

**NUCLEAR DATA AND MEASUREMENTS SERIES**

**ANL/NDM-99**

**Some Comments on the Effects of Long-Range Correlations in  
Covariance Matrices for Nuclear Data**

by

Donald L. Smith

March 1987

**ARGONNE NATIONAL LABORATORY,  
ARGONNE, ILLINOIS 60439, U.S.A.**

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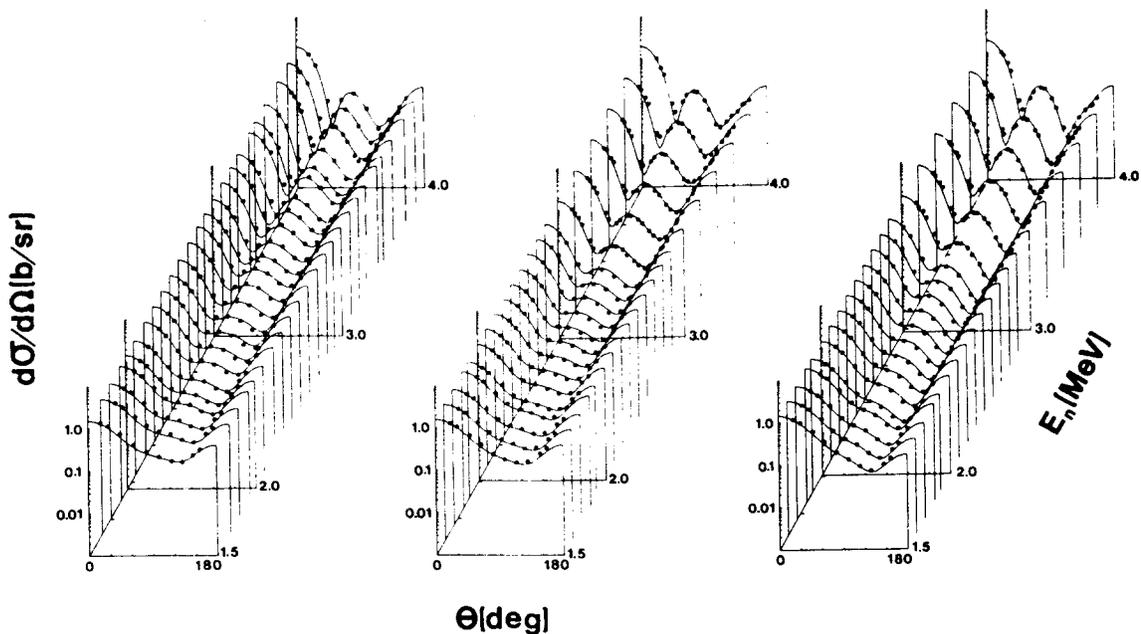
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ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS

Operated by THE UNIVERSITY OF CHICAGO

for the U. S. DEPARTMENT OF ENERGY

under Contract W-31-109-Eng-38

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NUCLEAR DATA UNCERTAINTIES. Covariance matrices. Long-range  
uncertainty correlations. Error propagation. Data evaluation.

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\*This work supported by the U.S. Department of Energy, Energy Research Programs, under contract W-31-109-Eng-38.

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SOME COMMENTS ON THE EFFECTS OF  
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ABSTRACT

Attention is called to the considerable sensitivity of many uncertainty calculations to the magnitude of the long-ranged correlations which appear in covariance matrices. If such correlations do exist, they must be included in order to properly assess the impact of the uncertainties in the data. If, however, certain assumed long-range correlations are unrealistic, then analyses involving such correlation information are almost certain to produce misleading results. The issue is discussed in general terms, and its importance is illustrated by examples based in part on recent work from this laboratory. Some practical suggestions are offered for dealing with the matter of correlations in instances where the available information is incomplete.

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\*This work supported by the U.S. Department of Energy, Energy Research Programs, under contract W-31-109-Eng-38.

## I. INTRODUCTION

During recent years there has been a pronounced increase in the utilization of detailed uncertainty information in the field of nuclear data research. In particular, it has become common practice to include either known or assumed correlations between various data in analyses involving uncertainties. Three notable applied areas are: i) reactor sensitivity calculations (e.g., Ref. 1), ii) neutron dosimetry (e.g., Ref. 2), and iii) nuclear data evaluations (e.g., Refs. 3 and 4). Considerable progress has been made in the development of procedures for utilizing information on covariances in such analyses. ENDF/B-V [5] marked the beginning for inclusion of covariance information in evaluated data files, and several other major data-file systems appear to be following this lead. Several guides to experimentalists on how to generate covariances for their measured results have been issued (e.g., Refs. 6 and 7). Some useful expositions on evaluation techniques are also available (e.g., Refs. 3 and 8).

The rapidly-expanding role of uncertainties in nuclear data research has resulted in a need to generate the covariance information which is employed by the formalisms associated with various new analytical procedures. Experimentalists are being urged to provide detailed uncertainty information (and commensurate documentation) in reports on their experimental results. Evaluators are expected (and in many cases required) to include covariance information (File 33 in the ENDF/B system [5]) along with their evaluated results. The covariance information which has evolved under these conditions varies widely in quality. Some reasons for this are discussed in Section II. The uneven quality of the available covariance information, and a growing realization that the results of analyses involving the use of covariances can be profoundly affected by their quality, are matters of growing concern within the small community of nuclear data investigators who are particularly knowledgeable in matters involving covariances (e.g., Ref. 9). Since these specialists are, by and large, dependant upon a wide range of sources for covariance information, it is essential that the issue be publicized widely across the entire community of nuclear data investigators. The main purpose for this communication is to address this matter.

