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THE IMPACT OF COVARIANCE INFORMATION ON CRITICALITY SAFETY
CALCULATIONS IN THE RESOLVED RESONANCE ENERGY RANGE

by

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Abstract

Resonance data play a significant role in the calculations of systems considered for criticality safety applications. K_{eff} , the major parameter of interest in such a type of calculations, can be heavily dependent both on the quality of the resonance data as well as on the accuracy achieved in the processing of these data.

If reasonable uncertainty values are available, in conjunction with their correlation in energy and among type of resonance parameters, one can exploit existing methodologies, based on perturbation theory, in order to evaluate their impact on the integral parameter of interest, i.e., K_{eff} in our case, in practical applications. In this way, one could be able to judge if the uncertainty on specific quantities, e.g., covariances on resonance data, have a significant impact and, therefore, deserve a careful evaluation.

This report, first, will recall the basic principles that lie behind an uncertainty evaluation and review the current situation in the field of covariance data. Then an attempt is made for defining a methodology that allows calculating covariances values for resolved resonance parameters. Finally, practical applications, of interest for criticality safety calculations, illustrate the impact of different assumptions on correlations among resolved resonance parameters.

Introduction

Resonance data play a significant role in the calculations of systems considered for criticality safety applications. K_{eff} , the major parameter of interest in such a type of calculations, can be heavily dependent both on the quality of the resonance data as well as on the accuracy achieved in the processing of these data. The reactor physicist is faced by a twofold problem, namely, to correctly process the basic nuclear parameters in order to produce multigroup cross sections, and to assess the effects of the uncertainties that affect these basic data.

The information on different types of cross sections, resonance parameters and other quantities of interest in the ENDF (Evaluated Nuclear Data File, Ref. 1) is based on the analysis of a variety of measurements as well as on applicable nuclear models. Since the discrepancies between different measurements can be significant and the nuclear models employed are far from being perfect, an interest in covariance information in the ENDF system has developed in recent years.

It is a fact that the covariance information in the present nuclear data is poor and is not adequate for a variety of its applications. The covariance information in the recent evaluations, such as ENDF/B-V, ENDF/B-VI, JENDL3.2, BROND2.2, and JEF2.2, is either not complete or is absent for a big variety of materials. The only rigorous way to provide that information is to perform a new evaluation incorporating covariance methodology. The construction of covariance information finds its origins at the experimental analysis stage. An experimenter is obliged to provide the most complete information possible on error components related to a particular experiment. Having that information, an evaluator can estimate the degree of “uncertainty” to be assigned to this measurement and others as well in order to provide that information to the users in the form of covariance files in ENDF/B format.

A number of reasons can be advanced to support the notion that uncertainty information is often crucial in nuclear data applications. These reasons are as diversified as the variety of nuclear data uses. Nevertheless, in nuclear technology fields, one is mostly interested in the impact of the initial data uncertainties on the key parameters such as safety coefficients of reactors. Using this fact as a base, one derives that not all-possible information that one can obtain and store as to the uncertainties of nuclear data might be necessary. Instead, one should bare in mind the eventual impact that one specific type of information can produce on the quantities of interest. This is to say that even in situations where information on the uncertainties is not available, this information might be irrelevant or might be estimated with a simpler procedure than a new evaluation.

If reasonable uncertainty values are available, in conjunction with their correlation in energy and among type of resonance parameters, one can exploit existing methodologies, based on perturbation theory, in order to evaluate their impact on the integral parameter of interest, i.e., K_{eff} in our case, in practical applications. In this way, one could be able to judge if the uncertainty on specific quantities, e.g., covariances on resonance data, have a significant impact and therefore deserve a careful evaluation.

This report, first, will recall the basic principles that lie behind an uncertainty evaluation and review the current situation in the field of covariance data. Then an attempt will be made for defining a methodology that allows calculating covariances values for resolved resonance parameters. Finally, practical applications, of interest for criticality safety calculations, will

illustrate the impact of different assumptions on correlations among resolved resonance parameters.

1.0 Uncertainty Methodology

The principles of uncertainty analysis and its applications to the fission reactor field are well documented (see, e.g., Ref. 2). We will simply recall here that we can represent a generic integral reactor parameter Q (such as K_{eff}) as a function of cross-sections:

$$Q = f(\sigma_1, \sigma_2, \dots, \sigma_J), \quad (1)$$

where $\sigma_1, \sigma_2 \dots \sigma_J$ represent cross sections by isotope, reaction type and energy range (or energy group, in a multi-group representation). The uncertainties associated to the cross section can be represented in the form of variance-covariance matrix:

$$C_\sigma = \begin{pmatrix} c_{11} & c_{12} & \dots & c_{1J} \\ c_{12} & c_{22} & \dots & c_{2J} \\ \dots & \dots & \dots & \dots \\ c_{1J} & c_{2J} & \dots & c_{JJ} \end{pmatrix}, \quad (2)$$

where the elements c_{ij} represent the expected values related to the parameters σ_j , and σ_i .

The variations of the integral parameter Q due to variations of σ can be expressed using perturbation theories (Ref. 3), to evaluate sensitivity coefficients S :

$$\delta Q/Q = \sum_j S_j \frac{\delta \sigma_j}{\sigma_j}, \quad (3)$$

where the sensitivity coefficients S_j are formally given by:

$$S_j = \frac{\partial Q}{\partial \sigma_j} \cdot \frac{\sigma_j}{Q}. \quad (4)$$

The variance of Q can then be obtained as:

$$\text{var}(Q) = \sum_{j,i} S_j S_i c_{ij}. \quad (5)$$

To exploit Eq. (5), one needs to obtain explicitly the S_j coefficients and to establish an appropriate variance-covariance matrix. In our particular case, we are interested in the K_{eff}

parameter so that the classical perturbation theory can be used for the calculation of the sensitivity coefficients. First, we consider the Boltzmann equations for the real Φ and adjoint Φ^* flux:

$$A\Phi = F\Phi / K_{\text{eff}}, \quad (6)$$

$$A^* \Phi^* = F^* \Phi^* / K_{\text{eff}}, \quad (7)$$

where A is the Boltzmann operator, F is the production operator, and K_{eff} is the multiplication factor of the system. Then, the sensitivity coefficients S for K_{eff} can be calculated as:

$$S = \frac{\sigma}{K_{\text{eff}}} \frac{dK_{\text{eff}}}{d\sigma} = \left\langle \Phi^*, \left(\frac{\partial A}{\partial \sigma} - \frac{\partial F}{\partial \sigma} \right) \Phi \right\rangle / I_f, \quad (8)$$

where $I_f = \langle \Phi^*, F\Phi \rangle$ is the normalization integral of the system, and ∂A and ∂F are the variations induced by the cross section uncertainties on the Boltzmann and production operators.

2.0 Covariance Evaluation

2.1 General Algebra of Covariances

We discuss here general features of methods used for the construction of a covariance matrix. The reader is referred to Ref. 4 for more detailed discussions.

A covariance matrix \mathbf{V}_X represents error information for all possible pairs of components X_i and X_j of a vector \mathbf{X} of dimension n . It is derived from a multivariate probability distribution function $p(\mathbf{X})$ as follows:

$$(\mathbf{V}_X)_{ij} = \text{cov}(X_i, X_j) = \langle \delta X_i \delta X_j \rangle = \langle X_i X_j \rangle - \langle X_i \rangle \langle X_j \rangle, \quad (9)$$

where $\delta X_i = X_i - \langle X_i \rangle$ and the symbol $\langle \rangle$ means that an average is to be taken with respect to $p(\mathbf{X})$. It is clear that if $i=j$, then the element $(\mathbf{V}_X)_{ii}$ simply reflects a variance (standard deviation squared) for the quantity $X_{i(j)}$.

Such quantities are commonly used to describe the propagation of errors through the well-known linear *Law of Error Propagation* (LEP). Let us consider a vector $\mathbf{Y}(\mathbf{X})$ of dimension m that is a function of the vector \mathbf{X} . This vector has components Y_k . Linear LEP suggests that \mathbf{Y} is a linear combination of all X_j . Nevertheless, the LEP approach can be generalized provided that the following conditions are satisfied: (a) \mathbf{Y} varies gradually over all the region of the most probable \mathbf{X} ; (b) the function $p(\mathbf{X})$ is localized in the vicinity of $\langle \mathbf{X} \rangle$, and (c) \mathbf{Y} is differentiable with respect to each X_j near $\langle \mathbf{X} \rangle$. In this case, \mathbf{Y} can be approximated by a first order Taylor series in the vicinity of $\langle \mathbf{X} \rangle$ as follows:

$$Y_k = Y_k(\langle X \rangle) + \sum_{j=1}^n \left(\frac{\partial Y_k}{\partial X_j} \right)_{X=\langle X \rangle} \delta X_j. \quad (10)$$

Introducing the notation $t_{jk} = (\partial Y_k / \partial X_j)_{X=\langle X \rangle}$ and $\langle Y_k \rangle \approx Y_k(\langle X \rangle)$ we obtain:

$$Y_k = \langle Y_k \rangle + \sum_{j=1}^n t_{jk} \delta X_j, \quad (11)$$

$$\delta Y_k = Y_k - \langle Y_k \rangle = \sum_{j=1}^n t_{jk} \delta X_j. \quad (12)$$

The matrix \mathbf{T} , whose components are t_{jk} , is called the sensitivity matrix. In terms of this matrix we can rewrite the preceding formula in its matrix form:

$$\delta Y = \mathbf{T}^+ \delta X, \quad (13)$$

where sign ‘+’ stands for transposition.

