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DATA INTERPRETATION, OBJECTIVE EVALUATION PROCEDURES AND MATHEMATICAL TECHNIQUES FOR THE EVALUATION OF ENERGY-DEPENDENT RATIO, SHAPE AND CROSS SECTION DATA*

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ABSTRACT

The evaluation of several energy-dependent cross sections which are of importance for practical applications is considered. The evaluation process is defined as the procedure which is used to derive the best knowledge of these cross sections based on the available direct experimental data information, and, using theoretical models, on the auxiliary data base. The experimental data base represents a multiple overdetermination of the unknown cross sections with various correlations between the measured values. Obtaining the least-squares estimator is considered as the standard mathematical procedure to derive a consistent set of evaluated cross section values. Various approximations made in order to avoid the monstrous system of normal equations are considered and the feasibility of the exact solution is demonstrated. The variance - covariance of the result, its reliability and the improvements obtained in iterative steps are discussed. Finally, the inclusion of auxiliary, supplementary information is considered.

I. INTRODUCTION

The subject of the present considerations and review is the evaluation of neutron cross sections which are of specific importance and thus have to be known with lesser uncertainties than others. This involves cross sections used in practical applications such as $^{235}U(n,f)$, $^{238}U(n,\gamma)$ as well as the standard cross

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sections (H(n,n), ^{6}Li(n,α), ^{10}B(n,α), ^{10}B(n,αγ), Au(n,γ)). For reasons which will become clear later on, some other cross sections are involved as well (^{6}Li(n,n), ^{10}B(n,n)). Following the intent of this meeting, we not only consider the state of the evaluations of these data but the evaluation process as well.

It should be clear from the outset that an evaluator is not expected to derive his opinion of the subject of the evaluation but the best knowledge of it. Nuclear data evaluations can be divided in historic terms into an

'Age of Archaic Evaluations',

where unjustifiable and subjective evaluation methods were used, an

'Age of Enlightenment',

where it was recognized that the archaic evaluation techniques had severe drawbacks, and an

'Age of Renaissance',

where it was discovered that exact solutions techniques were developed some 180 years ago. As in other areas of history, these periods cannot be sharply divided. But clearly, about 10 years ago, evaluation procedures for nuclear data were still in the 'Dark Ages' where archaic techniques were well entrenched, and appropriate methods were used only infrequently. Wild lines were drawn through data points and subjective opinion carried the day. It has been recognized in the last few years that appropriate techniqeus were well developed and applied in other disciplines of science and engineering and should be employed as well in the evaluation of nuclear data. Increasingly, improved techniques were used, but unfortunately, the archaic age is slow in dying: e.g., it would be easy to point out a number of evaluated cross sections in ENDF/B-V which were based upon one data set where many were available. Because of this staying power of unscientific, archaic methods, techniques and argumentation, it will be hard to avoid to point out fallacies which will be obviously recognized as such by many.

As we desire to derive the best knowledge of some quantities existing in nature, we have to consider what this knowledge consists of.

I.1. The Best Knowledge

The philosophy or theory of knowledge, developed by many important men, and culminating with Kant's 'Critique of Pure Reason' [1], tells us that knowledge has two sources: 'a priori', which is knowledge developed from reasoning along, and

'a posteriori', which is knowledge after the fact, e.g., after performing an experiment. As we are not in the area of logic or mathematics, where knowledge may be derived purely 'a priori', we have to be concerned whether our knowledge is purely 'a posteriori' or, to some extent, can be derived 'a priori'. Certainly, laws of nature have been found in physics, but the area applying to nuclear cross sections is still in a state of modeling and our knowledge is empirical, thus it is derived 'a posteriori'. A good example are cross sections which may be derived from the optical model. The optical model was not conceived 'a priori' but 'a posteriori' following the pioneering measurements of total neutron cross sections by Barshall [2] which showed systematic structure as a function of energy and nuclear mass. It was possible to predict other cross sections with this model. But, as measurements for such predicted cross sections became available, the model predictions were found in conflict with these experimental results. The conflicts lead to refinements of the model, in successive steps, changing the shape of the potential, adding a surface absorption potential, spin-orbit coupling, introducing non-local potentials, etc., always in response to disagreement with new measurement results. As of now, the optical model is still a model, of great value, but dependent on numerous parameters derived from fitting experimental data. It obviously follows that predictions with the optical model cannot be better than the quality of the whole of the experimental data base. This does not mean that optical model predicitons cannot be better, in some instances, than a singular experimental data set. A case in point is the total cross section of ^{233}U. The ENDF/B-IV evaluation used a line through the available experimental data. An optical model fit of these data would have provided a more physical shape but still erroneous values. It was appropriately recognized by evaluators for ENDF/B-V [3] that the experimental data for ^{233}U in the energy range below 1 MeV were in conflict with data for neighboring nuclei. A prediction based on a parameterization with data for other nuclei was utilized instead. However, then a new data set became available and the evaluation was changed to match this data set. Experimental data are uncertain, thus, the best knowledge of the ^{233}U total neutron cross section would be obtained by a simultaneous fit of the transactinides with the optical model, accounting for uncertainties of the data and the model. Such simultaneous optical model fitting is now being done, for example, by Madland and Young [4] and Poenitz [5].

The best knowledge of the quantities to be evaluated is derived by including all the direct and indirect information available. The primary source is the experimental data base, differential and integral, as our knowledge is 'a posteriori'. nuclear models and integral systems models provide the link between the data. Figure 1 shows a schematic of the maximum information leading to our evaluated (or best knowledge) cross section. This maximum information has been used, for example,

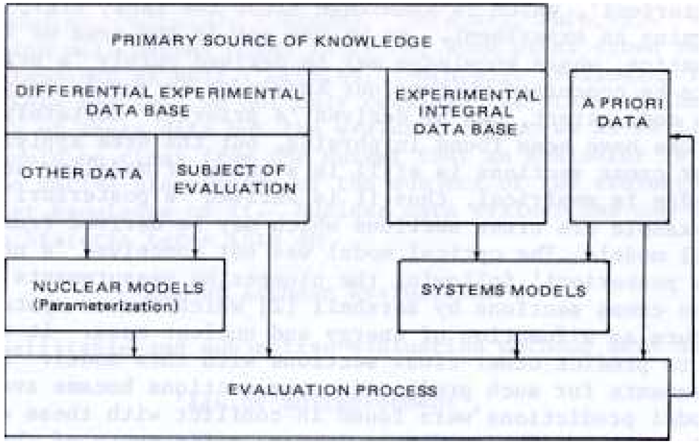

Fig. 1. Information Available for Cross Section Evaluations.

by Schenter's group [6] for the evaluation of fission product nuclei. The result of such evaluation (which includes the integral data) is often called an adjusted cross section set. An adjusted, best knowledge cross section set is justified and desirable, specifically in cases of sparce differential information, as in the case of fission product nuclear data.