Section II first explores the issue in rather general terms, with particular emphasis on some of the reasons why the problem exists in the first place. Then, specific examples are presented to illustrate the effects of long-range correlations in representative applications, mostly based upon experiences encountered in various investigations conducted in this laboratory. Section III offers some thoughts on how to deal with the problem, though no claim is made that this work offers a general solution for what is clearly a complex situation.

## II. DISCUSSION AND EXAMPLES

Before addressing the technical matters, it is worthwhile to provide a brief historical perspective of the issue. In earlier times for the nuclear data profession it was generally considered sufficient to merely provide an error estimate for each measured data point in a set. Though some statement regarding the relative importance of systematic and random errors might be offered in certain instances, it was very rare indeed to find a detailed breakdown of the error components within these two general categories, or to find specific information on the degree of correlation between the various systematic error components for the data points. Evaluations generally amounted to no more than eyeguides sketched through the available data points, and error specifications were not included in evaluated files. Evolution from this "Age of Darkness" into the "Age of Enlightenment" has been very well chronicled by Poenitz [3]. However, it appears that "enlightenment" may entail mixed blessings owing to the rather severe price that is often exacted from those who must deal with the issue in practical terms. An application of certain fundamental principles from mathematical statistics provided the nuclear data community with the blueprint needed to achieve progress in dealing with matters of uncertainty. Knowledge of the importance of dealing with a complete specification of uncertainties, i.e., of knowing the covariance matrix, has spread rapidly throughout the nuclear data community. Although there has been considerable activity within the community aimed at generating information of this nature, the quality of the results has been mixed.

In all fairness to the community, the provision of reliable covariance information in many realistic situations presents some very difficult problems, many of which have yet to be resolved to the satisfaction of everyone concerned. The sheer size of many experimental or evaluated data bases presents a problem in itself. In principle,  $n(n+1)/2$  distinct numbers are required to define the covariance matrix for a data set having  $n$  values (since covariance matrices are symmetric). If, e.g.,  $n=5000$  this amounts to more than  $1.25 \times 10^7$  values, an extremely-large number! Of course there are ways to alleviate this difficulty by representing covariance matrices as superpositions of several component matrices of considerably lower rank which require fewer numbers to parameterize. Such strategies are highly individualistic (i.e., they must be tailored to the particular situation in question) and are thus difficult to accommodate in general covariance-matrix practice without considerable approximation or compromise. Furthermore, it is generally no easy task to make reliable estimates of the essential parameters which comprise a covariance matrix. If an experiment is very complex, it is not a question of whether approximations will be made but rather of how they are to be made. This topic has been discussed in the literature (e.g., Refs. 6, 10-12). Finally, there is the matter of having to deal with cross-reaction and/or cross material correlation effects, an important

matter which has been seldom considered in practice, with the exception of a few standards and some dosimetry reactions. This troublesome consideration will eventually have to be dealt with in a scientifically-acceptable fashion by the nuclear data community, but it will not be discussed further in this report.

The nuclear data community obviously cannot abandon all the older data sets for which documentation is limited and the information needed to generate covariances is either lacking or inadequate. Data evaluators are therefore often forced into the position of having to exercise rather delicate subjective judgement in their endeavors. The reliability of subjective judgement is generally prone to wide variance, and the mixed quality of the existing File 33 content for ENDF/B-V supports this observation.

It would seem reasonable to expect that at least the minimum standards for generation of covariance matrices be met in practice. A covariance matrix should be real and symmetric (that insures that it will belong to the larger class of Hermitian matrices) and possess an inverse. Furthermore, a physically-reasonable covariance matrix ought to be positive definite (i.e., all the eigenvalues of the matrix ought to be positive). This insures that all real quadratic forms ultimately derived from the matrix (e.g., the chi-square statistics often referenced in least-squares adjustment procedures) will be positive definite. It is certainly not difficult to check whether a particular covariance matrix satisfies these basic mathematical properties, however there is abundant evidence that this has often not been done [3]. This problem, while important and probably amenable to resolution in the near term, is a separate one from the matter under consideration in this report. Therefore it will not be discussed further here.

It is evident that a major limitation in the generation of reliable covariance information is available time and manpower to do the work. Such activity is indeed very time and labor intensive. However, since worthy endeavors such as sensitivity analysis and unbiased data evaluation are highly dependent on the availability of reliable covariance information, achievements in this area cannot be realized by sidestepping the issue. There are some positive trends to consider which will help to alleviate the problem to some extent. It is clear that available computing power per unit cost is sharply on the rise, with no apparent limits in sight. This is an encouraging development from three points of view: First, it makes routinely feasible the rather laborious computations associated with the use of covariances. Second, it provides the means for storing and manipulating the large quantities of numbers which are involved in dealing with covariance matrices. Finally, it offers many possibilities for designing the integrated data-acquisition and data-processing systems which are required in order to generate reliable covariance information during the performance of experiments. Nevertheless, there will remain a number of unavoidable labor-intensive attributes to this work. In particular, the design of sophisticated algorithms for acquisition and analysis of data and the "archaeology" necessary in order to be able to

use much of the existing data base are unavoidable tasks. As a rule, if more is demanded from data, more thought and effort must be invested in the process of assembling it.