From the several preceding formulas it is then easily seen that:

$$\text{cov}(Y_k, Y_l) = \sum_{i=1}^n \sum_{j=1}^n t_{ik} t_{jl} \text{cov}(X_i, X_j). \quad (14)$$

The last expression makes a connection between the $m \times m$ covariance matrix \mathbf{V}_Y for \mathbf{Y} (with components $\langle \delta Y_k \delta Y_l \rangle$), and the $n \times n$ covariance matrix \mathbf{V}_X for \mathbf{X} (with components as defined in (9)) through the matrix \mathbf{T} :

$$\mathbf{V}_Y = \mathbf{T}^+ \mathbf{V}_X \mathbf{T}. \quad (15)$$

Sometimes one defines a so-called relative covariance matrix \mathbf{R} , introducing a correlation matrix \mathbf{C} , and fractional errors f_i and f_j of the quantities X_i and X_j :

$$R_{ij} = \frac{V_{ij}}{X_i X_j} = C_{ij} f_i f_j, \quad (16)$$

For convenience we drop the subscript ‘‘X’’ for \mathbf{R} , \mathbf{C} , and \mathbf{f} .

2.2 Experimental Statistical and Systematic Errors and Their Covariances

In a typical experiment there exist two types of errors: statistical and systematic. Distinguishing between these two types is somehow arbitrary. The statistical errors are generally related to the finite number of counts in the detector. If one could reach the limit of ‘infinite’ counts, this type of errors would be eliminated. The systematic errors are related to a particular way the experiment was conducted. Their components are the presence of background, calibration of detectors, etc. Therefore, in general one can write for the error of any measured quantity Y^j :

$$\delta Y^j = \delta Y_{st}^j + \delta Y_{sys}^j,$$

where δY_{sys}^j is statistical error component and δY_{sys} is systematic error component. δY_{sys} is the same for the whole data set, therefore, it does not carry an index. Since the statistical and systematic errors are uncorrelated $\langle \delta Y_{\text{st}}^j \delta Y_{\text{sys}} \rangle = 0$, and one easily obtains the expression for the covariance of the quantity Y:

$$\langle \delta Y^i \delta Y^j \rangle = \langle (\delta Y_{\text{st}})^2 \rangle \delta_{ij} + \langle (\delta Y_{\text{sys}})^2 \rangle.$$

It is seen that if the systematic error is zero, then the resulting covariance matrix would be diagonal. Thus, it is clear that it is the systematic error that introduces nondiagonal elements into the covariance matrix.

An experimenter usually corrects his data to account for background and calibration of the detector. This also applies to errors of measured quantities. By doing so, the data that initially depended only on recorded count rate C^j , become dependent on introduced correction procedures c_m : $\delta Y = \delta Y(c_m, C)$. This transforms the covariance matrix into:

$$\langle \delta Y^j \delta Y^k \rangle \cong \left(\frac{\partial Y^j}{\partial C^j} \right)^2 (\delta C^j)^2 \delta_{jk} + \sum_m \frac{\partial Y^j}{\partial c_m} (\delta c_m)^2 \frac{\partial Y^k}{\partial c_m}.$$

From the last formula, it is seen that an experimenter needs to report the variances and sensitivity coefficient expressed by the derivatives of the measured quantity.

Strictly speaking, a measurement of any physical quantity is nothing but determining a particular value of this quantity associated with its probability distribution function. In other words, what is measured is one or several possible outcomes of a trial (measurement) governed by a distribution of possible outcomes. In this respect, to report the most complete information one needs to provide the value of the measured quantity together with its probability distribution function. Clearly, such a way to record the information would not be very compact. One solution is to give not only the conventional two first moments of the distribution function (mean value and variance), but also higher moments of the probability distribution. This will allow for an evaluator to calculate/estimate the associated probability distribution in order to judge how reliable measured data are. For example, in case of lognormal distribution, the knowledge of higher moments assures not only the knowledge of the general shape of distribution, but also the knowledge of its skewness and kurtosis (third and fourth moments).

3.0 Covariance Information in the Current ENDF/B Format

From the simple mathematical background given in the previous sections, it is easily seen that there may exist several equivalent covariance representations for its storage and eventual applications. There are three interrelated quantities: the covariance matrix, correlation matrix, and actual uncertainties. For the proper storage of the information, two of these quantities must be recorded in the ENDF. For the user's convenience, the most logical and comprehensive choice is to record the relative standard error together with the correlation coefficients. The reasons for that are very simple. It is easier for a user to grasp and compare relative errors and absolute correlations compared to the absolute standard error and covariance. The covariance in itself is not a very convenient quantity to operate with. For a given error and correlation value, it is easy to comprehend what impact such ensemble has on the certainty of the data. For a given

covariance and absolute uncertainty on the quantity itself, one has to operate with the formulas in the previous section before getting a useful insight in the information obtained (Ref.5).

Despite these facts, the ENDF records the covariance information only by using either absolute or relative variances together with covariances. In the following ‘covariances’ mean the ENDF way to record the known information on the data uncertainties unless specified otherwise. Covariance information in ENDF/B format can be found in the files MF=31, 32, 33, 34, 35 and 40. Each of these files contains different type of information. The file MF=31 contains the covariances for the prompt, delayed and total number of neutrons per fission ν . The file MF=32 is used to provide the covariances for the resonance parameters. Finally, file MF=33 is reserved for the covariances for the cross sections of different reaction types. Within each MF, the covariances for different types of quantities are identified by MT numbers that represent subsections in the covariance portion of the evaluation. For example, the different MT numbers within files MF=32 and 33 provide covariances for different type of reactions; the different MT numbers within file the MF=31 differentiate between different ν types as described above. For the MF=33, “cross” covariances, i.e., covariances for different types of reactions or different isotopes may also be provided. Cross covariance information for different isotopes is important in the case where cross sections were deduced from the analysis of ratios of different cross sections. The fission cross section of ^{238}U is an example. The file MF=34 contains the angular distributions of secondary particles. The file MF=35 contains the energy distributions of secondary particles. The file MF=40 contains the production of radioactive nuclei.

ENDF gives a choice in recording the covariance information in direct and indirect ways. For this purpose, different flags NC and NI are assigned to specify the way to extract information from ENDF (Ref. 1). The NC and NI options represent the sub-subsections of an ENDF file. One uses NI option when the statistically independent sources of uncertainty for a given reaction pair need to be stored. Statistical independence imposes that one has to sum over all NI sub-subsections to obtain the required covariance for a pair of quantities. Every NI subsection can contain one or two energy grids, some constants and the parameter LB. This parameter imposes a processing code to use some specified sequence in order to reconstruct covariance for a particular quantity. One can find more technical details of the ENDF format in the manual of the module ERRORR of the code NJOY (Ref. 6).

On the other hand, when using NC, the covariances are described indirectly using different values of the flag LTY. These NC sub-subsections are useful when one desires to calculate the covariances based on the information given for the ratio of requested to some other (different or reference) quantity. The flag LTY describes three such situations and defines the way for a processing code (like NJOY) to extract the information and deliver the final covariances to the end users.

A lot of discussions in the international nuclear data community are dedicated to the choice of the most clear and appropriate format for the covariance information in ENDF. The nuclear data community tends now to agree that the most comprehensive and user-friendly format is NI-type format with an appropriate LB flag. If one is to keep the existing options for coding covariances in ENDF files, the most convenient form, in our opinion, is LB=5. This coding corresponds to the formulae [Eq. (16)]. Different factors in this formula need to be addressed in order to carry out the covariance generation process.

4.0 Current Status and Necessities in Nuclear Applications Community

The interest to covariance information in the nuclear applications community has risen in the past few years. The most obvious and conclusive reason for this rise of interest is the enormous effort that one dedicates nowadays to the assessment of safety of nuclear installations. Using the nuclear data with their uncertainties as a starting point, one strongly desires to know the degree of confidence that should be attributed to the theoretical and numerical treatment of different tasks in nuclear applications. A nuclear scientist who uses the nuclear data files for his applications should bare in mind the necessity to propagate the nuclear data errors through his calculations as rigorously as possible in order to arrive at understanding of uncertainties on his final product.

