ENDF/B-V covariance files onto a finer grid.[21] To minimize the extent to which such users will be tempted to make ad hoc changes to covariance files, ENDF-VI covariance evaluators for

reactions of particular importance are now being asked to employ narrower energy meshes than in the past in order to reduce the difficulties to be encountered by future evaluator-users of the covariance files.[22] Overlapping structures in energy and other techniques are suggested to reduce the occurrence of large changes in correlation as one crosses an arbitrary energy boundary.

CONCLUSION

Broadened format capabilities and the increased experience with covariance data that is now possessed by measurers, evaluators, and users should facilitate the generation of new evaluated covariance files that better meet the requirements for formal data adjustment. It remains for evaluators to employ the newly available techniques to determine if they meet the needs. Since some of these formats have become available only after most of the evaluation work on ENDF/B-VI is completed, they may not be so widely used for the first version of the new evaluated file.

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