The considerable attention focused on covariance matrices has led many workers to believe that inclusion of some sort of off-diagonal (correlation) content in data error specifications will automatically lead to improved results vis-a-vis what might be produced by endeavors in which such information is neglected. Proper treatment of reliable covariance information will indeed produce superior results. However, inclusion of faulty correlation information, even if the methodology is correct, may very well lead to results which are as unreliable as those produced by neglecting all of the correlations! This is an essential point which cannot be overemphasized. The nuclear data community must deal very carefully with covariances. Otherwise, the endeavors are likely to be counterproductive.

It is important to define the terms of this discussion. We assume that an  $(n \times n)$  symmetric covariance matrix  $\bar{V}$  with elements  $V_{ij}$  is associated with a set of  $n$  data points. The corresponding correlation matrix  $\bar{C}$  has elements  $C_{ij}$  defined by the relationship

$$C_{ij} = V_{ij} / (E_i E_j),$$

with

$$E_i = (V_{ii})^{1/2}.$$

If  $C_{ij} = \delta_{ij}$  (Kronecker delta, having the value 1 if  $i=j$  and 0 if  $i \neq j$ ), then the covariance matrix is said to be without correlations. However, if significant non-zero values  $C_{ij}$  are present in regions of the matrix  $\bar{C}$  far removed from the diagonal, then long-range correlations are said to be present. It is these correlations which are of greatest concern in the present context.

A straightforward hypothetical example will serve to illustrate why such correlations tend to have a strong influence on the outcome of analyses involving covariance matrices. Suppose that

$$S = \sum_{i=1}^n x_i.$$

The expected value of  $S$  is related to the expected values for the  $x_i$  according to the equation

$$\langle S \rangle = \sum_{i=1}^n \langle x_i \rangle.$$

Suppose also that  $\langle x_i \rangle = x$  for all  $i$ . Then  $\langle S \rangle = n x$ . The variance in  $S$  (denoted as  $\text{var}(S)$ ) is derived from the law of error propagation (e.g., Refs. 13-15). Thus,

$$\begin{aligned} \text{var}(S) &= \sum_{i=1}^n \sum_{j=1}^n (\partial S / \partial x_i) \text{cov}(x_i, x_j) (\partial S / \partial x_j) \\ &= \sum_{i=1}^n \sum_{j=1}^n \text{cov}(x_i, x_j) = x^2 \sum_{i=1}^n \sum_{j=1}^n f_i f_j \text{corr}(x_i, x_j), \end{aligned}$$

where  $\text{cov}(x_i, x_j)$  is an element of the covariance matrix for the set of values  $x_i$ ,  $\text{corr}(x_i, x_j)$  is the associated correlation matrix, and  $f_i$  and  $f_j$  are the fractional errors in  $x_i$  and  $x_j$ , respectively. Now consider the following two extreme cases: i) If the errors for the  $x_i$  are uncorrelated, then

$$\text{corr}(x_i, x_j) = \delta_{ij},$$

and

$$\text{var}(S) = x^2 \sum_{i=1}^n f_i^2.$$

Then, if  $f_i = f$  for each  $i$ ,

$$\text{var}(S) = n x^2 f.$$

Consequently,

$$\text{var}(S) / \langle S \rangle^2 = f^2 / n.$$

ii) If the errors in the various  $x_i$  are 100%-correlated, we can then treat all the  $x_i$  as being equivalent to  $\eta y_i$ , where all the error is concentrated in the common factor  $\eta$ , and each of the  $y_i$  is without error. It is then easy to show that

$$\text{var}(S) / \langle S \rangle^2 = \text{var}(\eta) / \eta^2.$$

By previous assumption,

$$\text{var}(x_i) / x_i^2 = f^2$$

for each  $i$ . Furthermore,

$$\text{var}(x_i)/x_i^2 = \text{var}(\eta)/\eta^2$$

since all of the error of  $x_i$  is in  $\eta$ . Therefore,

$$\text{var}(S)/\langle S \rangle^2 = f^2.$$

For this example, it is evidently the case that  $\text{var}(S)/\langle S \rangle^2$  falls in the range  $(f^2/n, f^2)$ , depending on the nature of the assumed correlations between the various  $x_i$ . For large  $n$ , the range of possibilities for the error in  $\langle S \rangle$  is sizeable. If, e.g.,  $f = 0.05$  (5% error) and  $n = 10$ , this corresponds to the difference between 1.6% and 5% in the error for  $S$ .

This simple example demonstrates that it is important to know the correlation parameters precisely and to take them into consideration in analyses of uncertainty. Experience in this laboratory has shown that unrealistic assumptions regarding long-range correlations are responsible for many of the pathological situations encountered in dealing with covariance matrices.

The File 33 formats provided in ENDF/B [16] may be partially responsible for the emergence of evaluated files with excessive long-range correlations. In ENDF/B, covariance information is recorded in energy-interval form [16]. It is observed that the selected intervals are often quite large (several MeV), possibly reflecting a desire to keep the File 33 content short, or possibly masking ignorance. The energy-interval form, however, forces 100% correlation for all values with energies falling within a particular specified interval, regardless of the structure of the file otherwise. As an example, it is observed that for  $^{60}\text{Ni}(n,p)^{60}\text{Co}$  all values in the range 3-5 MeV are treated as fully correlated by ENDF/B-V (see Refs. 5 and 17). The use of sub-sub sections in the ENDF/B covariance files provides a mechanism for tailoring the relative contributions of short-, medium- and long-range components of a covariance matrix, using the concept of superposition. This approach is, of course, a convenient and compact alternative to the provision of explicit covariances (also provided for in ENDF/B via the LB=5 option). While existing ENDF/B covariance file formats appear then to offer the flexibility needed by a skilled practitioner in order to provide adequate representations of realistic covariance matrices, there remains the potential for abuse in the hands of those with less experience and good intuitive judgement regarding these matters. Since it is likely that other covariance-file formats which could potentially be used in such applications have their own problematic limitations (though this is a matter which the nuclear data community should explore in the future), this observation should not be taken as a specific criticism of the contemporary ENDF/B formats.

