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UNIQUE DEFINITION OF NUCLEAR DATA ACCURACY

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Abstract

An approach to development of the unique definition of evaluated nuclear data accuracy suitable for reactor and other applications is proposed. In this connection the nature of experimental nuclear data errors is discussed and recommendations for the representation of the error components in publications are given.

A general algorithm is given for the calculation of the "unique" error important in applications - the error in the integral under the curve and in its general slope - on the basis of the representation of errors by a covariance matrix being obtained at the parametrization of experimental data by the least square method.

INTRODUCTION

Nuclear data the most important for fast reactors have been repeatedly measured and evaluated for more than a quarter of the century by many groups of authors but the measurements and evaluations of these values are being continued up to now and planned for the future.

This is caused by the dissatisfaction with the uncertainty value of obtained quantities. Besides, an increase in the accuracy of an experiment demands an increase of costs which are inversely proportional to the square of a tolerable uncertainty according to some estimations. Therefore quantitative determination of satisfactory accuracy is of great importance. There exists also a mathematical apparatus -

- "experiment planning" - which allows to find quantitatively the required data accuracy. To the problem being discussed this apparatus is applied in [1], [2], [3], [4]. It is necessary only to come to an agreement about the unique representation of the error based on the understanding of its structure, i.e. the nature of its components of various origin which have a different effect on the accuracy of calculated reactor parameters.

The great majority of reactor parameters depends on wide neutron spectra. Therefore the error components correlated over wide energy ranges and over some isotopes in a reactor are of great importance. Unique representation of these error components is of great concern because the most rigid requirements deduced in [1] - [4] are imposed just on the accuracy of these components. It is clear that all the considerations mentioned above will be also valid for the blanket of a fusion facility and in general for all cases when wide neutron spectra are important.

The question being considered here arose in connection with the discussion of the world-wide request list for neutron data (WRENDA) [7] at INDC. In particular, the discussion concerned the problem of reviews of state-of-the-art in the knowledge of some definite values by the evaluators which had performed corresponding evaluations. The point is that the errors indicated by them and characterizing the attained state of knowledge must be compared with the error value tolerated by users and shown in the same document. Comparison of attained and required accuracies must show if the efforts in refinement of the value under consideration should be continued or stopped. Naturally, this is possible only at the unique definition of quantities being compared. Formulation of the problem was discussed earlier in document [8].

ERROR STRUCTURE IN AN EXPERIMENT

An experimentator investigating the dependence of a function on an argument measures it usually at the argument

values being successively selected. In this case the dependence is obtained as a set of experimental points each of which has an error. Now we consider components of this error.

The first error component - the statistical one - shows itself directly in an experiment in the fact that the scatter is observed in the results of various sets of measurements.

This scatter is caused by the finiteness of the number of registered events and perhaps by other random factors. The experimentators consider that it is necessary to eliminate these random factors and they are satisfied if the scatter of some measurement sets is fully explained by the finiteness of the number of registered events, N, when the relative dispersion is equal to $\frac{1}{\sqrt{N}}$.

Irrespective of whether the scatter of measurement results is caused by the finiteness of the events number or not we denote this first error component by Δ statistical $\equiv \Delta_1$.

The second error component goes over to the measured value from the error of the standard used in measurements. Let us denote it by Δ standard $\equiv \Delta_2$.

The third error component is connected with possible disadvantages of the experimental set-up itself which results in a shift of the value under measurement. If the experimentator understands the causes of this shift or its part he introduces a calculational correction and evaluates a possible inaccuracy of this correction which is the third error component.

We denote it by Δ systematic $\equiv \Delta_3$.

This error can not stochastically vary from point to point because it results from the cause remaining constant or varying very slightly. Thus, this error component being correlated characterizes the error not of each point, but of the whole curve. The same considerations apparently can be attributed to Δ_2 or at least to its part and also to the next unknown error component.

The unknown error component is connected with disadvantages of the experimental set-up itself which result in the shift of the value under measurement what the experimentator himself does not know. We denote this component by Δ unknown systematic $\equiv \Delta x$.

The existence of Δx is just the reason of frequent discrepancies of the results of experiments performed with the use of various methods by values exceeding the errors declared by the experimentators.

The existence of Δx and its order of magnitude are revealed only when comparing the results in the process of evaluation. An important and a delicate task of an evaluator when revealing these discrepancies is the attribution of various values of Δx to the results of different authors. Fortunately, in some experimental works several various methods are used and in this case one can consider that for these works Δx is determined from the experiment.

The total error of an experimental point the authors of measurements usually calculate according to the formula

$$\Delta^2_{teep} = \Delta^2_1 + \Delta^2_2 + \Delta^2_3$$

because usually nothing is known about the last summand Δx. This representation is correct because three error components are not correlated with one another and the error of one point is characterized by this value correctly.