One may require, however, another approach, based on the intended use of the evaluated data. A separate evaluation of the differential data with utilization of the nuclear models provides for a "testing" of the integral systems modeling of experimental integral values. The large number of parameters involved in an integral system causes a diffusion of the lack of knowledge for some parameters (discrepancies) by distributing the blame between all of the parameters (cross sections). The French library data on the components of stainless steel provide an example. Though this library predicted available integral data very well, it was due to compensation and a design calculation for a different compositon of stainless steel would have resulted in erroneous predicitons [7].

Thus, in the following we restrict our considerations to the evaluation of differential data of the primary data base and the utilization of auxiliary information provided by the nuclear models.

I.2. Outline of an Objective Evaluation Process

One of several features of an objective evaluation process is not to select data based upon subjective judgment. However, the fitting of the available experimental nuclear data with nuclear models involves non-linear fitting of such monstrous

proportions that it is obviously beyond the range of present technology. This suggests to divide the evaluation process into steps as shown schematically in Fig. 2. The first major step consists of assembling the available experimental data, extraction of actually measured quantities, and the application of corrections to the reported values and their errors if such can be proven to be required. Updating constants ($T_{1/2}$) etc., used in the calculation of these values, recalculation of corrections with improved techniques (Monte Carlo) and data used in their calculations are acceptable. However, reintroduction of subjective methods (for example unjustified re-assignments of uncertainties) must be rejected.

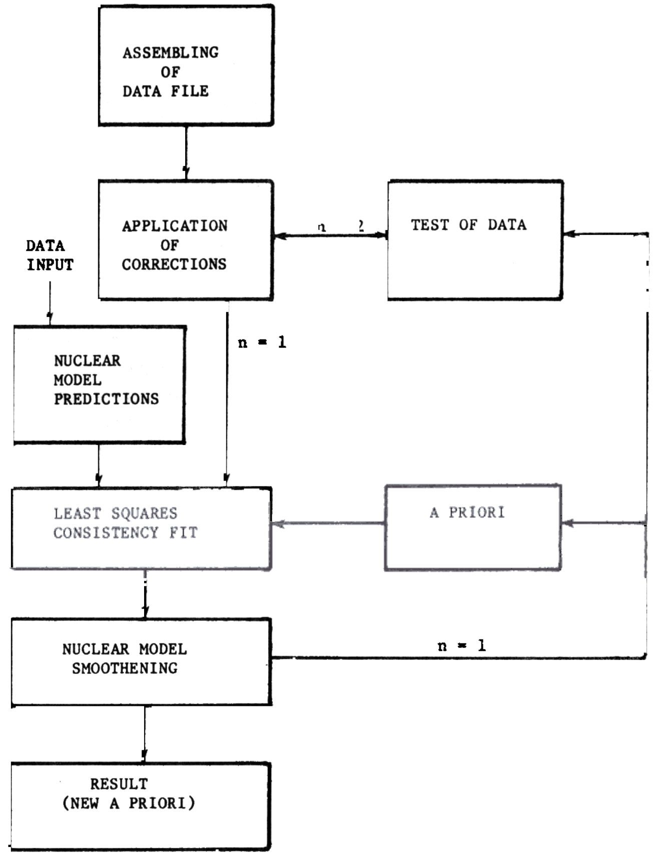

Fig. 2. Schematic of the Evaluation Procedure.

The second step is the evaluation of the experimental data in a simultaneous least-squares fit as discussed below which yields a consistent set of values which represent the est knowledge from the experiments. The third step is the tilization of nuclear models which permit to use auxillary ata information. The process is then repeated in iterative teps in order to obtain further improvements.

II. THE MEASUREMENT PROCESS AND INTERPRETATION OF THE EXPERIMENTAL DATA BASE

It is obvious that the evaluation process should be considered in context with the subject of the evaluation, the data base. An understanding of the measurement-process and the quantities derived appears required. Mathematical procedures can lead their own independent life, but the answer will surely be misleading if they are based upon a misconception of its elements. This may well be a danger we are facing now, as more and more evaluators become enchanted with powerful tools provided by statistical analysis, but do not understand the data base and thus "take off into a dream world".

II.1. Types of Measurements, Originally Measured Quantities

It must be realized that experimenters in the area of cross section measurements rarely present what they have measured. A measurement of the shape of the ratio of two cross sections, say $\sigma_{n,f}(^{235}U)/\sigma_{n,n}(^{1}H)$, will surely be presented as a measurement of the $^{235}U(n,f)$ cross section after using some reference for the H(n,n) cross section and normalization to some other absolutely measured or more or less arbitrarily choosen value. Comparison with other measurements are then made, differences pointed out and possible explanations given. All of which is an exercise in futility because the quantities measured were not the values discussed. This does not mean that the measurement was meaningless, in the contrary, it may have been an very important input for the quantity, for example a cross section shape, which was actually measured.

The first task for the evaluator, who wants to derive the best knowledge of one or several unknowns, is to rediscover the actually measured quantities, thus to reduce the given information to the truly new information obtained in the specific experiment. An example for the problems resulting from ignoring the originally measured quantities is the common procedure to evaluate a specific cross section for which N measurements are available without differentiating between K measurements which were made relative to the same reference cross secton and N-K absolute and independent measurements. Such procedure is identical to forming the average between 3 and 4 by calculating (3 + 3 + 4 + 4 + 4 + 4)/7 (assuming N=7 and K=5). Such fallacies may not be very obvious if correct and sophisticated techniques are used for the derivation of the evaluated cross section.

A measurement may have been presented as a cross section measurement over an energy range (E_k, E_i) but in reality the shape may have been measured in two segments, (E_k, E_ℓ), (E_j, E_i), (with $E_j < E_\ell$) and a normalization point obtained at E_n (with $E_k \leq E_n \leq E_i$). The true information obtained from these measurements which should be used as input for the evaluation are three sets of data: 1. the absolute value at E_n, 2. the segment in (E_ℓ, E_k), and 3. the segment in (E_j, E_i). The composite cross section should not be used, it will bias the evaluation as will be seen later on.

The types of measurements used to derive the data under present consideration are transmission experiments which yield total cross sections, reaction cross section or ratio measurements, shape measurements of cross sections or ratios which leave the normalization of the data undetermined, and absorption cross section measurements. Total cross sections are derived from the expression

$$\sigma_{tot}(E) = \frac{1}{a}\,\ell n\,\frac{C_o(E) - b_o - \sum_i b_{oi}(E)}{C(E) - b - \sum_i b_i(E)} \cdot \prod_j f_j(E) \qquad (1)$$

where a is the sample constant, b is a constant background and $b_i(E)$ an energy dependent background. The $f_j(E)$'s are correction factors, for example for deadtime, resonance self-shielding, etc. The $C_o(E)$ and $C(E)$ are the detector counts without and with the sample. Reaction cross sections are derived from

$$\sigma_x(E) = \frac{C_x(E) - b_x - \sum_i b_{xi}(E)}{C_n(E) - b_n - \sum_i b_{ni}(E)} \cdot \prod_i a_i \quad \prod_j f_j(E)\ , \qquad (2)$$