To illustrate the sort of difficulties which can result from the use of inadequate covariance information, we now consider an example based in part on Ref. 17. This is a simple case of what is usually referred to as sensitivity analysis, and it basically amounts to an application of the law of error propagation. What is sought here is the uncertainty in the calculated integral cross-section ratio of  $^{58}\text{Ni}(n,p)^{58}\text{Co}$  to  $^{60}\text{Ni}(n,p)^{60}\text{Co}$  for a continuous neutron spectrum arising from 7-MeV deuteron bombardment of a thick beryllium-metal target. The spectrum representation, including the covariance matrix, is based on the work of Crametz et al. [18]. The cross-section representations are from ENDF/B-V [5]. However, for purposes of demonstration, "hypothetical" covariance matrices are used in these computations. It is assumed that the cross section errors are 10% for both reactions from threshold to 20 MeV (i.e., across the entire energy range of the calculations). The correlation matrices used in the analysis are selected so that for each matrix all off-diagonal elements are identical. The values assumed are either 0, 0.25, 0.5, 0.75 or 1. The calculated integral ratio is, of course, insensitive to the uncertainty assumptions, but the error in this ratio varies according to the detailed error correlations. The results of this analysis appear in Table 1. The uncertainty in the calculated integral ratio changes by as much as a factor of two as the assumed long-range correlations are varied.

A similar concern arises in the use of least-squares adjustment procedures for the generation of cross-section evaluations, e.g., GMA [3], GLUCS [19] or UNFOLD [20]. The procedures inherent in each of these computer algorithms demand detailed input covariances for the data files included. In those instances where knowledge of the uncertainties is fragmentary, or misleading, there is a considerable risk that poorly estimated long-range correlations will adversely impact upon the outcome of the evaluation process.

To demonstrate this, we consider here an evaluation which was conducted recently in this laboratory for  $^{59}\text{Co}(n,\alpha)^{56}\text{Mn}$  (Ref. 21). The concept of this evaluation is as follows: It was observed that the ENDF/B-V [5] evaluation provides a reasonably good representation of all the data which were available when this evaluation was performed (ca. 1970). Since that time, however, there have been a number of new data points reported in the vicinity of 14 MeV, plus one differential data set which spans most of the threshold-energy region. It was decided to use these new data to adjust the previous evaluation in the manner described in Ref. 20. A special evaluation of the data in the vicinity of 14 MeV was performed recently by Evain et al. [22]. This work led to a single evaluated value with high accuracy at 14.7 MeV. It was decided to treat this as a single data point which is representative of all the new detailed experimental information available in the 13-15 MeV energy range. Furthermore, a new measurement from this laboratory [23], performed after the evaluation of Evain et al. [22], produced an independent value at 14.74 MeV. This point was

also included in the evaluation procedure. Finally, the new data in the threshold region ( $< 10$  MeV), also from work performed in this laboratory, were included. The adjustment procedure, accepting all the available information without alteration, produced the results indicated in Fig. 1. It is evident that the new differential data in the threshold region were consistent with the prior information, so the adjustment procedure produced a negligible change there. However, the new information in the 14-MeV region led to a noticeable increase in the evaluated cross section. In fact, it is obvious that the adjustment procedure simply renormalized the shape of the a priori cross section from about 12-18 MeV. The reason this happened is that the covariance matrix for this reaction which was obtained from ENDF/B-V, and thus is the a priori covariance matrix for the adjustment procedure, indicates that the entire region from 12-18 MeV must be treated as fully correlated. The new information in this energy region can therefore serve only to force a renormalization of a shape factor which is otherwise treated as unalterable. Consequently, the effects of strong long-range correlations cannot be readily purged by the accumulation of new information. Since such a situation is clearly quite non-physical, it is evident that strong long-range correlations should not be assumed unless there is very good justification.

In this example, a more reasonable solution for the evaluation was obtained by relaxing the excessively-stringent long-range correlations. The magnitudes of the total errors (variances) were adjusted only slightly so as to provide better continuity from group to group in the adjustment process. However, the long-range correlations were reduced to 0.2, a modest level. A short-to-medium range correlation pattern was arbitrarily introduced. It had the property that adjacent groups (separated by 0.5 MeV) were assumed to be 0.75 correlated, once-removed groups 0.5 correlated, twice-removed groups 0.25 correlated, and all other groups correlated to 0.2 as indicated above. The results of this analysis are indicated in Fig. 2. A solution which is far more consistent with the realities of this problem was obtained. The new information in the vicinity of 14 MeV now affects the evaluation in that region as it should, but it does not have an excessive effect on the evaluation at energies far removed.