It is clear that the correct and most comprehensive covariance information can only be obtained by collecting all possible experimental data and analyzing them with the most accurate theoretical models. The task of an experimentalist is to provide precise and complete information, surely to the possible extent, on the uncertainties of quantities measured along with sensitivity coefficients of possible sources of those uncertainties. In fact, the experimenter should try to separate as much as possible the correlated sources of uncertainties to arrive at uncertainties with correlation coefficients zero. For an evaluator, it is always better to have larger number of uncorrelated sources of uncertainties than have to incorporate the correlation information into the evaluated files. A supplementary way to deduce or better say, refine, the covariance information is to use the results of integral experiments (such as, for example, the measurements of K_{eff}) to verify, and possibly to correct the covariance information on the initial nuclear data. Our point of view is that this method definitely can prove useful in a number of situations; nevertheless it does not represent a correct and comprehensive approach in refining the covariance information.

Unfortunately, the covariance information in the current ENDF files is poorly represented. It does not cover all the reactions and isotopes which are of interest to the nuclear application community. In the light of what has been said above and taking into account the degradation of funding in the area of nuclear evaluation, the first priority for the ENDF evaluation is to incorporate at least the uncertainty quantities for the variety of reactions and isotopes as needed. In measurements, it is much more straightforward and comprehensive to attribute errors to a quantity than to assess the correlation coefficients.

As we mentioned above, the fully correct and comprehensive way to produce covariance information is to collect and analyze all available measurements. The existing theoretical models should be used to produce the best fit possible to the experimental data through, for example, the generalized least square method. Along with following this path, some techniques were developed to detect inconsistent nuclear data sets to eventually correct/eliminate them from the analysis (Ref. 7). Nevertheless, in current situation of poor funding for nuclear data activities, a number of attempts were made to construct covariance data without thorough examination of the experimental results. Although, this is not a most comprehensive approach, it does display its utility in certain applications such as nuclear criticality safety. In this case, one is interested in assessing the influence of the initial (nuclear) data uncertainties on the criticality of new systems/configurations. To study methods/tools to be applied to a new system, one uses the set of benchmarks for known, analyzed, and validated critical experiments. These cover a certain region of applications differentiating from each other by, for example, composition, geometry

or/and energy spectra. A number of approaches were developed to estimate the ‘degree of similarity’ for a new system in question versus a set of well-established benchmark calculations (Ref. 8). These include generalized linear-least-square methodology, uncertainty analysis techniques, and sensitivity coefficients methods. The final objective of these approaches is to deduce whether the existing set of nuclear data and calculation tools can be used for a new system that one wants to study. In such instances, one might not need a very well-established set of uncertainties/correlation data (although this would be preferred).

In such cases, a reasonable estimation of uncertainties and correlations could be proposed. For example, Argonne National Laboratory was requested to develop such an approach for the criticality safety community. Reference 9 deals with establishing covariances based on comparison of deviations between different existing evaluations for creating uncertainties and estimation of correlation coefficients based on the physics of the system in question. To do so, the cross sections processed into energy groups were intercompared for all existing evaluations (ENDF/B-V, ENDF/B-VI, JENDL, BROND and JEFF). Another example is the prior absence of covariance information in JENDL which forced the evaluators to create covariances that are not fully based on the analysis of all experimental results, but on the combination of ‘expert judgment’ with the errors coming from the nuclear models themselves (Ref. 10). For instance, in the resolved resonance energy range, this approach uses one (a priori the best) set of experimental data to assess uncertainties in the parameters of nuclear models used in evaluation. These are assessed once again by simply calculating the deviation between experimental points and calculations. The resulting differences were attributed to the ‘uncertainties on nuclear model parameters’, therefore, an evaluator can propagate these uncertainties through the nuclear models calculations to finally obtain covariance on desired quantity (cross section, resonance parameters, etc.)

It is difficult to say a priori what impact a quantity’s uncertainty will have on the variance of the final and desired result. The following example illustrates a situation where to create covariances, one might consider using methods not at all or only partially based on the analysis of experimental data. Consider a simple linear dependence of a calculated quantity Y on the measured quantity X : $Y = a \times X$. The Law of Error Propagation (LEP) in this case is simply expressed by the Taylor series development: $\Delta Y = a \Delta X$. Now, if $a \ll 1$, then even if the uncertainty in measured quantity X might be very large, its impact on the uncertainty in calculated quantity Y becomes very small. This is to say that even in situations where information on the uncertainties is not available, this information might be irrelevant or might be estimated with simpler procedures than a new evaluation. On the other hand, if $a \gg 1$, one falls into the situation of so-called error amplification. In this situation, it is extremely important to improve the knowledge of the covariances on the initial nuclear data.

4.1 Filling in the Absent Information on Covariances

To fulfill the blanks in the existing covariance information, several points should be considered. The first is to identify crucial and missing information on covariances. It is easy to deal with ‘missing’ part, but determining the crucial information for applications is a more complicated matter. To identify the importance of missing information, one must consider either all possible applications of the covariance in question or a particular set of applications one is interested in. It is time consuming and unnecessary to consider all possibilities for the covariance

applications. If this needs to be done, it is much more logical and coherent to remake the evaluations which will include the complete covariance information. In the case of a set of particular applications, one might be satisfied with estimated/simplified approaches to create covariance information as discussed above. Nevertheless, in such a situation, one still needs to consider how important this covariance information is for this particular set of applications by examining the range of these applications and the methods/tools used for their analysis. Furthermore, as to the availability of the reported experimental uncertainties/correlations, one should look for a reason why this information is missing. The reason might be threefold: (a) the information on covariances is created and exists, but not properly used/processed; (b) the information is missing with a large support from the nuclear data measurements results, and (c) the information is missing and there is a poor experimental base for its creation. The last reason clearly appeals to an estimation of covariances that might not be fully based on the analysis of experiments. Although, at this point, we need to understand what is the best way to generate missing information: through the regular and rigorous evaluation procedure or by estimation. If the last option is in order, we must propose the estimation methods, examples of which are discussed in the previous section. Finally, once all the steps are completed, one should estimate the impact of obtained covariance for the chosen set of applications and define the domain and restrictions on applicability/use of proposed methodologies.

4.2 Current Status of Covariance Information in the Resonance Range

Determining covariances (uncertainties plus correlation coefficients) in smooth cross section energy ranges, i.e., thermal and fast, is straightforward. The measurement uncertainties reported by experimentalists are used in the fitting procedures to obtain uncertainties on cross sections. The final uncertainties are recorded in ENDF files as described in previous sections. A number of tools exist to process this information and deliver it to the applications.

In the resonance domain, the situation is not that simple. In this case, one a priori needs to record the uncertainties of the widths of individual resonances and corresponding short- and long-range correlations between resonances. The code SAMMY (Ref. 11) for the experimental analysis includes the capability to create covariance files for the resonance range.

The nature of final uncertainties produced by SAMMY depends on the manner to introduce input data into the code. In principle, the code uses the experimental data with corresponding uncertainties as input parameters. This assumes that the experimental data are free of experimental errors (such as the normalization and background correction parameters, self-shielding corrections, etc.) with exception of statistical ones. Therefore, in this case, the uncertainty matrix of input data is a priori diagonal (represented by the experimental transmission points along with their uncertainties). At the level of small groups of resonance, the short-range correlations (correlations between different types of widths and/or resonances) can be relatively easily assessed. These correlations are due to the methods of calculation used in SAMMY. The information on covariances of group cross sections deduced in this manner will not contain the long-range correlation since these correlations essentially depend on the systematic errors mentioned above.

In order to get an insight into the long-range correlations between different resonances, some of experimental errors mentioned above (Ref. 12) (for example, the normalization and background correction parameters) are forced to serve as input data for SAMMY and are allowed

to vary during the fitting procedure. As a result, the final, fitted resonance parameters can be calculated along with the correlations between these resonance parameters and normalization and background correction parameters. According to Ref. 12, the covariance information on resonance parameters from ORNL is available for Gd, Al and Si.

As described briefly above, current JENDL evaluations also contain the information on resonance parameters based on the uncertainties of nuclear models parameters. These are already present in the JENDL files and it should be possible to process them with the code NJOY. As reported in Ref. 10 the covariance file are available for Li, C, O, Na, Ti, Fe, ^{233}U , ^{235}U , ^{238}U , ^{239}Pu , ^{240}Pu , and ^{241}Pu .

5.0 Assessment of Covariance on Group Cross Sections

To judge how crucial the covariance information in the resonance domain is or could be in a variety of criticality safety applications, one can perform a relatively simple sensitivity study. A set of covariances for resonance cross sections should be used in a certain representative criticality calculation. Given the absence of resonance parameters covariances in the ENDF, one might use the covariances calculated without the involvement of the experimental data analysis. In this section, we present an approximate methodology to construct covariance matrix for the group cross sections based on uncertainties and correlations of resonance parameters. This methodology is ad-hoc and is not based on the analysis of experimental data, but instead on several physical assumptions. Development of this methodology will serve us to evaluate the importance of covariances on resonance parameters in nuclear applications. This evaluation is performed for two well-established benchmark examples described in the following sections.

