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Uncertainty Information of Experimental Data and Nuclear Models

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ABSTRACT

A straightforward derivation is presented for the covariance matrix of evaluated cross sections based on the covariance matrix of the experimental data and propagation through nuclear model parameters.

I. *INTRODUCTION*

In an evaluation of nuclear data, the evaluator would ideally attempt to utilize and preserve all valid information contained in the experimental data base, as well as utilize the knowledge available from and through nuclear models and their associated auxiliary parameter data base. In the case of neutron cross sections, this usually calls for a simultaneous evaluation of several cross sections if correlations between such cross sections exist. This is the case for the "standards", and several cross sections of importance for reactor neutronics which will be considered here as an example. The experimental data for ^{6}Li(n,α), ^{10}B(n,α), ^{197}Au(n,γ), ^{238}U(n,γ), ^{235}U(n,f), ^{238}U(n,f) and ^{239}Pu(n,f) are correlated not only because some measurements of different cross sections were carried out with the same detectors or samples, but also because cross section ratios and sums (e.g. total cross sections for the light nuclei) were measured as well. For this reason it has been decided to evaluate these cross sections simultaneously for ENDF/B-VI.[1] Such simultaneous evaluation is especially desirable in this case as covariance information for these cross sections, as well as cross material covariances are of specific importance for applications and can be derived in a natural way.

Different theoretical models would be invoked for the evaluation of these cross sections, i.e. the R-matrix theory for the light nuclei (see for example Ref. 2) and the statistical/optical model for the reaction cross sections of the heavy nuclei (see for example Ref. 3). The use of these theoretical models is desirable for various reasons. One is the use of additional data, e.g. angular distributions, polarization and inverse reaction data through R-matrix theory for the light nuclei, and to impose physical gross structure, e.g. inelastic competition cusps, on the heavy nuclei cross sections. Another is that theoretical models provide smooth cross sections where experimental data may result in unreal structure due to statistical uncertainties and data inconsistencies.

The simultaneous fitting of the correlated experimental data with a combined R-matrix and statistical/optical model computer code would provide a multi-model parameter set and its covariance which would be used for the subsequent derivation of the evaluated cross sections and their covariance by error propagation. Though this would be the most satisfying and direct approach, it can be easily guessed that it would severely tax the present computer capabilities in both running time and storage and addressing space. A stepwise approach is discussed here which has been or may be used in parts of an evaluation proposed for ENDF/B-VI.

II. GENERALIZED LEAST-SQUARES EVALUATION OF EXPERIMENTAL DATA

A first and substantial reduction of the amount of data which have to be handled by a nuclear model code can be achieved by a generalized least-squares fit of the experimental data (about 450 data sets with more than 10,000 data values). A parameter space of ~ 1000 appears desirable in order to represent thermal parameters, energy integrals below 10 KeV, and pointwise cross sections which reflect the gross structure of the cross sections above 10-20 KeV on an appropriate energy grid. From the generalized least-squares fit one obtains the refinement vector

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

with covariance

$$C_\delta = (A^T C_m^{-1} A)^{-1} \qquad (2)$$

(see for example Ref. 4) which is to be applied to an a priori parameter vector (arbitrary, except for the applicability of the linearity approximation). The A is the design matrix with elements equal to the first coefficients of the Taylor series expansion of the measured quantities (A^T is its transpose), and M is the measurement vector. With appropriate transformation,[5] C_M is the correlation matrix of the measured data. That a parameter space of this size can be handled with today's computer capabilities has been demonstrated with the generalized least-suqares program CMA in 1980[6] and this step is now part of an evaluation proposed for ENDF/B-VI.[1]

III. THE ADDITION OF NEW OR AUXILIARY DATA

Additional data for the evaluated parameters may be available, e.g. new experimental data, integral data, or data which have been derived from quantities which are not part of the parameter space (for example angular distributions) with the help of a nuclear model. Integral data have been excluded from the evaluation proposed for ENDF/B-VI, with the well-justified exception of the ^{252}Cf spectrum averaged fission cross sections of ^{235}U and ^{239}Pu, in order to keep the problem of differential data uncertainties and reactor modelling uncertainties a separate issue. New data could easily be accommodated by rerunning GMA. However, the data obtained from a nuclear model cannot, in general, be added as an input set to the GMA data base because its covariance matrix is singular.[6] Instead, these data can be utilized with the well-known formalism used in "adjustment" procedures (see for example Ref. 7) if they are uncorrelated with the data used in the first step of the evaluation. Using the first-step result of the parameter vector as a priori one obtains a simplified second-step adjustment vector[8]

$$\delta_2 = C_\delta A_2^T (A_2 C_\delta A_2^T + C_2)^{-1} M_2 \qquad (3)$$

with covariance

$$C_{\delta 2} = C_\delta - C_\delta A_2^T (A_2 C_\delta A_2^T + C_2)^{-1} A_2 C_\delta . \qquad (4)$$