### III. CONCLUSIONS AND RECOMMENDATIONS

Efforts to insure that improvements are made in the way that covariance information is generated and utilized in the future ought be directed along three general lines: i) Improved methods for obtaining and documenting the covariance information from experiments must be developed and followed. ii) Rigorous evaluation procedures must continue to be developed and practiced, and improvements in evaluated data file formats should be sought. and iii) Good judgement, based on an understanding of the significance and impact of covariance information, must be exercised in the utilization of covariances for various applications.

There is little that can be done to alter some of the unfavorable consequences of past experimental and data-compilation efforts. Therefore, emphasis must be placed on establishing improved standards for the acquisition, analysis, reporting and compilation of future experimental data. To this end, only a few comments are offered in this report.

The single most important factor may very well be the matter of education. It is essential that experimentalists acquire a working familiarity with statistical methods and the basic concepts of uncertainty. Consideration of uncertainties ought to be an integral part of experimental planning since the essential information needed to determine uncertainties usually needs to be developed very early in the experimental process. Experience has shown that a posteriori analysis of uncertainties can lead to very dubious results, particularly if an analysis is conducted long after the measurements are over. It was indicated above that contemporary availability of very impressive computing power provides most laboratories with many opportunities from this point of view. Methods for developing reliable covariance information during the experimental process have been suggested in the literature (e.g., Refs. 6, 10-12). The work of the ORELA group provides a particularly impressive model in this regard (e.g., Ref. 12). It is evident that considerable thought and effort will be required to meet the necessary standards in this area, but the task appears to be a tractable one. Proper reporting of detailed uncertainty information is equally important, and is also a matter requiring improved definition of standards. There are some issues and problems in this regard which need to be resolved. Some covariance specialists feel that experimenters should not provide explicit covariance matrices for their data, but rather should limit themselves to a complete listing of all the explicit error components and their correlations between the data points. From this information, covariances can be readily constructed as needed (e.g., see Ref. 6). Others feel that explicit covariance matrices should be provided. An obvious solution to this controversy would be to suggest that both demands be met in reporting data. This leads to a second troublesome issue, namely the manner in which such information should be reported. As was mentioned in Section II,

covariance information can be very voluminous. It is often impractical to report such information in journal articles, or even in laboratory reports. It would seem then that computer files are the storage medium of choice in most instances. Fortunately, there exist provisions for the inclusion of such information in nuclear data archival systems, e.g., in the international EXFOR system. They should be more widely exploited.

Next we turn to consideration of nuclear data evaluation processes. Since most computational applications involving nuclear data use evaluated information, this is a very important issue. It would appear that the more recent least-squares methods and procedures which have been developed (and also exploited in a number of instances) for performing unbiased evaluations are capable of yielding acceptable results provided that the information in the corresponding available data bases is adequate in scope, quantity and consistency to provide a sound basis for statistical analysis. It is also evident that the execution of these procedures is very demanding of time and labor, primarily because of inadequacies in the existing data bases and/or difficulties in gathering the available information. Shortcomings in existing evaluations, particularly in the area of covariances, seem to have developed primarily because many of these evaluations were not rigorous. It is suggested, then, that a goal for the future should be to address as many evaluation activities as possible in a rigorous fashion, particularly for data sets upon which certain important contemporary applications are heavily dependent. At the outset this approach will no doubt be quite laborious, but the situation should improve as the quality of the available data bases improves in time (especially from the point of view of uncertainties). When rigorous, unbiased evaluation methods are used, the resulting covariance information is certain to be of better quality. One reason is because the procedures themselves tend to guard against the introduction of excessive long-range correlations, and they also insure that the covariances produced possess the proper mathematical properties (e.g., positive definiteness).

It is also recommended that careful attention be given by evaluators to the selection of grid structures for their evaluations, particularly the grids selected for the specification of covariances. It has been common practice to select coarser grid structures for covariance information than for the specification of cross sections, the argument being that less precision is needed for the former. The danger inherent in this assumption results from the fact, mentioned above, that values for all energies within a grid interval are treated as fully correlated. So long as the ENDF/B formats for covariances are retained in present form (and there are some clear advantages to this form), it is suggested that the grid structures used for evaluations be suitably refined to avoid inadvertent introduction of long-range correlations. If one is faced with the task of generating covariance information under less than ideal conditions, then it would seem better to err in the direction of providing estimates of long-range correlation components which are too weak rather than too strong. In

that way, new and more reliable data which are considered in future evaluations will not be prevented by the excessively restrictive conditions mandated by long-range correlations from having a beneficial impact on the knowledge-refinement process.

Finally, we come to the question of how to deal with flawed covariance information in analytical applications. Experience has shown that the error estimates (or variances) are often quite reasonable, whereas the implied correlation information is a source of difficulty (e.g., see the example provided in Section II). If it is evident that a problem with long-range correlations exists only because the grid structure employed in the specification of covariance information is too coarse, one possible way to deal with the situation would be to arbitrarily refine the grid structure, while at the same time generally preserving the magnitudes of the indicated variances. Another approach would be to essentially eliminate the long-range correlations (or reduce them sharply) and arbitrarily replace them with a short-range correlation pattern such as the one used in the example above. Neither of these approaches constitute an ideal solution because they both involve more subjectivity than is desirable. Nevertheless, blind application of available covariance information, particularly when it is strongly suspected that there are flaws, is very likely to be even less desirable in practice.