In nuclear applications, one operates with cross sections processed into a certain energy group structure. These groups are defined in a way that, for a particular reaction x and group G , the reaction rate within this group is conserved, i.e.,

$$\sigma_x^G \phi_G = \int_{E_G}^{E_{G+1}} \sigma_x(E) \phi(E) dE \quad \text{with} \quad \phi_G = \int_{E_G}^{E_{G+1}} \phi(E) dE. \quad (17)$$

The flux $\phi(E)$ is not known a priori, and thus group cross sections (group constants) can be estimated only either by iterations or by using a certain flux shape that approximates well the flux in a particular system under study.

Generally, the cross sections $\sigma_x(E, \bar{p})$ depend not only on energy E but also on the number of parameters \bar{p} such as resonance parameters and nuclear models parameters. In this study, we will focus on the influence of the resonance parameters covariances on the group cross sections covariances, therefore, we consider only resonance parameters dependence in \bar{p} . In this case, the group cross section variations are expressed as follows:

$$\delta \sigma_x^G = \sum_i \frac{\partial \sigma_x^G}{\partial p_i} \delta p_i. \quad (18)$$

It is numerically difficult to deal with such a large number of parameters (for example, ^{235}U has about 3000 resolved resonances). Therefore, we propose here to group resonance

parameters in packages, based on the physical assumptions that we will discuss later. In other words, we rewrite the previous expression as:

$$\delta\sigma_x^G = \sum_g \sum_{i \in g} \frac{\partial\sigma_x^G}{\partial p_i} \delta p_i^g, \quad (19)$$

where p_i^g is a set or resonance parameters that belong to the package g , $i \in g$. Now, one can construct the covariance matrix for the group cross sections:

$$\langle \delta\sigma_x^G, \delta\sigma_x^{G'} \rangle = \sum_i \sum_j \frac{\partial\sigma_x^G}{\partial p_i} \frac{\partial\sigma_x^{G'}}{\partial p_j} \langle \delta p_i, \delta p_j \rangle = \sum_g \sum_{g'} \left(\sum_{i \in g} \frac{\partial\sigma_x^G}{\partial p_i^g} \sum_{j \in g'} \frac{\partial\sigma_x^{G'}}{\partial p_j^{g'}} \langle \delta p_i^g, \delta p_j^{g'} \rangle \right). \quad (20)$$

Now we make several assumptions about the packaging of resonances. First, we suppose that all resonances inside of each package are 100% correlated. Second, we assume that each resonance within a package contributes the same amount to the package cross section.

The first assumption means that within each package δp_i^g can be replaced by its ‘package value’ δp_g , i.e., the index i of individual resonances is dropped within the package. This quantity describes a simultaneous variation of the same kind of resonance parameters within a package. The resonance parameter covariance matrix will no longer depend on individual resonances, but on packages of resonances: $\langle \delta p_i^g, \delta p_j^{g'} \rangle \rightarrow \langle \delta p_g, \delta p_{g'} \rangle$.

The second assumption permits us to replace the sums of derivatives of the group cross sections with respect to individual resonance parameters by a derivative with respect to the package parameters:

$$\sum_{i \in g} \frac{\partial\sigma_x^G}{\partial p_i^g} \rightarrow \frac{\partial\sigma_x^G}{\partial p_g}.$$

If each resonance’s contribution is the same, then the sum of partial derivatives will be proportional to the derivative with respect to the simultaneous change of all parameters in the package. The proportionality constant is the inverse of the number of resonances in the package.

Under these assumptions, the expression for the group cross sections covariance matrix becomes:

$$\langle \delta\sigma_x^G, \delta\sigma_x^{G'} \rangle = \sum_g \sum_{g'} \frac{\partial\sigma_x^G}{\partial p_g} \frac{\partial\sigma_x^{G'}}{\partial p_{g'}} \langle \delta p_g, \delta p_{g'} \rangle. \quad (21)$$

The described packaging of resonances does not have to correspond to the group cross section structure, but should be chosen to satisfy the two assumptions discussed above. It is noteworthy that at the limit of small packages containing only one resonance, the resulting formula [Eq. (21)] is equivalent to the initial definition of the group covariance matrix [Eq. (20)].

It is now necessary to introduce a way to characterize the covariance matrix for the packages of resonance parameters $\langle \delta p_g, \delta p_{g'} \rangle$. This covariance matrix can be rewritten as follows:

$$\langle \delta p_G, \delta p_{G'} \rangle = \delta p_G \delta p_{G'} C_{p_G p_{G'}} ,$$

where $C_{p_G p_{G'}}$ is the correlation matrix for resonance parameters. To evaluate the upper and lower bounds of the impact that this covariance matrix produces on the group cross sections, it is necessary to consider limiting cases of full ($C=1$) and zero ($C=0$) correlations. It is also worthy to study intermediate situations. To begin with, we can assume that the correlations between the packages of resonance parameters are equal 0.5. However, a more elaborate approach can be proposed. This approach is the adaptation of the formalism proposed earlier in Ref. 9. In fact, the correlations C between two packages of resonance parameters g and g' will compose of two factors: long-range correlations L and short range correlations S . In other words, the correlation between two packages g and g' are given as a product of two factors:

$$C_{gg'} = L_{gg'} S_{gg'} . \quad (22)$$

The long-range correlations decrease as the distance in energy between quantities increases. This suggests an exponential behavior of such a correlation function. In order to illustrate this behavior, we write the long-range correlations in the following way:

$$L_{gg'} = 1 - \alpha \frac{|\bar{E}_g - \bar{E}_{g'}|}{\varepsilon} , \quad (23)$$

which is a first-order approximation of an exponential. In this expression, \bar{E}_g and $\bar{E}_{g'}$ are medium energies of groups g and g' , and ε is the total resonance energy range. The constant α is generally confined between 1 and 2. In this study, $\alpha=1.5$ is assumed. Note that this expression gives right limiting cases for close and remote resonance packages.

The short-range correlations are characterized by the similarity of errors of the package resonance parameters. It is given by:

$$S_{gg'} = \frac{\min(\Delta p_g, \Delta p_{g'})}{\max(\Delta p_g, \Delta p_{g'})} .$$

This expression accounts also for the sign of correlation between pairs of packages.

Numerically, the calculation of all components in Eq. (21) is straightforward. To illustrate the procedure, an example based on the resonance structure of ^{235}U was considered. A program was written to permit reading and modifying part of the ENDF tape relevant to the current study (MF=2, MT=151, resolved resonance parameters). This is done in order to calculate the derivatives in Eq. (21) taking the initial, unperturbed ENDF tape as a reference.

The sensitivity of the group cross sections to the resonance parameter uncertainties was first investigated using a 33-group structure shown Table 1. The code NJOY is used to process around 3000 resolved resonances of ^{235}U with Reich-Moore formalism. In this example, all neutron partial widths Γ_n were perturbed by +10% in the energy range 40 to 2000 eV (the energy range in 33-group structure that contains resonances). Figure 1 presents the relative variations of the group cross sections resulted from the perturbation of Γ_n . It is seen that the capture cross section is changed up to 9% by 10% change of Γ_n .

The hypothesis introduced earlier was also tested for resonances of ^{235}U isotope. The spacing between resonances of ^{235}U in the same energy range was first examined. Figure 2 represents the difference of the energies of neighboring resonances normalized to the total energy range considered (1 to 2300 eV). It is seen that the distance between resonances is relatively uniform, and its contribution to the whole resolved resonances energy range is less than fractions of a percent. Figures 3 and 4 show the ratio of partial widths to the sum of corresponding partial widths. It is seen from these figures that if the resolved resonances energy range is subdivided into a number of packages (let say 10), then from a statistical point of view, the contribution of each resonance to the group cross section does not exceed $\sim 10\%$ in a rough estimation.