M_2 is the "measurement" vector of the cross sections derived from the nuclear model, C_2 is the corresponding covariance matrix, and A_2 is the coefficient matrix for the additional data. C_δ is the covariance matrix of the "first-step" evaluated parameters and follows from Eq. (2). C_δ is non-singular but C_2 is in general singular; however, in the one example of interest here, it has been shown that $A_2 C_\delta A_2^T + C_2$ can be inverted.[6] This "second-step" approach of adding more complex data information (as angular distributions, polarization etc.) is currently being considered as an option for the evaluation proposed for ENDF/B-VI. Another option of combining theoretical nuclear model results with evaluated pointwise data has been discussed elsewhere.[1] In either case, it proved necessary in the example discussed here to use some cross section data which could have been used in the first step of the evaluation in the nuclear model fit.[1]

IV. THE UTILIZATION OF NUCLEAR MODELS

Though some data obtained from a nuclear model can be utilized in a "second-step" procedure as shown in Section III, the desire to use a multi-model fit of the pre-evaluated cross sections remains. The main advantage of a separate "second-step" addition of data derived from a nuclear model is that a final step requires less complicated nuclear model modules, i.e. modules which only calculate the cross sections which are the objects of the evaluation, and thus require less computer time and space. The total parameter space is somewhat reduced as only the cross sections described by the nuclear models can be included in the fit, i.e. thermal parameters and energy interval integrals are excluded.

For this third step of the evaluation in which the pre-evaluated cross sections are fit with a multi-nuclear model code, the (cross section) parameters evaluated in the prior steps become measureable quantities, m_i, which can be derived from nuclear models, and the nuclear model parameters become the new parameters. Assuming an a priori nuclear model parameter vector p, the adjusted quantity (evaluated cross section) is again based upon a Taylor series expansion

$$f_i(\vec{p}) = f_i(\hat{p}) + \sum_j \frac{\partial f_i(\vec{p})}{\partial p_j} (p_j - \hat{p}_j) = m_i, \qquad (5)$$

$$= f_i(\hat{p}) \; (1 + \sum_j S_{ij}\delta_j), \qquad \delta_j = \frac{p_j - \hat{p}_j}{\hat{p}_j}$$

where $f_i(\hat{p})$ is the derived quantity obtained from the nuclear model based upon the a priori parameter vector p. The

$$S_{ij} = \frac{\hat{p}_j}{f_{i(p)}} \; \frac{\partial f_i}{\partial p_j}$$

are the coefficients of the "sensitivity" matrix which replaces the coefficient matrix A in Eqs. (1) and (2). The derivatives, $\partial fi/\partial pi$ are obtained from the nuclear model either in analytical form (R-matrix) or from finite differences. The adjustment vector δ for the nuclear model parameters and its covariance can be obtained with analogous use of Eqs. (1) and (2). However, p needs to be close to the final solution $\vec{p}$ in order for the linearity assumption (Eq. (5)) to hold. This can be achieved by prior non-linear fitting of the cross sections of individual nuclei by simple χ^2 minimization. At this stage, other cross sections can be included in order to further constrain some parameters. Alternatively, if a nuclear model parameter set and its covariance are available based upon data which are uncorrelated with the m_i's, δ and its covariance can be obtained from Eqs. (3) and (4). In this case, the uncertainties of the a priori nuclear model parameters restrain the adjustment called for by the additional data. The covariance matrix of the evaluated quantities, $fi(\vec{p})$, follows from error propagation from the covariance matrix of the parameters[8-10]

$$C_f = DC_pD^T,$$

where D is the matrix of the derivatives, $\partial fi/\partial pj$, and C_p is from Eq. (2) or (4). Formally, the covariance of the evaluated cross sections, C_f, is derived from the covariance of the measured data, C_M, by propagation through the covariance of the nuclear model parameters, C_p. Additional uncertainties which are due to the approximations of the nuclear models are ignored at this point.

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