**ACKNOWLEDGEMENT**

**This work has been supported by the U.S. Department of Energy, Energy Research Programs, under contract W-31-109-Eng-38.**

## REFERENCES

1. C.R. Weisbin, E.M. Oblow, J. Ching, J.E. White, R.Q. Wright and J. Drischler, "Cross Section and Method Uncertainties: The Application of Sensitivity Analysis to Study Their Relationship in Computational Benchmark Problems", Conference on Nuclear Cross Sections and Technology, Washington, D.C., March 3-7, 1975, edited by R.A. Schrack and C.D. Bowman, NBS Special Publication 595, p. 825 (1975).
2. J.J. Wagschall, B.L. Broadhead and R.E. Maerker, "Least-Squares Methodology Applied to LWR-PV Damage Dosimetry, Experience and Expectations", Conference on Nuclear Cross Sections for Technology, Knoxville, Tennessee, October 22-26, 1979, edited by J.L. Fowler, C.H. Johnson and C.D. Bowman, NBS Special Publication 594, p. 956 (1980).
3. W.P. Poenitz, "Data Interpretation, Objective Evaluation Procedures and Mathematical Techniques for the Evaluation of Energy-Dependent Ratio, Shape and Cross Section Data", Proceedings of the Conference on Nuclear Data Evaluation Methods and Procedures, Brookhaven National Laboratory, Upton, N.Y. 11973, September 22-25, 1980, edited by B.A. Magurno and S. Pearlstein, BNL-NCS-51363, p. 249 (1981). Also, private communication (1987).
4. J.H. Marable, "The Adjustment of Group Cross Sections Based on Integral Experiments in Fast Benchmark Assemblies", Proceedings of the Conference on Nuclear Data Evaluation Methods and Procedures, Brookhaven National Laboratory, Upton, N.Y. 11973, September 22-25, 1980, edited by B.A. Magurno and S. Pearlstein, BNL-NCS-51363, p. 117 (1981).
5. "Evaluated Neutron Data File, ENDF/B-V", ENDF/B Summary Documentation, compiled by R. Kinsey, ENDF-201, 3rd Edition, Brookhaven National Laboratory (1979).
6. Donald L. Smith, "Covariance Matrices and Applications to the Field of Nuclear Data". ANL/NDM-62, Argonne National Laboratory (1981).
7. W. Mannhart, "A Small Guide to Generating Covariances of Experimental Data", PTB-FMRB-84, Physikalisch-Technische Bundesanstalt, Braunschweig, F.R. Germany (1981).
8. F.H. Froehner, "Principles and Techniques of Data Evaluation", KfK 4099, Kernforschungszentrum Karlsruhe, F.R. Germany (1986).
9. IAEA Specialists' Meeting on Covariance Methods and Practices in the Field of Nuclear Data, Rome, Italy, November 17-19, 1986, proceedings to be published as an INDC report.

10. Donald L. Smith, "Non-Evaluation Applications for Covariance Matrices", ANL/NDM-67, Argonne National Laboratory (1982).
11. D.L. Smith, "On the Relationship Between Micro and Macro Correlations in Nuclear Measurement Uncertainties". Accepted for publication in Nuclear Instruments and Methods in Physics Research (Section A).
12. D.C. Larson, N.M. Larson, J.A. Harvey, N.W. Hill and C.H. Johnson, ORNL/TM-8203, Oak Ridge National Laboratory (1983).
13. E. Parzen, Modern Probability Theory and Its Applications, John Wiley and Sons, Inc., N.Y. (1960).
14. J.E. Freund, Mathematical Statistics, Prentice-Hall, Inc., Englewood Cliffs, New Jersey (1962).
15. W. Mendenhall, Introduction to Probability and Statistics, Wadsworth Publishing Company, Inc., Belmont, California (1967).
16. "Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF/B-V, ENDF-102, edited by R. Kinsey (1979) and revised by B.A. Magurno (1983), Brookhaven National Laboratory.
17. D.L. Smith, J.W. Meadows and M.M. Bretscher, "Integral Cross Section Measurements for  ${}^7\text{Li}(n,n't){}^4\text{He}$ ,  ${}^{27}\text{Al}(n,p){}^{27}\text{Mg}$ ,  ${}^{27}\text{Al}(n,\alpha){}^{24}\text{Na}$ ,  ${}^{58}\text{Ni}(n,p){}^{58}\text{Co}$  and  ${}^{60}\text{Ni}(n,p){}^{60}\text{Co}$  Relative to  ${}^{238}\text{U}$  Neutron Fission in the Thick-Target  ${}^9\text{Be}(d,n){}^{10}\text{B}$  Spectrum at  $E_d = 7 \text{ MeV}$ ", ANL/NDM-93, Argonne National Laboratory (1985).
18. A. Crametz, H.-H. Knitter and D.L. Smith, "Thick-Target  ${}^9\text{Be}(d,n){}^{10}\text{B}$  Neutron Spectrum at  $E_d = 7 \text{ MeV}$ ", Nuclear Data for Science and Technology, edited by K.H. Boeckhoff, D. Reidel Publishing Company, Dordrecht, Holland, p. 902 (1983).
19. D.M. Hetrick and C.Y. Fu, "GLUCS: A Generalized Least-Squares Program for Updating Cross-Section Evaluations with Correlated Data Sets", ORNL/TM-7341 (ENDF-303), Oak Ridge National Laboratory (1980).
20. Donald L. Smith, "A Least-Squares Method for Deriving Reaction Differential Cross Section Information from Measurements Performed in Diverse Neutron Fields", ANL/NDM-77, Argonne National Laboratory (1982).
21. J.W. Meadows, D.L. Smith and R.D. Lawson, to be published.