Table 1. 33 Energy Group Structure

Group	Energy Boundaries (eV)	
	Upper	Lower
1	1.96400E+07	1.00000E+07
2	1.00000E+07	6.06500E+06
3	6.06500E+06	3.67800E+06
4	3.67800E+06	2.23130E+06
5	2.23130E+06	1.35300E+06
6	1.35300E+06	8.20800E+05
7	8.20800E+05	4.97870E+05
8	4.97870E+05	3.01900E+05
9	3.01900E+05	1.83100E+05
10	1.83100E+05	1.11090E+05
11	1.11090E+05	6.73700E+04
12	6.73700E+04	4.08600E+04
13	4.08600E+04	2.47880E+04
14	2.47880E+04	1.50300E+04
15	1.50300E+04	9.11800E+03
16	9.11800E+03	5.53080E+03
17	5.53080E+03	3.35400E+03
18	3.35400E+03	2.03400E+03
19	2.03400E+03	1.23410E+03
20	1.23410E+03	7.48500E+02
21	7.48500E+02	4.53900E+02
22	4.53900E+02	3.04320E+02
23	3.04320E+02	1.48600E+02
24	1.48600E+02	9.16600E+01
25	9.16600E+01	6.79040E+01
26	6.79040E+01	4.01600E+01
27	4.01600E+01	2.26000E+01
28	2.26000E+01	1.37090E+01
29	1.37090E+01	8.31500E+00
30	8.31500E+00	4.00000E+00
31	4.00000E+00	5.40000E-01
32	5.40000E-01	4.14000E-01
33	4.14000E-01	thermal

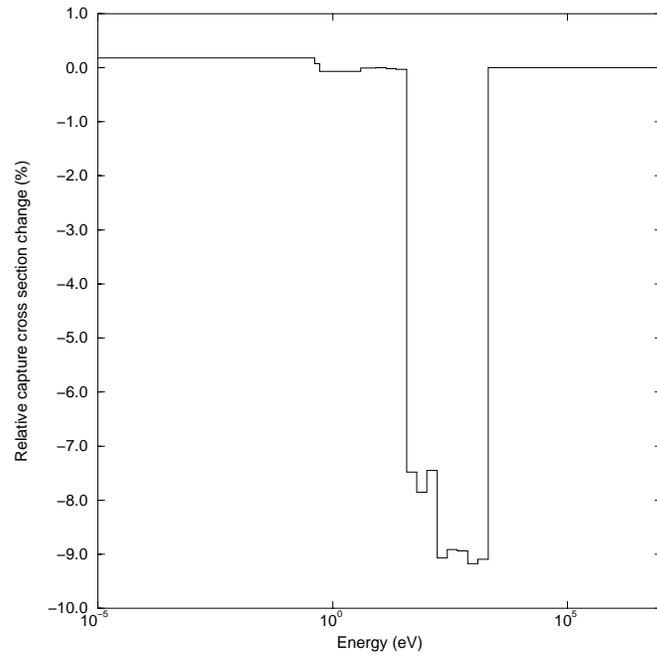


Fig. 1. Impact of the 10% Change in Neutron Width on the Capture Cross Section of ^{235}U

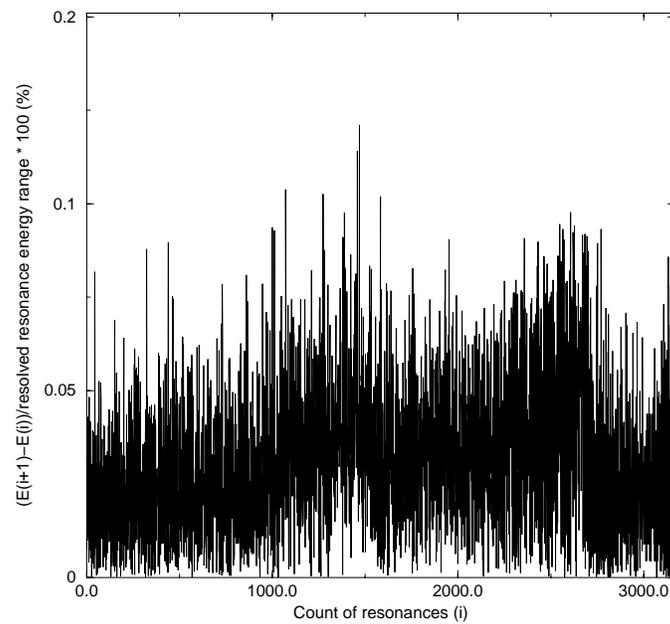


Fig. 2. Spacing of Capture Resonances for ^{235}U : the Difference between Neighboring Resonance Energies i and $i+1$ Divided by the Total Energy Interval

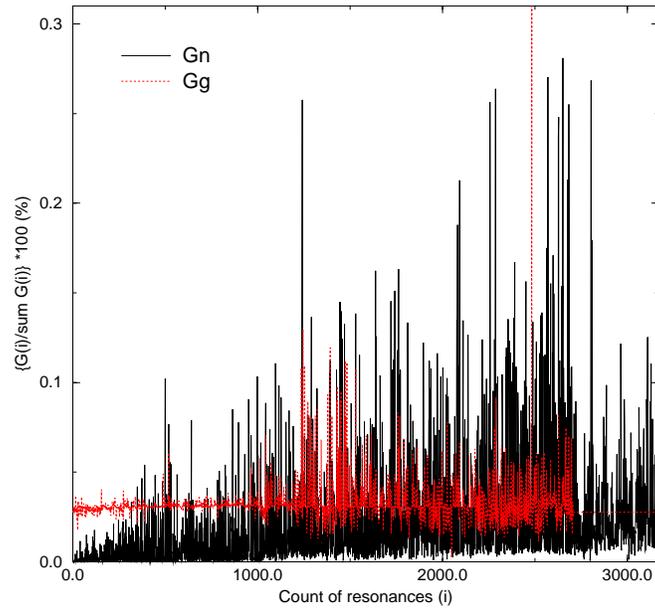


Fig. 3. The Ratio of the Radiative (G_n) and Neutron (G_g) Widths of ^{235}U Resonances (count i) to the Sum of Corresponding Widths Performed Over All Resonances

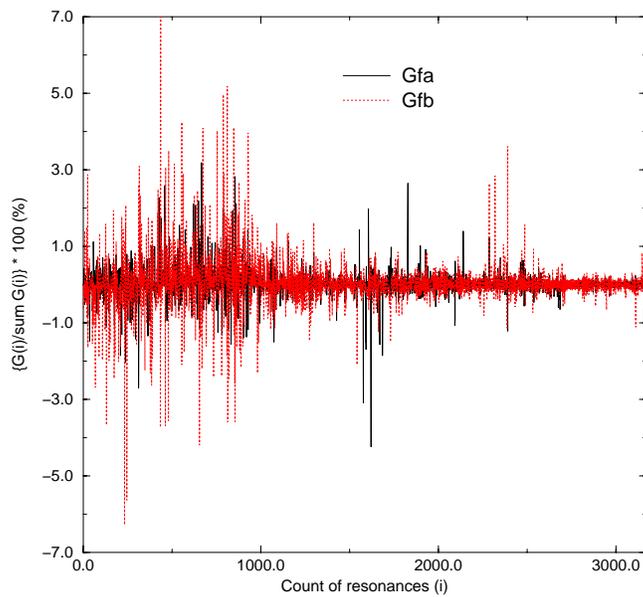


Fig. 4. The Ratio of the Fission Channel a (G_{fa}) and Fission Channel b (G_{fb}) Widths of ^{235}U Resonances (count i) to the Sum of Corresponding Widths Performed Over All Resonances

5.1 Calculation of Covariances

We describe here the procedure used to calculate covariances for the group cross sections with the formalism described in the previous section. This procedure consists of several steps described below. A program was written to accomplish these steps.

1. Packaging of resonances was chosen to correspond to the group structure: $g=G$. Thus, since all terms in the sum are zero except for those with $g=G$, one directly obtains:

$$\text{cov}(\sigma_x^G, \sigma_x^{G'}) = \langle \delta\sigma_x^G, \delta\sigma_x^{G'} \rangle = \frac{\partial\sigma_x^G}{\partial p_G} \frac{\partial\sigma_x^{G'}}{\partial p_{G'}} \langle \delta p_G, \delta p_{G'} \rangle.$$

2. Derivatives $\frac{\partial\sigma_x^G}{\partial p_G}$ are replaced with $\frac{\Delta\sigma_x^G}{\Delta p_G}$, $\Delta p_G = \text{frac} * \bar{p}_G$ with $\text{frac}=0.01\%$. This fractional

change was determined from the behavior of numerical derivatives: the value of the derivative seems to stabilize at $\text{frac}=0.01\%$. Also $\bar{p}_G = \sum_{i \in G} p_i / n_G$, n_G is the number of resonances in the

group G . The analysis includes the following: (1) a program reads an ENDF tape and changes all resonances parameters by an amount frac specified by the user in the specified energy range (corresponding to the packages of resonances); (2) a new, modified portion MF=2, MT=151 is created and then inserted into the initial ENDF tape; (3) the modified tape is processed; (4) the difference between group cross sections processed with unchanged ENDF tape and group cross sections processed with modified ENDF tape gives the $\Delta\sigma_x^G$.

3. The covariances for the resonance parameters are determined by:

$$\langle \delta p_G, \delta p_{G'} \rangle = \delta p_G \delta p_{G'} C_{p_G p_{G'}},$$

where δp_G are assumed to be 10% of \bar{p}_G .

4. The correlations between resonance parameters $C_{p_G p_{G'}}$ are calculated as described in the previous section: $C_{p_G p_{G'}} = 1 - 1.5 \left| \bar{E}_G - \bar{E}_{G'} \right| / \varepsilon$. In this expression $\bar{E}_G, \bar{E}_{G'}$ are medium energies of each group, ε is the total resonance energy range.

Finally, the relative covariance matrix therefore is:

$$\left\langle \frac{\delta\sigma_x^G}{\sigma_x^G}, \frac{\delta\sigma_x^{G'}}{\sigma_x^{G'}} \right\rangle = \left(\frac{1}{\sigma_x^G} \frac{\Delta\sigma_x^G}{\Delta p_G} \delta p_G \right) \left(\frac{1}{\sigma_x^{G'}} \frac{\Delta\sigma_x^{G'}}{\Delta p_{G'}} \delta p_{G'} \right) C_{p_G p_{G'}},$$

where $\left(\frac{1}{\sigma_x^G} \frac{\Delta\sigma_x^G}{\Delta p_G} \delta p_G \right)$ is the relative change of σ_x^G when p_G changes by δp_G .