But it would be incorrect to form the table: argument, function, Δ_{teep}.

The fact is that at this representation one would like to draw a curve through the points with errors by the least square method but this assumes the errors of neighbouring points to be non-correlated. But in reality there is no correlation between neighbouring points only for the component Δ_1. On the contrary, for all remaining error components taking into account their origin one assume in the first approximation that there exists the total correlation between the points. In other words, all the components with

the exception of Δ_1 shift the whole curve completely upwards or downwards and Δ_1 affects its form. If we draw the curve by the least square method using Δ_{teep} the form of this curve will be smoothed because some its peculiarities will be wrong treated as statistically unstipulated. It would not take place when using Δ_1 instead of Δ_{teep}. On the other hand, the error of an integral under the curve at a great number of points. Can be highly lowered because the total error is considered as the statistical one, decreased by $\sqrt{N}$ times with the increase of the "N" - number - points on the curve. At the correct treatment only the contribution to the integral from Δ_1 will be decreased with the increase of points number. The growth of the experimental points number in the given experiment can not affect other error components but Δ_1 .

RECOMMENDATION FOR REPRESENTATION OF ERRORS OF EXPERIMENTAL VALUES

The error component Δ_1 non-correlated in various points and following directly from the measurements should be represented point by point. All other error components obtained as a result of the analysis of the experimental set-up and corresponding calculation or from literature should be represented separately with the specification of correlative properties, either with the help of formulae, either by algorithms description or in the table form. The total error of an experimental point can be presented in some characteristic points.

UNIQUE DEFINITION OF ERROR AND THE EVALUATION ALGORITHM AT WHICH IT IS REALIZED

The unique definition of error is necessary for establishing a common language between users, evaluators and measurers of nuclear data in the process of planning the work on data refinement.

When the user is speaking about a tolerable value of error, the evaluator - about a decrease of error achieved in the last experiments, and the experimentator - about his ability of measuring a value to a certain error, it is necessary that the same word "error" have the same meaning. Search of this meaning should be started from considering the aim of activities, i.e. ensuring an assigned accuracy of reactor calculation. From general considerations on the breadth of neutron spectra in fast reactors it is clear that the error components correlated over a broad energy range, i.e. affecting the integral under the cross-section curve and, may be, the general slope of this curve, should affect the calculation accuracy. And, on the contrary, the error component determining the inaccuracy of the curve detailed trend cannot influence significantly.

In accordance with this, for a unique definition of error of a function we take the errors of several functionals of this function which would characterize its normalization, general large-scale trend, etc. In the simplest case such functionals are the integral for characterizing the normalization and the first moment for characterizing the slope.

What are the requirements to the evaluation procedure to determine correctly the errors of the evaluated data and, specifically, of the above functionals?

First of all, the following remark should be made.

The commonly used programs of the least-squares method, for example, the program of the curve representation with the use of polynoms, assume the errors to be non-correlated, statistically independent. Therefore, with the use of these programs it is quite justified to draw a curve through the points of a single experiment assigning to these points the error Δ_1 . But an attractive possibility to draw a curve through the points of several works at once, with assigning a total error to each point, should be rejected as an incorrect one. Let us explain this. There are two groups of experimental points from two works carried out by different methods and presenting the same function. They differ from one

another by some value characterizing the systematic error value Δ_x. Now by assigning total errors to the points of both experiments according to the formula $\Delta^2_{teop} = \Delta_1^2 + \Delta_x^2$ and drawing a curve through them by the least-squares method we obtain an error in the integral of this curve equal on its order of magnitude to $\Delta_{teop}/\sqrt{N}$, where N is the number of points in both experiments. But it is obviously an erroneous conclusion because this error is determined by Δ_x and cannot decrease with the number of points on the curve.

Therefore, taking into account this remark, the evaluation process should consist of the following stages: 1) Reduction of results to one standard, introduction of corrections for systematic errors found out by the time of evaluation, rejection of works not satisfying some criteria or assigning a considerable systematic error Δ_x to them. 2) Parametrization by the least-squares method of experimental curves of separate works or groups of works performed by the same method. In this case information about uncertainties resulting from statistical uncertainties of each experimental work is presented, in corresponding covariance matrices. The algorithm for obtaining the error of the functional of the parametrized curve from the covariance matrix is described in Appendix. Let us denote these errors by Δ_{fp}. 3) The procedure of obtaining a single evaluated function from several parametrized curves will not be discussed here. If such a method keeping information about errors exist, then it would be sufficient to apply the algorithm described in Appendix to a correspondingly parametrized function and to its covariance matrix to obtain a "unique" error. But irrespective of the method used for obtaining the evaluated curve the information on uncertainties of its functionals can be obtained by considering a statistical ensemble of functionals of the curves taken from separate works. When considering this ensemble we can consider it as an ensemble of measuring methods, systematic errors of each method being now considered as random ones. Therefore, to obtain the mean functional

and its dispersion let us use the formulae of the least-squares method:

$$F = \frac{1}{N} \frac{\sum F_i / \Delta^2_{iF}}{\sum 1 / \Delta^2_{iF}} \quad ; \quad \Delta^2_F = \frac{1}{\sum 1 / \Delta^2_{iF}} \qquad (a)$$