22. Bernard P. Evain, Donald L. Smith and Paul Lucchese, "Compilation and Evaluation of 14-MeV Neutron Activation Cross Sections for Nuclear Technology Applications: Set I", ANL/NDM-89, Argonne National Laboratory (1985).
23. J.W. Meadows, D.L. Smith, M.M. Brestscher and S.A. Cox, "Measurement of 14.7-MeV Neutron-Activation Cross Sections for Fusion", accepted for publication in Annals of Nuclear Energy.

**Table 1:** Variation in the Uncertainty of a Calculated Integral Cross Section Ratio with Magnitude of the Assumed Long-Range Correlations for the Reaction Cross Section Errors\*

$\sigma_1$ Correlation	$\sigma_2$ Correlation				
	0	0.25	0.5	0.75	1
0	7.1	8.4	9.6	10.6	11.5
0.25	8.4	9.6	10.6	11.5	12.4
0.5	9.6	10.6	11.6	12.4	13.2
0.75	10.7	11.6	12.4	13.2	14.0
1	11.6	12.5	13.3	14.0	14.7

\*Results in the table correspond to percent errors in the integral ratio

$$R = \int_0^{20 \text{ MeV}} \sigma_2(E) \phi(E) dE / \int_0^{20 \text{ MeV}} \sigma_1(E) \phi(E) dE.$$

Here  $\sigma_1$  represents the  $^{60}\text{Ni}(n,p)^{60}\text{Co}$  reaction while  $\sigma_2$  represents the  $^{58}\text{Ni}(n,p)^{58}\text{Co}$  reaction. ENDF/B-V [5] values are employed in the calculations for both cross sections. The spectrum  $\phi$  is produced by 7-MeV deuterons incident on a thick beryllium metal target. The representation and covariance matrix for this spectrum are drawn from the work of Crametz et al. [18]. They are kept fixed. Hypothetical covariance information is employed for the two reaction cross sections for purposes of demonstration, as discussed in Section II. A 10% error is assumed for each cross section from threshold to 20 MeV. All the off-diagonal elements of the correlation matrices used for a particular cross section are then assumed to be the same. The values these constant long-range correlations are assumed to take are those indicated in the table.

## FIGURE CAPTIONS

Figure 1: Experimental data and evaluations for the  $^{59}\text{Co}(n,\alpha)^{56}\text{Mn}$  reaction. Old data are indicated by (X), recent results from this laboratory by (O). Curve A is ENDF/B-V [5]. Curve B is a revised evaluation based on a least-squares composition of ENDF/B-V and results from this laboratory. The covariance information provided for ENDF/B-V is used without alteration for this analysis.

Figure 2: Experimental data and evaluations for the  $^{59}\text{Co}(n,\alpha)^{56}\text{Mn}$  reaction. Old data are indicated by (X), recent results from this laboratory by (●). Curve A is ENDF/B-V [5]. Curve B is a revised evaluation based on a least-squares composition of ENDF/B-V and results from this laboratory. The covariance information provided for ENDF/B-V is modified somewhat to dampen the effects of long-range correlations on the analysis, as described in Section III.