5.2 Results for Covariance Matrix

The covariance matrices were calculated for the following cross sections: capture and fission cross sections of ^{235}U and elastic cross section of ^{56}Fe . These cross sections were calculated relative to the change of neutron resonance width Γ_n . Tables 2 through 5 summarize the results.

Relatively high correlations can be observed in most groups and for the three types of cross sections. This is largely due to selected formalism. The constant α in Eq. (23) was chosen to be 1.5. Reducing this constant will allow lowering the correlation coefficients. We also note, that Tables 3 through 5 only display correlations for groups with non-zero uncertainties (covariances).

Table 2. Group Cross Section Uncertainties $\left(\frac{1}{\sigma_x^G} \frac{\Delta\sigma_x^G}{\Delta p_G} \delta p_G \right)$

Group	²³⁵ U Capture	²³⁵ U Fission	⁵⁶ Fe Elastic
33	1.21E-02	0.00E+00	0.00E+00
32	0.00E+00	0.00E+00	0.00E+00
31	0.00E+00	5.03E-02	0.00E+00
30	1.10E-01	6.22E-02	0.00E+00
29	9.11E-02	9.21E-02	0.00E+00
28	1.20E-01	8.04E-02	0.00E+00
27	9.44E-02	9.72E-02	0.00E+00
26	1.20E-01	8.45E-02	0.00E+00
25	1.35E-01	1.14E-01	0.00E+00
24	5.63E-02	1.17E-01	0.00E+00
23	7.06E-02	7.60E-02	0.00E+00
22	8.78E-02	1.11E-01	0.00E+00
21	8.91E-02	5.14E-02	0.00E+00
20	8.37E-02	1.40E-01	0.00E+00
19	8.57E-02	8.92E-02	0.00E+00
18	3.59E-02	3.33E-02	0.00E+00
17	0.00E+00	0.00E+00	0.00E+00
16	0.00E+00	0.00E+00	0.00E+00
15	0.00E+00	0.00E+00	0.00E+00
14	0.00E+00	0.00E+00	0.00E+00
13	0.00E+00	0.00E+00	5.31E-02
12	0.00E+00	0.00E+00	0.00E+00
11	0.00E+00	0.00E+00	1.81E-02
10	0.00E+00	0.00E+00	2.60E-02
9	0.00E+00	0.00E+00	2.60E-02
8	0.00E+00	0.00E+00	2.56E-02
7	0.00E+00	0.00E+00	2.98E-02
6	0.00E+00	0.00E+00	0.00E+00
5	0.00E+00	0.00E+00	0.00E+00
4	0.00E+00	0.00E+00	0.00E+00
3	0.00E+00	0.00E+00	0.00E+00
2	0.00E+00	0.00E+00	0.00E+00
1	0.00E+00	0.00E+00	0.00E+00

Table 3. Correlations of Group Cross Sections for ^{235}U Capture

G\G'	33	30	29	28	27	26	25	24	23	22	21	20	19	18
33	1.000													
30	0.998	1.000												
29	0.996	0.998	1.000											
28	0.994	0.996	0.998	1.000										
27	0.990	0.992	0.994	0.996	1.000									
26	0.984	0.986	0.987	0.990	0.994	1.000								
25	0.973	0.975	0.977	0.979	0.983	0.989	1.000							
24	0.955	0.957	0.959	0.961	0.965	0.972	0.982	1.000						
23	0.926	0.928	0.930	0.932	0.936	0.943	0.953	0.971	1.000					
22	0.879	0.880	0.882	0.884	0.888	0.895	0.906	0.923	0.952	1.000				
21	0.800	0.802	0.803	0.806	0.810	0.816	0.827	0.844	0.873	0.921	1.000			
20	0.670	0.672	0.673	0.676	0.680	0.686	0.697	0.714	0.743	0.791	0.870	1.000		
19	0.456	0.458	0.459	0.462	0.465	0.472	0.483	0.500	0.529	0.577	0.656	0.786	1.000	
18	0.102	0.104	0.106	0.108	0.112	0.119	0.129	0.147	0.176	0.224	0.303	0.433	0.647	1.000

Table 4. Correlations of Group Cross Sections for ^{235}U Fission

G\G'	31	30	29	28	27	26	25	24	23	22	21	20	19	18
31	1.000													
30	0.999	1.000												
29	0.997	0.998	1.000											
28	0.995	0.996	0.998	1.000										
27	0.991	0.992	0.994	0.996	1.000									
26	0.984	0.986	0.987	0.990	0.994	1.000								
25	0.974	0.975	0.977	0.979	0.983	0.989	1.000							
24	0.956	0.957	0.959	0.961	0.965	0.972	0.982	1.000						
23	0.927	0.928	0.930	0.932	0.936	0.943	0.953	0.971	1.000					
22	0.879	0.880	0.882	0.884	0.888	0.895	0.906	0.923	0.952	1.000				
21	0.800	0.802	0.803	0.806	0.810	0.816	0.827	0.844	0.873	0.921	1.000			
20	0.670	0.672	0.673	0.676	0.680	0.686	0.697	0.714	0.743	0.791	0.870	1.000		
19	0.456	0.458	0.459	0.462	0.465	0.472	0.483	0.500	0.529	0.577	0.656	0.786	1.000	
18	0.103	0.104	0.106	0.108	0.112	0.119	0.129	0.147	0.176	0.224	0.303	0.433	0.647	1.000

Table 5. Correlations of Group Cross Sections for ^{56}Fe Elastic Scattering

G\G'	13	11	10	9	8	7
13	1.000					
11	0.934	1.000				
10	0.866	0.932	1.000			
9	0.755	0.821	0.889	1.000		
8	0.571	0.637	0.705	0.816	1.000	
7	0.268	0.334	0.401	0.513	0.697	1.000

6.0 Practical Applications

In order to illustrate the possible impact on quantities of interest for the criticality safety community, the resonance cross section correlations and uncertainties evaluated in the previous section were applied to the estimation of K_{eff} uncertainty. Specifically, two well-known problems were considered. The first one is representative of a fast spectrum system, even if the presence of a large quantity of iron in the core in addition to a stainless steel reflector contributes to soften the neutron energy spectrum. This is the case of the Uranium/Iron Benchmark Assembly. The second application is the ZEUS critical assembly. This is a system that has an intermediate neutron energy spectrum where one can expect a larger impact of uncertainty on resonance parameters.

The sensitivity coefficients for K_{eff} are calculated by solving Eqs. (6) and (7) in multigroup form using the BISTRO S_n code (Ref. 13), and then evaluating the sensitivity coefficients using the perturbation calculation modules of the ERANOS system (Ref. 14). The uncertainty modules of the ERANOS system are also used to calculate the final uncertainty by the means of Eq. (5).

In order to evaluate the bounds of the impact of covariances of the resonance parameters, three different hypotheses have been considered on the correlation among the multigroup variances: no correlation, full correlation, and the evaluated correlations that have been calculated in the previous section.

6.1 The Uranium/Iron Benchmark Assembly

This benchmark assembly (Ref. 15) consists of a ^{235}U (93% enriched)/iron cylinder reflected by stainless steel (see Fig. 5).