In this case the condition of $\frac{1}{N}\sum (F-F_i)^2/\Delta^2_{iF} = 1$ (b) will not be satisfied if we take $\Delta_{iF} = \Delta_{1iF}$. It is necessary to include in Δ_{iF} the known systematic errors Δ_{3iF} and, may be, to assign the unknown Δ_{xiF}. Assuming all the curves to be reduced to one standard, we do not take into account the component Δ_{2iF} at this stage. Thus,

$$\Delta^2_{iF} = \Delta^2_{1iF} + \Delta^2_{3iF} + \Delta^2_{xiF}$$

Strictly speaking, Δ_{xiF} should be assigned in accordance with the quality of methods but so that the condition (b) is satisfied.

From the point of view of applications the correctness of the evaluated curves should be verified by comparison of their functionals with the values obtained by formulae (a). As for the "unique" errors, they are also determined by the latter formulae (a) and (b).

In conclusion it should be noted that for the functionals considered we may take not the integral and the first moment but, for some important reactor parameter, the integral of the product of a cross-section by flux and importance of neutrons. In some cases it may prove that important is not an error within a broad energy range, as it has been said above, but an error in parameters of some resonance, for example, of the 3 keV sodium resonance. Functionals determining blocking coefficients, i.e. sensitive to the detailed trend of a curve can be also considered.

From the above it is clear that the proposed approach to the unique definition of the error is a sufficiently general one.

A P P E N D I X

The Error of the Parametrized Curve Functional

Let $f(x, a_0, a_1 \dots a_n)$ be a function the parameters of which are determined from the condition of the best, in the sense of the least-squares method, description of the experimental points set. $F(a_0, a_1 \dots a_n)$ is the functional of the "f" function, and D_{ij} is's the covariance matrix characterizing dispersions - squares of parameter errors (diagonal terms) and covariances of parameter errors (non-diagonal terms).

To calculate the functional F dispersion it is necessary, first of all, to find the sensitivity coefficients of the functional to parameter variation, i.e., partial derivatives of the functional over the parameters $\partial F/\partial a_i \quad i = 0, 1, \dots n$, the set of which forms the vector $\{\partial F/\partial a_i\}$.

The dispersion of the functional F, i.e. the square of its error, is expressed by the formula:

$$\Delta^2_{1F} = \left| \frac{\partial F}{\partial a_0} \quad \frac{\partial F}{\partial a_1} \dots \frac{\partial F}{\partial a_n} \right| \times \begin{vmatrix} D_{00} & D_{01} & \dots & D_{0n} \\ D_{10} & D_{11} & \dots & D_{1n} \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ D_{n0} & D_{n1} & \dots & D_{nn} \end{vmatrix} \times \begin{vmatrix} \frac{\partial F}{\partial a_0} \\ \frac{\partial F}{\partial a_1} \\ \vdots \\ \frac{\partial F}{\partial a_n} \end{vmatrix} \qquad (p.1)$$

where the sign "x" denotes matrix multiplication. Thus, this algorithm extracts from the detailed information about the error the component we are interested in.

As a simple example let us consider a function presented by a series over the Legendre polynomials in the range of arguments from -1 to +1, i.e. in the range of orthogonality of these polynomials. In case of the energy dependence of the

functions in the interval E_1 to E_2, by transformation of the argument:

$$x = -\frac{E_2 - E}{E_2 - E_1} + \frac{E_1 - E}{E_1 - E_2} .$$

we will get into the above mentioned interval of arguments.

So, let

$$f(x, a_0, a_1 \dots a_n) = \sum_{i=0}^{n} a_i P_i(x)$$

then

$$F_0 = \int_{-1}^{1} f(x, a_0, \dots a_n) dx = 2a_0 \qquad F_1 = \int_{-1}^{1} x f(x, a_0 \dots a_n) = \frac{2}{3} a_1$$

$$\frac{\partial F_0}{\partial a_i} = 2\delta_{0i} \quad i = 0, 1 \dots n \qquad \frac{\partial F_1}{\partial a_i} = \frac{2}{3}\delta_{1i} \quad i = 0, 1 \dots n$$

$$\Delta^2_{1F_0} = 4D_{00} \qquad \Delta^2_{1F_1} = \frac{4}{9} D_{11}$$

If the polynomials were not orthogonal, or the functionals had weight, or parametrization were more complicated, e.g., presentation of the resonance curve by a multilevel formula, then such simplification of the algorithm would not take place and calculations should be carried out by the general formula (p.1).

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