where $C_x(E)$ and $C_n(E)$ are the count rates for the observed reaction and the neutron detector, respectively. The a_i are independent on energy and stand for sample masses, efficiency calibrations etc. The $f_j(E)$ are energy dependent corrections and the energy dependence of the counting efficiencies. The same expression [2] applies for ratio measurements with $C_n(E) \rightarrow C_y(E)$ and $\sigma_x(E) \rightarrow R_{xy}(E) = \sigma_x(E)/\sigma_y(E)$. In a shape measurement (cross section or ratio), the product $\prod_i a_i$ remains undetermined and only the energy dependence of the cross section is obtained: $S(E) = C \cdot \sigma(E)$ with $C = \prod_i a_i$ an unknown factor. The central expressions in (1) and (2) can be restated as

$$\frac{C_x(E)\left(1 - \frac{b_x}{C_x(E)} - \frac{\Sigma\, b_{xi}(E)}{C_x(E)}\right)}{C_n(E)\left(1 - \frac{b_n}{C_n(E)} - \frac{\Sigma\, b_{ni}(E)}{C_n(E)}\right)} \;, \qquad (3)$$

which shows that background corrections are energy dependent correction factors. Equations (1), (2) and (3), obvious to the experimenter, were recounted here in order to show that i) no additive terms occurs, and ii) the shape measurement is a measurement of the energy dependence of the cross section with an undetermined factor and not an undetermined bias. An evaluator who uses polynomials in fitting experimental data will not find support for an interpretation of the a_0-term of the polynomial as a background of the measured values. In addition, the constant background which enters as an energy dependent background-to-foreground ratio is usually small and well determined, thus of negligible error and not adjustable.

II.2. Overdetermination of the Data Base

If several measurements exist for the same unknown quantity, it is well recognized that an overdetermination exists and it is well accepted, that the best estimator for the quantity is obtained as a weighted average of the measured values. This is the least-squares-estimator, if it is based on the minimization of the sums of the squares of the deviations between the measured values and the average value.

Another form of overdetermination exists if a value was measured for one quantity, another value for a second quantity, and a third measurement was made, for example for the ratio or sum of the two quantities. Obviously, three values were measured for only two unknown quantities.

These two types of overdetermination are dealt with mathematically identical. However, we note here that an important difference may exist which makes the second type more valuable for obtaining an unbiased estimator: Measurements of the same quantity may be subject to similar errors, specifically the psychological error explained below, and thus result in an biased evaluated value. Measurements of different quantities are more likely to be subject to different errors and therefore more probably provide a data base with overall random errors.

Absolute measurements of several cross sections are of equal value (assuming equal accuracy) and our best knowledge of any one of these cross sections is determined by all of the measurements if ratio measurements between them are available. Because of the equivalence of any absolute measurement, a real justification for declaring some cross sections "standards" or even "primary standards" and "secondary standards" does not

exist. However, defining some cross sections as "standards" because their physical behavior provides for convenient detection schemes has resulted in a concentration of absolute measurements on these cross sections. This permits us to limit our considerations to these "standards" and some cross sections which are important for applications and for which therefore also absolute measurements were carried out.

Removal of the second type of overdetermination is sometimes referred to as a consistency fit or a simultaneous evaluation of several cross sections. Such simultaneous evaluations were carried out, for example, for the thermal parameters [8], and for standard, fission and capture cross sections [9,10].

II.3. Errors, Uncertainties, and Correlations

It is assumed that the experimental values have been reported in terms of the following parameters.

E	The average energy at which a value was measured,
ΔE	The uncertainty of this energy,
R_{es}	The energy resolution or energy spread,
σ, R	The measured cross section or ratio,
$\Delta\sigma$	The total uncertainty of the measured value,
$\Delta\sigma_{st}$	The statistical uncertainty of the measured value

It is a basic feature of the measuring process to result in uncertain values. The true uncertainty is composed of several components, which may be subdivided as follows [9, 11, 12]:

$\Delta\sigma_R$	The normalization uncertainty, which is the uncertainty of a, $\prod_i a_i$ in Eqs. (1) and (2). This is an energy independent systematic uncertainty and thus totally correlated for all measured values $\sigma(E_i)$. It contains the uncertainties of the sample masses, calibration etc.
$\Delta\sigma_S$	The energy dependent systematic uncertainties which were estimated or calculated from the uncertainties of models and parameters used to calculate corrections, background subtraction, energy dependence of efficiencies, etc. Because of the energy dependence of these uncertainties, these errors correlate the measured values only par-

tially, often causing larger correlations for values at adjacent energies than between values measured at substantially different energies.

$\Delta\sigma_{st}$ The statistical uncertainty caused by the limited number of events counted for the primary reaction rates as well as for the background. Note that the statistical error may become a totally correlated systematic error if a shape measurement is normalized to an absolute value or if two segments are normalized to one another in the overlap range.

$\Delta\sigma_a$ The accidental error which may be revealed by repeating the identical experiment (i.e. reproducibility),

$\Delta\sigma_u$ The unknown error, which is systematic in nature and caused by not recognizing necessary corrections or underestimating uncertainties,

$\Delta\sigma_{ps}$ The psychological error which is caused by satisfaction with agreement obtained with values reported by others, thus neglecting the search for additional effects in the measuring process or equipment which would require corrections, or, the opposite, that is the dissatisfaction with a disagreement with prior reported values and the subsequent search for one-directional corrections.

The last three error sources affect the evaluation in a similar way, that is, as an unkonwn error. However, their differences help to understand some effects, for example historical trends in reported cross sections as shown in Ref. 9.

We may differentiate between two types of correlations in considering the interdependence between different measured values caused by correlated errors:

i) Measurements of a cross section or ratio at different energies in one experiment are usually made with the same sample and detectors, thus all values are partially correlated.

ii) Measurements of different cross sections may be based upon the same neutron detection technique and thus causes these measurements to be correlated. Correlations between different measurements of the same cross section may be caused because the same sample or the same detector was used.

Figure 3 shows schematically how the different types of errors will influence an evaluation and what the correlation matrix for the energy-dependent measurement will look like. We assume for this demonstration an absolute measurement of a cross section as a function of energy and one additional independent measurement obtained only at one energy.