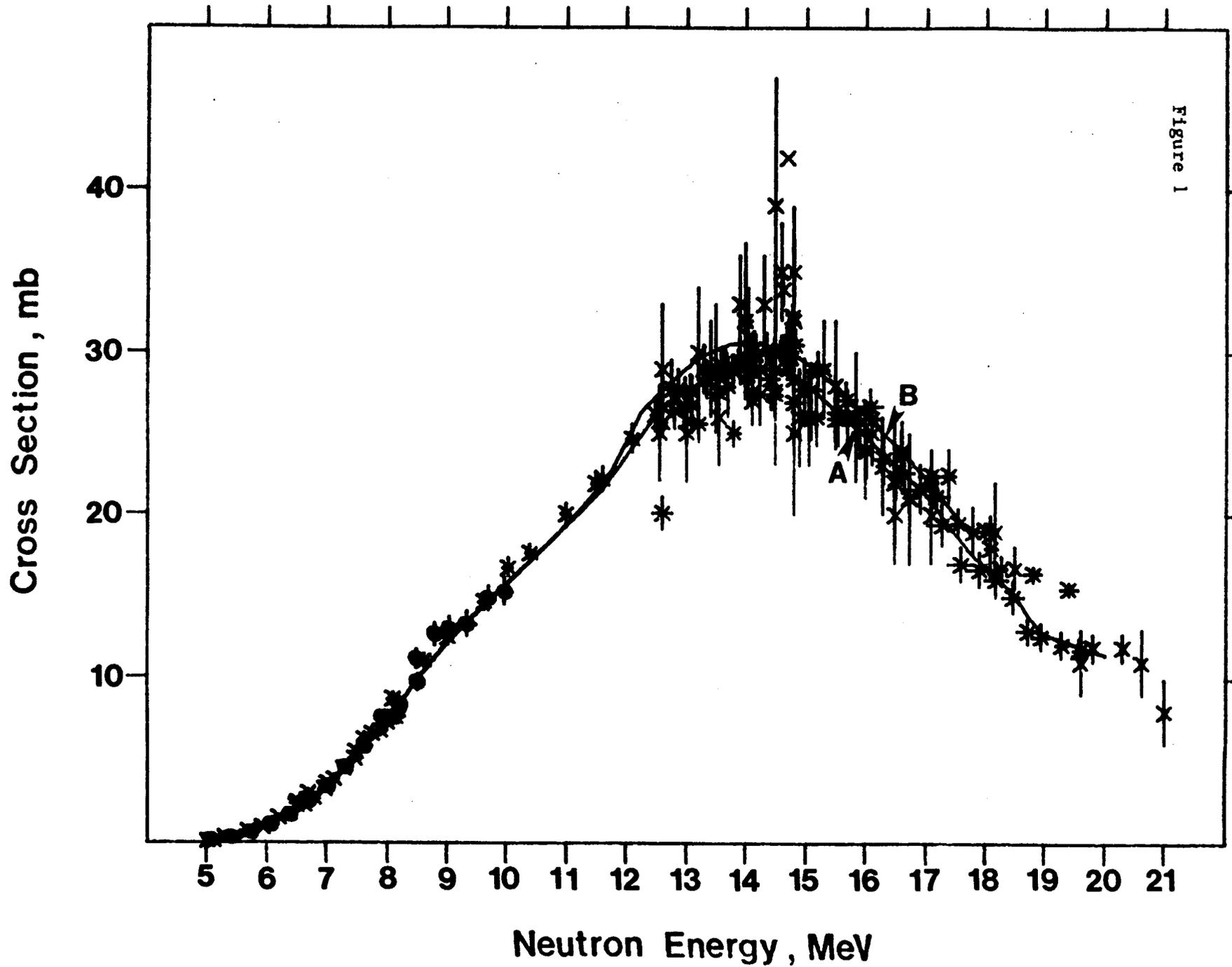


Figure 1

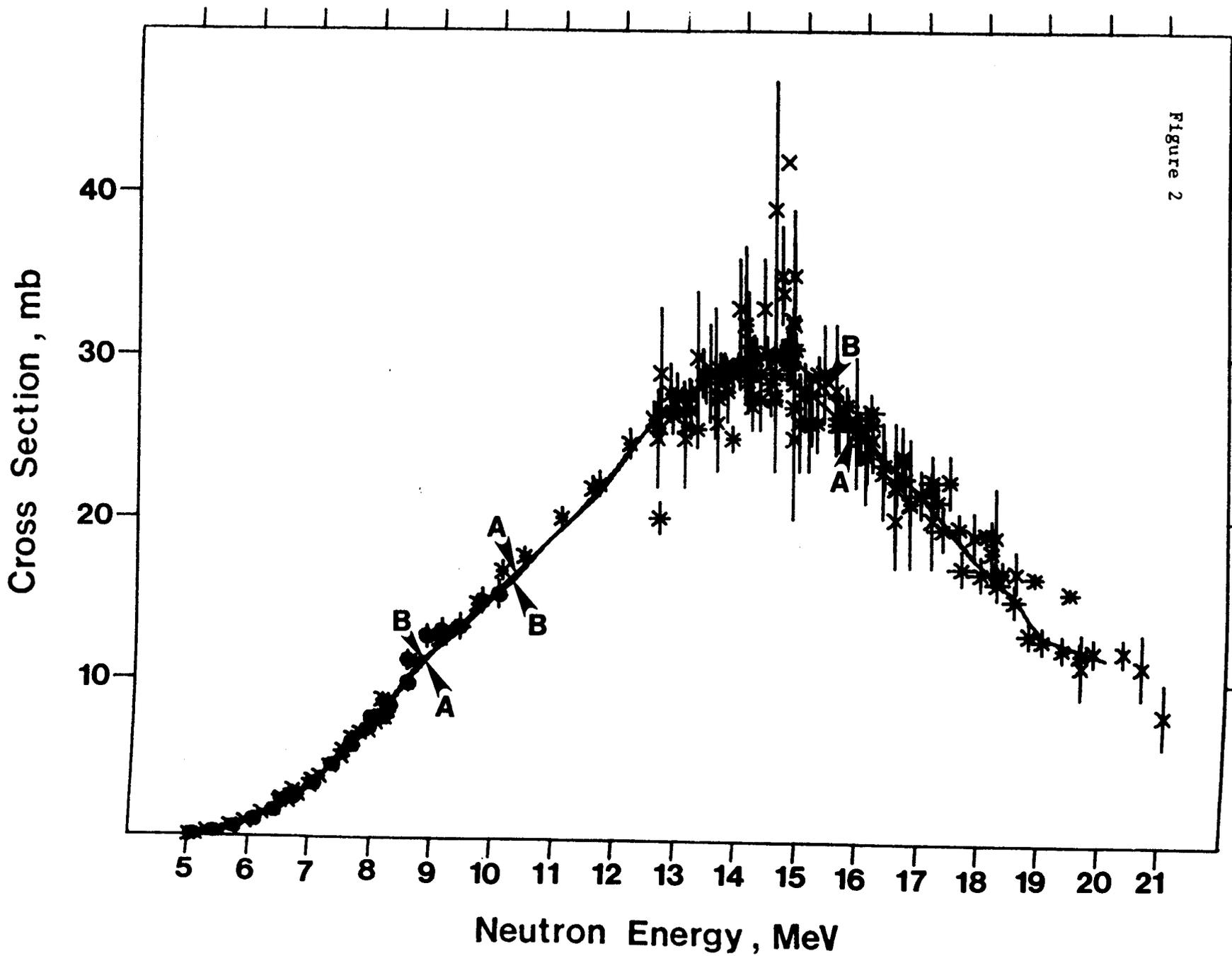


Figure 2