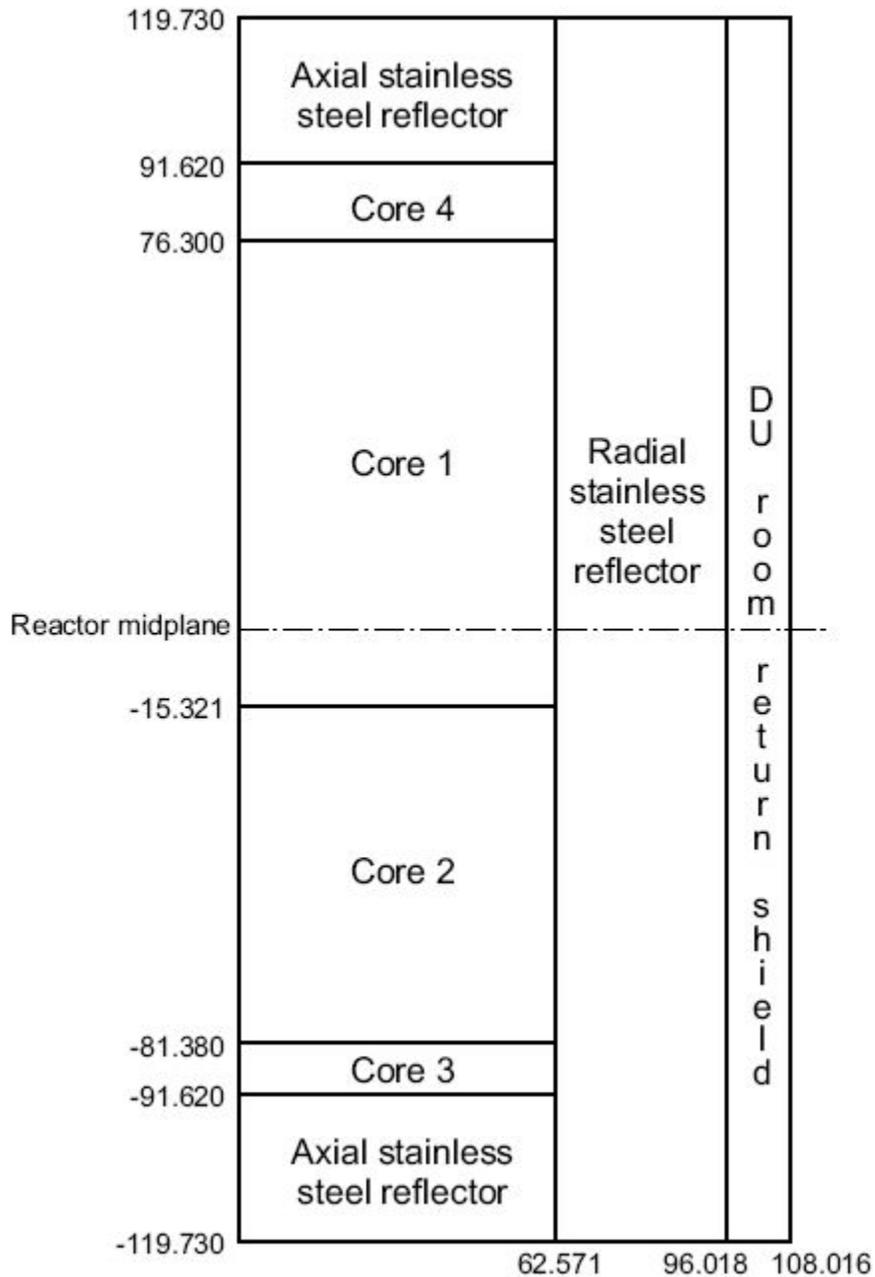


Fig. 5. Uranium/Iron Benchmark Geometry

Real and adjoint fluxes were calculated in the 33-group energy structure shown in Table 1 and S_8 approximation.

For the sake of simplicity, the four core regions were homogenized into one single composition. Cross sections were generated by the ECCO (Ref. 16) cell code with a JEF2.2 based library. The resulting core average flux spectrum is shown in Fig. 6.

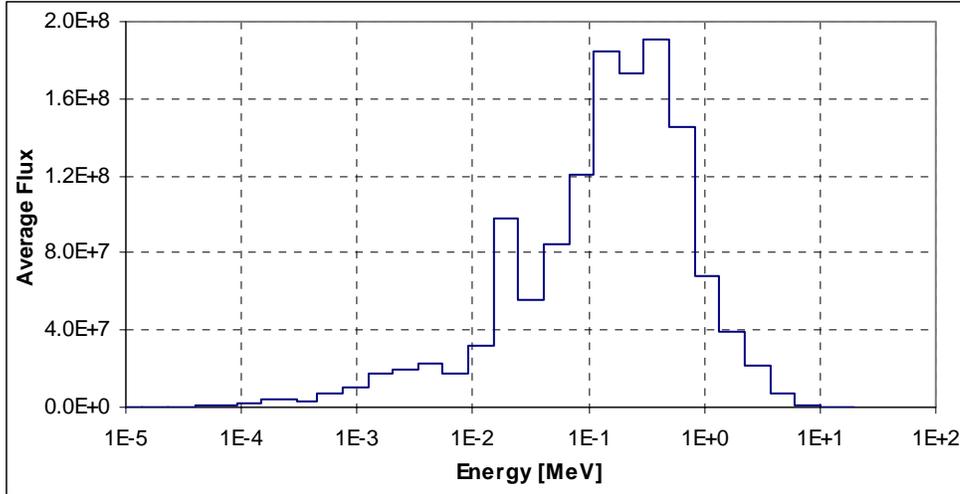


Fig. 6. Uranium/Iron Benchmark Core Averaged Flux Spectrum

As it can be observed, the spectrum is of the fast type. One can notice that the presence of a large amount of iron in the core composition in conjunction with the absence of a blanket region before the stainless steel reflector has the effect to shift non-negligible portion of the flux to the region of the resolved resonance of ^{235}U that starts around 2 KeV. Uncertainty results for the ^{235}U capture and fission, and the ^{56}Fe elastic cross section determined using the variances and covariances of Tables 2 through 5 are shown in Tables 6, 7, and 8. Only groups that give significant contribution to the total uncertainty are shown.

Table 6. K_{eff} Uncertainty of the Uranium/Iron Benchmark Assembly Due to ^{235}U Capture Uncertainties with Different Assumptions on Energy Group Correlation. Total is obtained by statistically combining individual values.

Group	No Correlation	Evaluated Correlation	Full Correlation
18	2.74E-04	8.70E-04	1.43E-03
19	8.33E-04	1.95E-03	2.40E-03
20	6.72E-04	1.91E-03	2.18E-03
21	5.94E-04	1.82E-03	2.06E-03
22	2.55E-04	1.22E-03	1.38E-03
23	4.54E-04	1.58E-03	1.82E-03
24	1.84E-04	1.02E-03	1.18E-03
25	1.73E-04	9.77E-04	1.15E-03
26	2.26E-04	1.11E-03	1.30E-03
27	1.03E-04	7.53E-04	8.90E-04
28	5.68E-05	5.59E-04	6.62E-04
29	3.88E-05	4.62E-04	5.47E-04
30	1.91E-05	3.24E-04	3.84E-04
Total	1.41E-03	4.46E-03	5.31E-03

Table 7. K_{eff} Uncertainty of the Uranium/Iron Benchmark Assembly Due to ^{235}U Fission Uncertainties with Different Assumptions on Energy Group Correlation. Total is obtained by statistically combining individual values.

Group	No Correlation	Evaluated Correlation	Full Correlation
18	5.48E-04	1.79E-03	2.89E-03
19	1.70E-03	4.02E-03	4.89E-03
20	2.08E-03	4.69E-03	5.33E-03
21	6.37E-04	2.74E-03	3.10E-03
22	6.19E-04	2.67E-03	3.06E-03
23	8.50E-04	3.05E-03	3.56E-03
24	5.31E-04	2.42E-03	2.84E-03
25	2.62E-04	1.70E-03	2.01E-03
26	2.71E-04	1.72E-03	2.05E-03
27	1.95E-04	1.46E-03	1.74E-03
28	7.11E-05	8.82E-04	1.06E-03
29	6.84E-05	8.65E-04	1.04E-03
30	1.96E-05	4.63E-04	5.55E-04
31	2.56E-05	5.29E-04	6.34E-04
Total	3.08E-03	9.01E-03	1.070E-02

Table 8. K_{eff} Uncertainty of the Uranium/Iron Benchmark Assembly Due to ^{56}Fe Uncertainties with Different Assumptions on Energy Group Correlation. Total is obtained by statistically combining individual values.

Group	No Correlation	Evaluated Correlation	Full Correlation
7	7.14E-04	1.60E-03	2.19E-03
8	7.80E-04	1.96E-03	2.28E-03
9	6.79E-04	1.90E-03	2.14E-03
10	8.76E-04	2.08E-03	2.40E-03
11	3.25E-04	1.30E-03	1.52E-03
13	3.46E-04	1.29E-03	1.57E-03
Total	1.60E-03	4.21E-03	5.01E-03

From Tables 6 through 8, it can be seen that correlations play quite a significant role. When full correlation among the groups is assumed, the total uncertainty can increase by more than a factor of 3 relative to the uncorrelated case. The K_{eff} uncertainties reported above are due uniquely to the +10% Γ_n widths variation of resolved resonances. It is also likely that one can expect similar results for other important resonance parameters. One concludes that in order to avoid additional uncertainty on criticality calculations, a relatively good accuracy is needed on resonance parameters.

As expected, the fission of ^{235}U contributes more to the K_{eff} uncertainty than the other reactions. It is interesting to note that the contribution of the ^{56}Fe elastic scattering uncertainties is comparable to that of the ^{235}U capture, and it is coming from the fast component of the spectrum. Finally, it is noted that the results for the case with evaluated correlations are very similar to the results for the case with full correlations. This is mainly due to the relatively high values of estimated correlations as described in Eq. (23). Although the expression in Eq. (23) is based on reasonable assumptions, it needs to be validated using experimental information.

6.2 The ZEUS Critical Assembly

The ZEUS assembly (Ref. 17 and Fig. 7) consists of a cylindrical core region containing interspersed plates of highly enriched uranium metal and graphite that are surrounded on all sides by a metallic copper reflector. As in the previous case, a simplified R-Z cylindrical geometry was adopted and real and adjoint fluxes were calculated. The corresponding averaged flux spectrum is shown in Fig. 8.