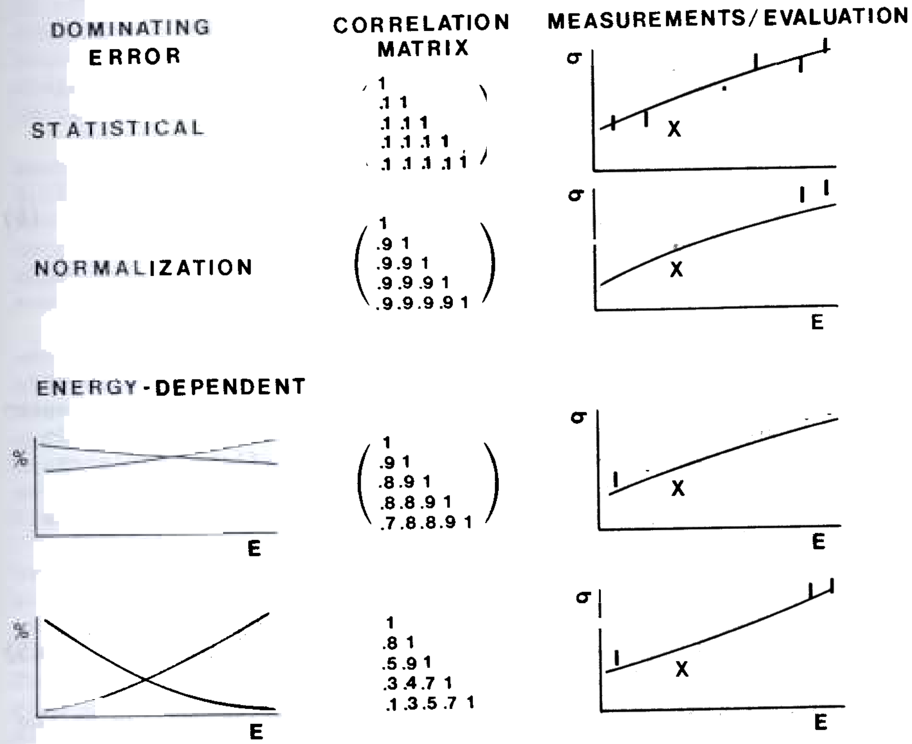

Fig. 3. The Effect of Dominating Errors on an Evaluation. The Correlation Matrix is Shown for the Energy-Dependent Measurement.

Our knowledge is improved only at the energy where the additional measured value was obtained if the dominating error is statistical. However, our knowledge is improved over the whole energy range by the additional independent measurement if the dominating error is due to the normalization. The effect on the evaluation result for dominant energy dependent errors is similar as for the case of dominant normalization errors if the energy dependence of the systematic errors is weak. Strongly energy dependent systematic errors cause a "flexibility" of the shape measured in the one experiment.

An additional cross section uncertainty is caused by the energy dependence of the cross section and the energy uncertainty, ΔE. This can be derived approximately from

$$\Delta\sigma_E^{\ 2} = \left(\frac{\partial\sigma}{\partial E}\right)^2 \Delta E^2 + \sum_i \left(\frac{\partial\sigma}{\partial f_i}\right)^2 \left(\frac{\partial f_i}{\partial E}\right)^2 \Delta E^2$$

$$+ 2 \sum_{i,k} \frac{\partial\sigma}{\partial f_i} \frac{\partial f_i}{\partial E} \frac{\partial\sigma}{\partial f_k} \frac{\partial f_k}{\partial E} \Delta E^2 \tag{4}$$

where the first term is the cross section uncertainty caused by the energy dependence of the cross section and the second term is that caused by the energy dependence of efficiencies and corrections. The third term is a pairwise sum which causes a reduction if two of the factors have the opposite energy dependence. The first term usually suffices because of the second-order nature of corrections and the choice of flat-efficiency detectors. The same expression [4] applies for ratio measurements with $\sigma \rightarrow R$. However, the cross section uncertainty of a cross section measured relative to another cross section and used as such in the evaluation is given by

$$\Delta\sigma_E^{\ 2} = \left(\frac{\partial\sigma}{\partial E}\right)^2 \Delta E^2 + \left(\frac{\partial\sigma_R}{\partial E}\right)^2 \Delta E^2 - 2 \frac{\partial\sigma}{\partial E} \frac{\partial\sigma_R}{\partial E} \Delta E^2 \quad , \tag{5}$$

A measured value differs from the true cross section by the true errors:

$$\sigma_i = \sigma_o + \sum_{k=1}^{m} p_{ik} \frac{\partial\sigma_i}{\partial f_{ik}} \Delta f_i + v_i \tag{6}$$

where σ_i is the measured value, σ_o is the true cross section $\partial\sigma_i/\partial f_{ik}$ is the sensitivity of the cross section to the k.th factor used to derive the measured value, and Δf_{ik} is the estimated uncertainty for this factor. The p_i have some distribution (normal if the uncertainty is statistical) but are unknown. Also unknown is the additional unknown error v_i.
It is not possible to determine the true errors (along with the true value σ_o) because the system of equations obtained with repeated measurements remains hopelessly underdetermined.

II.4. Energy Range, Average Cross Sections, Fluctuations

The energy range choosen for an evaluation which has the aim of obtaining the best knowledge must be selected based on regions of available absolute data information. A limited energy range may be of interest for particular applications, for example fast reactor design calculations. The best knowledge of the cross sections in this range is not only determined by measurements within this range but by well known absolute thermal and 14 MeV cross sections as well. Energy dependent absolute and shape measurements provide the link between the range of interest and such particular sources of information as values at .0253 eV and 14 MeV.

We are interested here in the evaluation of average cross sections. At thermal energy this is simply the value at 0.0253 eV. In the resolved resonance range bin average values would be used. Above the resolved resonance range the cross section values at specific energies, averaged over fluctuations which exist for some of the cross sections in the unresolved energy range, are the subject of the evaluation.

Experimental values measured in a range of fluctuating cross sections depend on the resolution of the measurement and require a correction in order to obtain average cross section values. Such corrections can be obtained from high resolution measurements which are available for Au(n,γ), ^{238}U(n,γ) and ^{235}U(n,f). Where such measurements are not available (e.g. above 100 keV) an error may be estimated by extrapolation from the high resolution data available at lower energies [15, 16, 17].

For many evaluations an energy grid is established for which cross section values are obtained [9, 12, 13, 14, 17]. The energy grid density should be choosen to present the gross structure of the cross section. Somewhat different techniques are used to obtain "experimental values" at these grid points. The method used here and at previous occasions [12] is demonstrated in Fig. 4. Experimental values from one data set which are within the range given by the centers between neighboring energy grid points are extrapolated to the grid point by using the shape obtained from (in sequence of preference)

i) an analytical a priori representation of the cross section (for example available for the H(n,n) cross section)

ii) a polynomial fit through neighboring points of an a priori cross section.

The weighted average value is then obtained at the grid energy point. The error of this point consists of the minimum systematic error of the contributing data values and a reduced statistical error.

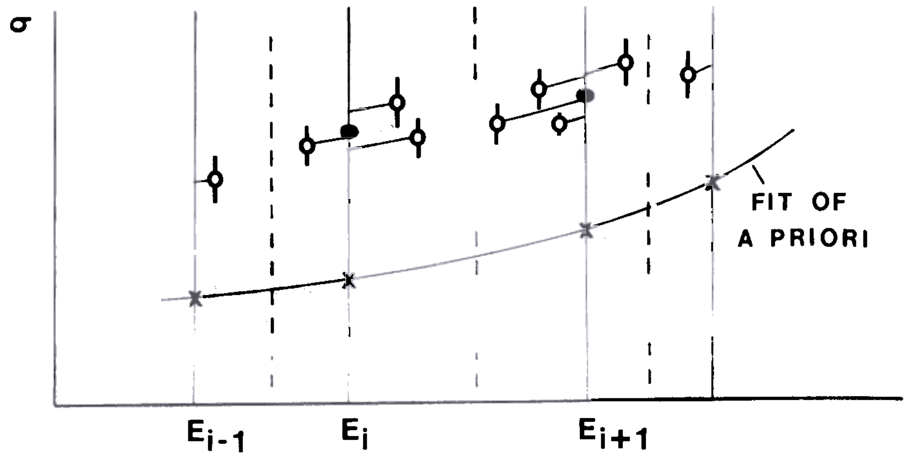

Fig. 4. Energy Grid and Procedure to Obtain "Experimental" Values at a Grid Energy.

Another approach is used by Schmittroth and Schenter [14], who introduce triangle or "roof" functions centered around the grid point. This procedure corresponds to the above, using linear extrapolation. Bhat [13] uses a polynomial fit of the difference between the experimental values and an a priori cross section. The latter procedure requires that grid values are only picked where data are in the vicinity of the grid energy. Tagesen et al. [27] form the average of data points adjacent to the grid point (correcting for the energy dependence of the cross section) and assign as an error the average error which appears to be an overestimate.

III. THE EVALUATION OF THE EXPERIMENTAL DATA

III.1. The Least-Squares-Estimator

The method of least-squares-evaluation of overdetermined data was devised by Gauss [18] (in prep school) and independently by Legendre [19] about 180 years ago. Though Legendre's publication on the subject actually preceded that by Gauss, the latter appears to be most frequently credited with this method in the literature, presumably because it has been generally accepted that he used the technique for some 10-15 years prior to its publication in all his calculations, and because he provided a foundation for the theory of least-squares-estimation (actually three successive explanations, the second basing on maximum likelihood estimation, previously derived by Bernoulli, and the third, the most general, based on the requirement of an unbiased estimator of minimum variance).

The unknown quantities in our consideration are the cross sections $\sigma_\ell(E_i)$, where ℓ refers to a specific reaction and E_i to the energy grid values. The energy grid must be identical for all cross sections; however, not all cross sections need to be included at all grid points. Additional unkonwn quantities are the normalization factors, a_k, of the cross section shape and ratio shape measurements. We denote the unknowns in consecutive order with $\sigma_1, \sigma_2 \ldots \sigma_j, a_1, a_2 \ldots a_\ell$, where $\sigma_1, \sigma_2 \ldots \sigma_i$ are the cross sections at consecutive energy grid points for one of the cross sections, $\sigma_{i+1}, \sigma_{i+2} \ldots \sigma_k$ those for another, etc.

The values obtained from the experimental data at the grid points with the procedure described above provide the n measured values

$$m_i = f(\sigma_1, \sigma_2 \ldots \sigma_j; a_1, a_2 \ldots a_\ell) \qquad i = 1 \ldots n \tag{7}$$

which overdetermine the system of $j + \ell$ unknown quantities with $n - j - \ell$ degrees of freedom. The least-squares-procedure to remove the overdetermination is to make adjustments, v_i, on the measured values, m_i, in order to obtain a consistent set of values

$$m'_i = m_i + v_i \tag{8}$$

Making such adjustments, v_i, is justified because the measured values have errors, ε_i, and we may set $v_i = \varepsilon_i$. We minimize the adjustments such that

$$F = \sum_i v_i^2 = \text{Min} \tag{9}$$

In order to obtain a linear relationship between the measured values, errors, and variables, σ_i, a_k, we make a Taylor-series expansion of f around prior estimated values of σ, a, which we denote $\hat\sigma$, $\hat a$

$$f(\sigma_1, \sigma_2 \ldots \sigma_j; a_1, a_2 \ldots a_\ell) = f(\hat\sigma_1, \hat\sigma_2 \ldots \hat\sigma_j; \hat a_1, \hat a_2 \ldots \hat a_\ell)$$

$$+ (\sigma_1 - \hat\sigma_1) \left.\frac{\partial f}{\partial \sigma_1}\right|_{\hat\sigma,\hat a} + (\sigma_2 - \hat\sigma_2) \left.\frac{\partial f}{\partial \sigma_2}\right|_{\hat\sigma,\hat a} + \ldots$$

$$\ldots + (a_1 - \hat a_1) \left.\frac{\partial f}{\partial a_1}\right|_{\hat\sigma,\hat a} + \ldots \tag{10}$$

and neglect the higher order terms. In addition, we substitute

$$\delta_i = \frac{\sigma_i - \hat{\sigma}_i}{\hat{\sigma}_i} \qquad \rho_k = \frac{a_k - \hat{a}_k}{\hat{a}_k} \tag{11}$$

and make a transformation of the measured values

$$M_i = \frac{m_i - f(\hat{\sigma}_1, \hat{\sigma}_2, \ldots \hat{\sigma}_j; \hat{a}_1, \hat{a}_2 \ldots \hat{a}_\ell)}{\Delta m_i} \tag{12}$$

where Δm_i is the squareroot of the variance of the measured value, m_i, i.e. the standard deviation. The set of linear equations which we obtain is

$$M = \frac{\hat{\sigma}_i}{\Delta m}\,\delta_i + \varepsilon \qquad \text{for cross section measurements} \tag{13a}$$

$$M = \frac{\hat{\sigma}_i/\hat{\sigma}_k}{\Delta m}\,\delta_i - \frac{\hat{\sigma}_i/\hat{\sigma}_k}{\Delta m}\,\delta_k + \varepsilon \qquad \text{for ratio measurements} \tag{13b}$$

$$M = \frac{\hat{\sigma}_i}{\Delta m}\,\delta_i + \frac{\hat{\sigma}_k}{\Delta m}\,\delta_k + \ldots + \varepsilon \qquad \text{for total cross section measurements} \tag{13c}$$

$$M = \frac{\hat{a}_\ell\hat{\sigma}_i}{\Delta m}\,\delta_i + \frac{\hat{a}_\ell\hat{\sigma}_i}{\Delta m}\,\rho_\ell + \varepsilon \qquad \text{for cross section shape measurements} \tag{13d}$$

$$M = \frac{\hat{a}_\ell\hat{\sigma}_i/\hat{\sigma}_k}{\Delta m}\,\delta_i - \frac{\hat{a}_\ell\hat{\sigma}_i/\hat{\sigma}_k}{\Delta m}\,\delta_r + \frac{\hat{a}_\ell\hat{\sigma}_i/\hat{\sigma}_k}{\Delta m}\,\rho_\ell + \varepsilon$$

for a ratio shape measurement, and (13e)

$$M = c_i\delta_i + c_{i+1}\,\delta_{i+1} + \ldots \ldots + \varepsilon \tag{13f}$$

$$C_i = \frac{\phi_i\ \Delta E_i}{\sum \phi_k \Delta E_k} \cdot \frac{\hat{\sigma}_i}{\Delta m} \qquad \text{for an average cross section measurement.}$$

Equations (13a-f) give the expressions obtained for the different types of measurements considered here. Expressions for other quantities can be obtained as easily.