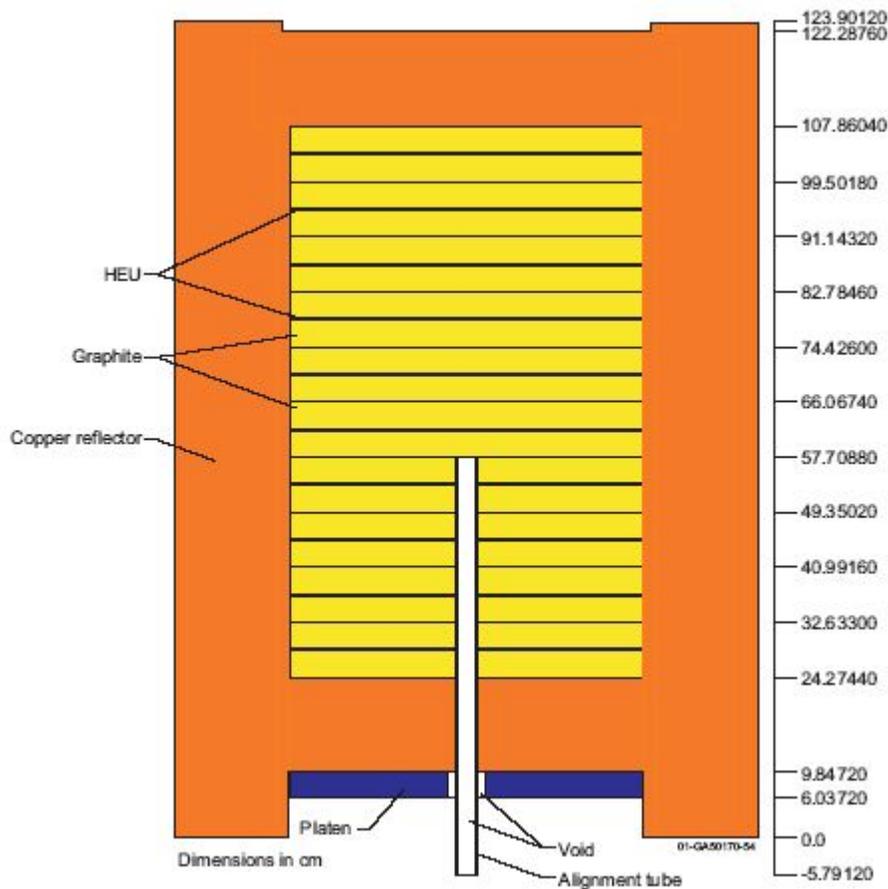


Fig. 7. Schematic View of the ZEUS Assembly

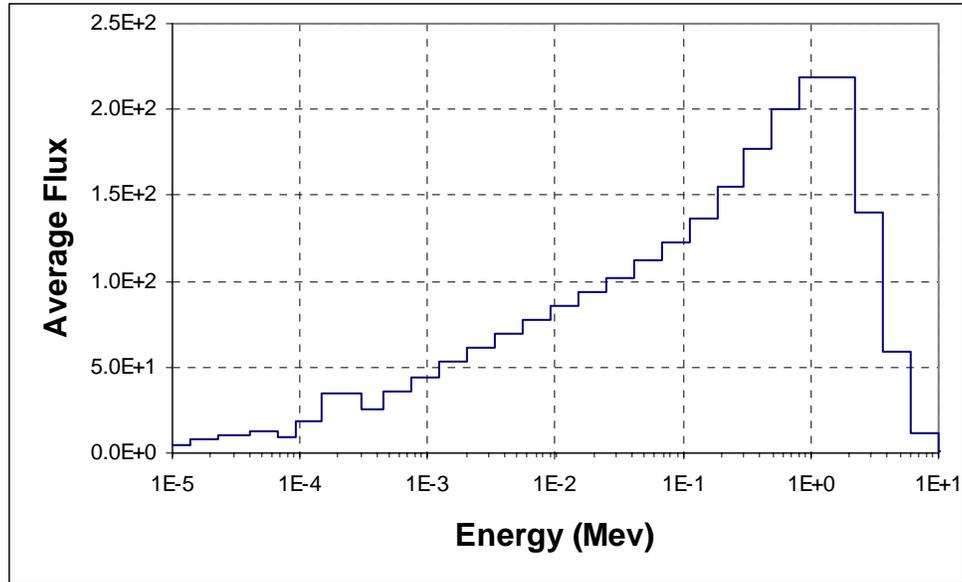


Fig. 8. ZEUS Assembly Core Averaged Flux Spectrum

As one can expect, due to the large amount of graphite in the core composition, there is a significant part of the spectrum in the intermediate region. Because, ^{12}C has no resonance structure in its data, the uncertainty evaluation was limited to the ^{235}U contribution. Results for the capture and fission cross sections are shown in Tables 9 and 10.

Table 9. K_{eff} Uncertainty of the ZEUS Assembly Due to ^{235}U Capture Uncertainties with Different Assumptions on Energy Group Correlation.

Total is obtained by statistically combining individual values.

Group	No Correlation	Evaluated Correlation	Full Correlation
18	3.42E-04	1.33E-03	2.60E-03
19	1.09E-03	3.47E-03	4.55E-03
20	1.18E-03	4.07E-03	4.72E-03
21	1.02E-03	3.98E-03	4.42E-03
22	7.27E-04	3.43E-03	3.75E-03
23	9.16E-04	3.84E-03	4.19E-03
24	5.76E-04	3.08E-03	3.35E-03
25	6.47E-04	3.25E-03	3.55E-03
26	1.02E-03	4.03E-03	4.42E-03
27	7.48E-04	3.47E-03	3.80E-03
28	7.16E-04	3.39E-03	3.73E-03
29	5.60E-04	3.01E-03	3.31E-03
30	4.80E-04	2.79E-03	3.07E-03
33	2.66E-05	6.66E-04	7.31E-04
Total	2.92E-03	1.223E-02	1.392E-02

Table 10. K_{eff} Uncertainty of the ZEUS Assembly Due to ^{235}U Fission Uncertainties with Different Assumptions on Energy Group Correlation.
Total is obtained by statistically combining individual values.

Group	No Correlation	Evaluated Correlation	Full Correlation
18	6.57E-04	2.46E-03	4.58E-03
19	1.84E-03	5.85E-03	7.52E-03
20	3.03E-03	8.22E-03	9.46E-03
21	1.14E-03	5.39E-03	5.98E-03
22	1.61E-03	6.41E-03	7.06E-03
23	1.81E-03	6.76E-03	7.45E-03
24	1.59E-03	6.34E-03	7.02E-03
25	9.46E-04	4.93E-03	5.47E-03
26	1.04E-03	5.14E-03	5.73E-03
27	1.04E-03	5.12E-03	5.72E-03
28	5.03E-04	3.59E-03	4.01E-03
29	5.95E-04	3.89E-03	4.36E-03
30	1.87E-04	2.20E-03	2.46E-03
31	2.86E-04	2.71E-03	3.04E-03
Total	5.15E-03	1.951E-02	2.243E-02

Results confirm the conclusions observed for the uranium/iron benchmark. The increased sensitivity of the resonance parameters due to the intermediate type of spectrum of the system produces both larger total uncertainties as well as larger effects when correlations are taken into account. This indicates that, for future studies, the ZEUS assembly would be a good candidate to illustrate the impact of correlations among resolved resonance parameters, in particular for ^{235}U .

7.0 Conclusions

Resonance data play a major role in criticality safety calculations. Therefore, it is very important to assess uncertainties that are related not only to the specific parameters that are used for evaluating the cross sections, but also that associated with correlations among the different resonance parameters. The interest of this work was not to precisely quantify the impact of covariance information in the resonance domain, but to judge how important such information is for the applications.

We reviewed the basic principles that lie behind an uncertainty evaluation and review the current situation in the field of covariance data. Then, because of the lack of tools for correctly evaluating the variances and correlations among resolved resonance parameters, a methodology to estimate these values was developed. This methodology is based on a number of physical assumptions that we tested on the example of ^{235}U resonances. Relatively high correlations can be observed in most groups for the capture and fission cross sections of ^{235}U , and elastic scattering cross section of ^{56}Fe .

In order to estimate the impact of calculated uncertainties and correlations on K_{eff} , two well-known criticality safety benchmark problems were considered. Furthermore, we focused on these two practical applications to illustrate the impact of different assumptions on the correlation values (no correlation, full correlation and evaluated correlation). The calculated uncertainties on K_{eff} show that resonance parameters need a careful evaluation in order to minimize their associated uncertainty, and, consequently, the uncertainty on integral parameters. Correlations among parameters cannot be ignored without having a significant impact on calculations.

In order to correctly quantify the importance of correlations, an appropriate tool based on the analysis of experimental data is needed. The methodology that has been proposed leads to quite high values of correlations. In the future, we need to confirm these types of results by using a tool that is based on experimental values and nuclear modeling information.

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