These equations can be written as a matrix equation

$$M = A\ \delta + \varepsilon \tag{14}$$

where M is the measurement vector, A is the coefficient matrix, δ is the vector of the unknowns (actually containing ρ as well), and ε is the error vector. We obtain the least-squares estimator for δ by minimization of the scalar

$$F = \varepsilon^T C_M^{-1}\ \varepsilon = (M - A\delta)^T C_M^{-1}\ (M - A\delta) \tag{15}$$

where C_M is the variance - covariance matrix of M, and T denotes the transpose. We assume that the variance - covariance matrix, C_m, of the measurements, m_i, is known and obtain the variance - covariance matrix, C_M, from

$$C_M = Q\ C_m\ Q^T \tag{16}$$

where for a linear transformation, as above,

$$Q = \begin{pmatrix} \frac{\partial M_1}{\partial m_1} & \frac{\partial M_2}{\partial m_1} & \cdots \\ \frac{\partial M_1}{\partial m_2} & \frac{\partial M_2}{\partial m_2} & \cdots \\ \vdots & \vdots & \end{pmatrix} \tag{17}$$

Choosing the transformation Eq. (12) results in the correlation matrix of the originally measured values

$$\text{VAR-COVAR (M)} = C_M = \text{COR (m)} \ . \tag{18}$$

According to the Gauss-Markov-theorem, extended to correlated measurements by Aitken, the least-squares-estimator is an unbiased estimator with minimum variance. Minimization of F is achieved with

$$\frac{\partial F}{\partial \delta_i} = 0 \tag{19}$$

which yields the normal equations for δ,

$$\delta = (A^T C_M^{-1} A)^{-1}\ A^T C_M^{-1} M \tag{20}$$

and following from error propagation

$$C_\delta = (A^T C_M^{-1} A)^{-1} \tag{21}$$

as the variance - covariance matrix of the least-squares-estimator δ. The results for the σ's are derived from the δ's and the variance - covariance matrix, as above, from C_δ

$$\sigma = (1 + \delta) \cdot \hat{\sigma} \quad , \ a = (1 + \rho) \cdot \hat{a} \quad , \ C_\sigma = Q\ C_\delta\ Q^T \ , \tag{22}$$

Q, of course, derived from the different transformation.

Using, as an approximation, the assumption of uncorrelated data yields

$$C_M = I \quad ,$$

the identity matrix, and therefore

$$\delta = (A^T A)^{-1} A^T M \tag{23}$$

with

$$C_\delta = (A^T A)^{-1} \tag{24}$$

We note that $A^TC^{-1}A$ and $A^TC^{-1}M$ in Eq. 20 have the same structure and we can include M as an additional column vector in A. Instead of inverting C we could then resolve the linear equation system $A = CB$, where $B = A^TC^{-1}A_{r+1}$, which is computationally faster and more accurate. Likewise, the solution, δ, can be obtained from the resolution of the linear equation system $(A^TB_r)\delta = A^TB_{r+1}$, if we are not interested in the variance - covariance of the solution, δ.

The formalism summarized above is represented in textbooks too many to reference here, some of the more handy for applications are given in Ref. 20. In some of these FORTRAN programs ready to use for obtaining the solution, $\delta = (A^TC^{-1}A)^{-1} (A^TC^{-1}M)$, are given, but usually only usable for small n. Software packages for matrix inversions and the resolution of linear equation systems are readily available. At Argonne, a software package, LINPAC, is available which was developed at Argonne in cooperation with other laboratories and universities and is extremely efficient [21].

The coefficient matrix, A, is of size $N(=n) \times R(=j+\ell)$. Its structure is shown in Fig. 5. The elements, α_{ik}, are the coefficients from the Taylor series expansions (Eqs. 13a-f). Usually no more than three elements in a row are nonzero. However, for total cross section values, each partial cross section has a nonzero entry. For average cross section data as many entries as there are unknowns for this cross section are nonzero. Columns are similarly nearly empty. But for shape data there are as many entries as experimental values in the set. The coefficient matrix consists of submatrices given by the experimental data sets as indicated in Fig. 5.

The correlation matrix, C_M, is of size N x N and its structure is shown in Fig. 6. It consists of submatrices around the diagonal which correspond to the correlation matrices of particular data sets, and nonzero off-diagonal blocks which contain the correlation coefficients between different experiments.

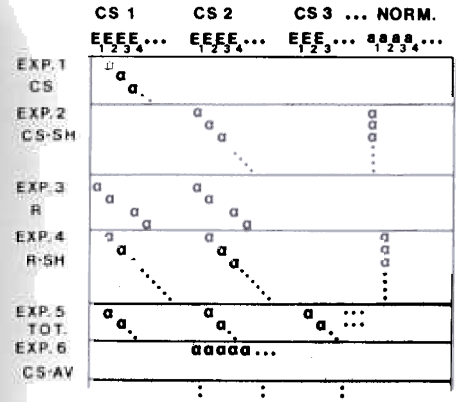

Fig. 5. The Entries into the Coefficient Matrix, A.

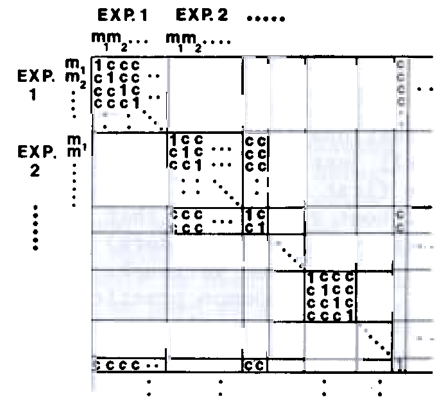

Fig. 6. Schematic of the Correlation Matrix, C.

A consistency least-squares-fit of measured values for two activation cross sections of ^{115}In, a ratio between them, and an absorption cross section at thermal energy [22] may serve as a very simple example for the application of the above formalism to nuclear data. Four experimental values were available for only two unknowns and a least-squares-fit provided a consistent set of values. The same procedure was used to obtain consistent data for several energy-dependent cross sections by employing Eq. 23 [9]. The formalism has been applied more recently for the evaluation of single cross sections as a function of energy using Eq. 20 [42, 14].

The size of the presently considered system is not quite that simple. We are concerned about the simultaneous evaluation of ~10 cross sections, an energy grid of ~100 points appears desirable, and about 10 measurements are available per cross section (less for some, more for others; also ratio and total cross section measurements would have to be counted). Thus, we estimate that $N \sim 10^4$. We find that the correlation matrix, C, alone exceeds computer core memory by several orders of magnitude. Since we recognized that many elements of the coefficient matrix, A, and the correlation matrix, C, are zero, sparce matrix storage and handling might be used (a sparce matrix software package, for example is available at the Harwell Software Library). Inversion of the correlation matrix as well as the subsequent matrix multiplication would take days and appears cost-prohibitive.

III.2. Approximations Used to Avoid the Monstrous System of Normal Equations and Their Shortcomings

The easiest way out of the seemingly huge system of normal equations (Eq. 20) would be to find approximations which are well justified. Before considering such approximations, let us first consider a procedure which is commonly used (probably without realization that it is an approximation to the correct least-squares procedure) and yields a biased estimator which is not of minimum variance.

It is common practice to normalize cross sections, most often obtained relative to another cross section, at thermal energies. Evaluators use such data by updating to the most recent reference cross sections and thermal cross section value. Then they obtain an (hopefully weighted) average values at all energies higher than thermal. Subsequently the possible agreements or discrepancies are pointed out and commended or lamented. The procedure appears to be logical as the thermal value is the preferable absolute value available for these measurements. However, this procedure represents a separation of the general least-squares problem into two steps, each of which may have been handled by the least-squares method. The separation introduces an approximation and results in a biased estimator which does not have minimum variance. The difference between the "logical" use of the available information and the least-squares procedure is shown in Fig. 7. The answer is, of course, different. The difference (the bias) can be easily estimated. It will be $\lesssim 0.3\%$ if the shape values differed by ~10%, thus it is small compared with the data difference. However, the difference for the variance may be much larger, depending on its derivation for the "logical" procedure.

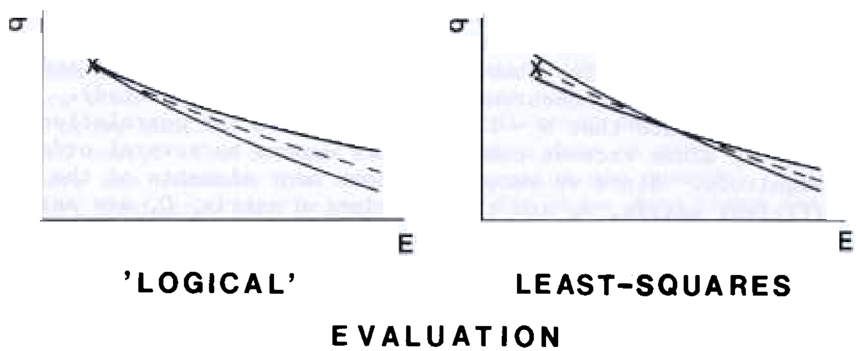

Fig. 7. Comparison of a "Logical" and the Least-Squares Evaluation.

Next, we consider approximations intentionally made to avoid the size of the system given with Eq. 20. The major problem appears to be the correlations which require Eq. 20 to be used instead of Eq. 23. Correlations between experimental data sets can be easily removed. Three different cross sections measured by the same experimentalists using the same neutron flux detection technique or the same calibrated neutron detector provide information for one of these cross sections, say $\sigma_1(E)$, and the ratio between the other two, $R_{23}(E) = \sigma_2(E)/\sigma_3(E)$. Measurements of a cross section with the same sample as used in another measurement of the same cross section can be used as a shape data set. The correlations are removed in each of these examples without loosing much information. Most other sources for correlations between different data sets were already removed by using the originally measured quantities, e.g. ratios, for the evaluation.

The major source of correlations between values of one data set seems to be due to the normalization (mass, efficiency, etc.). To give an example: The recent absolute measurements of the ratio between the cross sections $^{235}U(n,f)$ and $H(n,n)$ by Kari [23] have a total uncertainty of ~3% of which ~2.5% are due to the normalization and ~1% due to statistics. Other measurements, mostly for the shape of a cross section or ratio, have small systematic and thus negligible correlated errors. For example, the measurements of the shape of $\sigma_{n,f}(^{235}U)/\sigma_{n,n}(H)$ by Carlson and Patrick [24] have an uncertainty of ~2-3% but only a 0.5% systematic uncertainty.

This suggests to separate the evaluation of the shape from the evaluation of the normalization. The data would be treated as totally uncorrelated for the shape evaluation and as totally correlated for the evaluation of the normalization. We immediately recognize that we obtain a biased estimator as a consequence of separating the evaluation into two steps as shown above. However, because the bias appears to be very small, this will be acceptable. This procedure was used in various evaluations [9, 12, 25].

The evaluation of the shape can be carried out in several ways:

i) The energy dependent absolute data and the shape data are normalized to an 'a priori' cross section and then a least-squares estimator is obtained [9]. The discontinuity of the available data information may result in a dependence on the a priori cross section which might not be removed in iterative steps.

ii) The unknown normalization contained in the equations [13] can be removed by Gaussian elimination. This corresponds to forming the ratio of the measured shape data (or absolute data) to a value at any energy, $R_{ik} = a\cdot\sigma(E_i)/a\cdot\sigma(E_k)$. The evaluation of the ratios, R_{ik}, by least-squares methods then defines the shape of the cross section [25].

iii) Another method recently devised to avoid the small bias introduced by separating the shape evaluation from the normalization evaluation consists of shifting the shape "up or down" parallel to the σ - axis. This corresponds to adding or subtracting a constant to the measured values which appears to be in contradiction to the way the experimental data are derived (see Eqs. 1-3, the normalization is a factor, thus "shifting" would be only permissible on a logarithmical scale). The problems this procedure creates can be easily demonstrated if the shape measurements change over a large range. For example, suppose two measurements of $^{235}U(n,f)$ were quoted at thermal energy with 587b and 585b and at 30 keV with 2b and 1.9b, respectively, and they were shifted to a new normalization value of 583b at thermal. The result at 30 keV would be -1.05b.

III.3. The Solution of the Least-Squares Problem

We realize that Gauss and his contemporaries must have faced a similar problem (as we do today) with the large number of the normal equations. Of course, their data base was small compared to ours, maybe 100-200 values where we have 10^4. However, they did not have a computer. And indeed, Gauss points out in his supplement on the theory of least-squares [26] that, if a new data value becomes available, the calculation does not have to be repeated but the new value can be easily combined with the prior result. Gauss proceeds to provide proof for this and draws the obvious conclusion that reduced calculational effort will result by subdividing a large data base and to obtain subset-estimators which are to be combined in a subsequent step.

Using this suggestion, we first rearrange the sequence of the experimental data sets in such a way, that those which are correlated appear in one block. This results in a correlation matrix shown in Fig. 8. A convenient feature of a super-matrix of this type is that its inverse has the same structure and consists of the inverses of the submatrices. The subdivision of the matrix is given by the correlated and uncorrelated data sets. The simple rules of matrix multiplications immediately lead to the conclusion that $C^{-1}A$ has again a subdivision by data blocks, as shown also in Fig. 8. Multiplication with the transpose of the coefficient matrix, A^T, however, does not retain this separation. But we realize that the resulting matrix $B = A^TC^{-1}A$ has elements, β_{ik}, which are additive contributions from the different data blocks. The triple products which contribute to the element, β_{ik}, can be arranged in a similar geometric structure as the structure of the matrix, C. The result of the above is that we do not need to store the huge correlation matrix, C, we do not need to invert it, which reduces the problem of computer

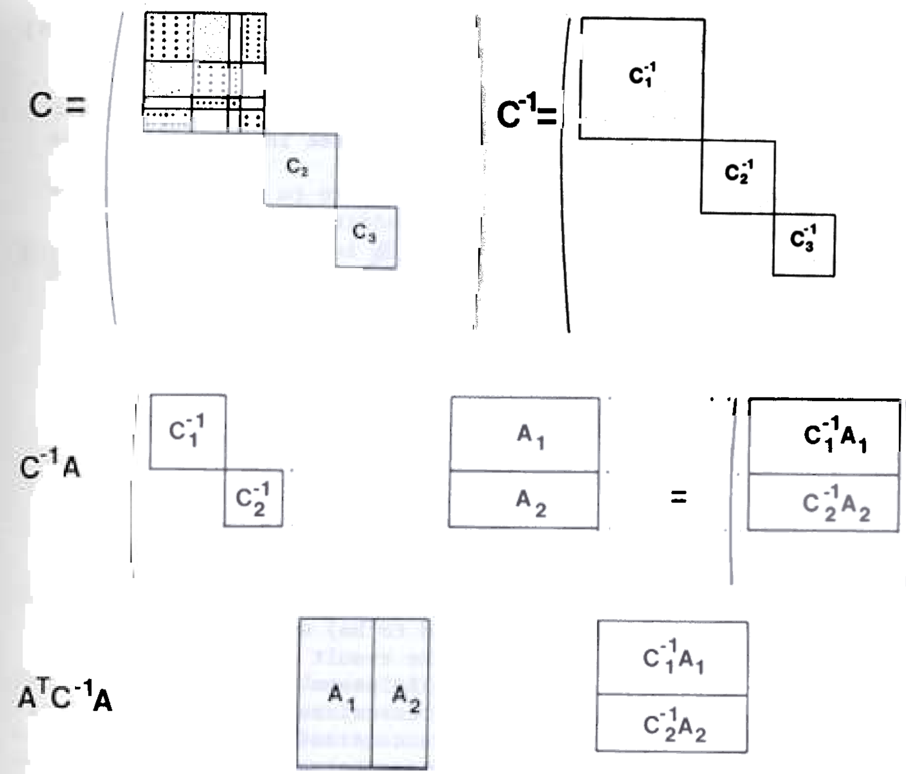

Fig. 8. The Reordered Correlation Matrix, C, and the Separation of Experimental Data Blocks in A^TC A.

time and storage space by several orders of magnitude. The contributions of the matrix product $A^TC^{-1}A$ to the elements β_{ik} can be obtained by handling one correlated or uncorrelated data block at the time. Sparce matrix storage and handling can be employed for the A matrix which further reduces the size of the required DO - loops.

The addition of a new data set, once a solution has been obtained, becomes as straightforward as shown by Gauss [26] and has been extended to correlated data as well [28]. The solution after evaluating i experimental data blocks and obtaining a new, (i + 1)th block which is uncorrelated with the previous data is obtained from

$$\delta_{i+1} = C_{\delta_{i+1}} A^T_{i+1} C^{-1}_{i+1} M_{i+1} \qquad (25)$$

$$C^{-1}_{\delta_{i+1}} = C^{-1}_{\delta_i} + A^T_{i+1}\, C^{-1}_{i+1}\, A_{i+} \qquad (26)$$

It has been shown by Schmittroth [45] that the inversion of the matrix in Eq. (26) which is required for use in Eq. (25) can be avoided.

It appears that the simplest procedure to add new information would be to do this directly by addition to the matrix elements, β_{ik}. A new measurement which is correlated with a data set previously included in the evaluation would require to first subtract the contribution from this set, combine it with the new data and then to add the new correlated block. Use of iterative steps in the evaluation appears also more straightforward by working directly with the β_{ik}'s.

III.4. The Variance - Covariance of the Result

Using the evaluation method outlined above provides the variance - covariance matrix of the result, $(A^TC^{-1}A)^{-1}$ for correlated data, and $(A^TA)^{-1}$ for uncorrelated data. We note that off-diagonal nonzero correlation coefficients occur even if the original data were (or were assumed to be) uncorrelated. The source for these correlations of the result are the ratio and total cross section measurements. It seems to be an obvious advantage to obtain the variance - covariance matrix as integral part of the evaluation process. In contrast, subsequent derivation of the uncertainty information appears to lead to many problems. For example, if the evaluation was biased, the subsequent derivation of the uncertainty will be unsymmetric.

The large amount of data contained in the correlation matrix usually causes it to be given in a reduced form. Care must be taken not to improperly extrapolate such information. The evaluated results still have a random error contribution. Thus extrapolation should not be to the diagonal 1.0 but to a lower value (see Fig. 9). However, if the evaluation result of the experimental data was subsequently fitted with a nuclear model, correlation increases for adjacent energies and a shape of the correlation matrix indicated by the dashed line in Fig. 9 can be expected.

The variance - covariance matrix in the above formalism is derived from error propagation, based on the assumption of random errors. Thus the variance of the estimator of a set of values, σ_i, with weights, w_i, is given by

$$V = \frac{\sum w_i\,(\sigma_i - \sigma)^2}{(n-1)\quad w_i} \qquad (27)$$

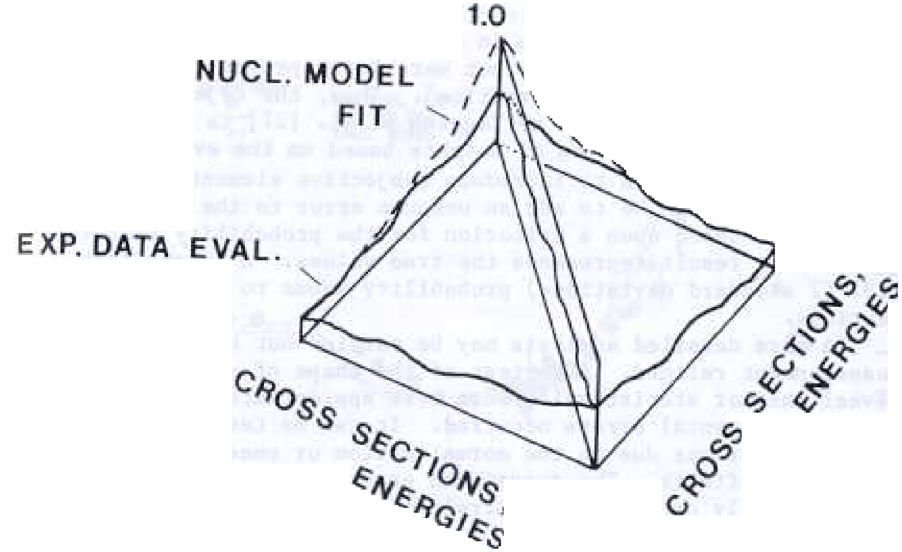

Fig. 9. Graphical Representation of the Correlation Matrix of the Result.

This probably will underestimate the true uncertainty of the result as the errors are not truely random. The problem has been often discussed but no unique answer exists. Grigoryan et al. [29] adjust the variance based upon differences between the external and internal errors by various combinations thereof, based upon prior work by Birge [30]. Tagesen et al. [27] select the larger of the external or internal error. Peelle [31] used a χ^2 test and suggests to increase the uncertainties by $\sqrt{\chi^2}$.

III.5. The Use of the Solution and its Variance - Covariance in Iterative Steps and Additional Analysis.

There are several reasons for using iterative steps, e.g. repeating the evaluation after a result was obtained. A rather trivial reason is that the Taylor-series expansions, Eqs. (13a-f), result in some cases in non-zero higher order terms. Of greater concern must be the influence of discrepant data on the result, specifically if such data are quoted with small (internal) errors. Usachev [32] points out that the evaluator obtains an improved knowledge of the quantity and thus has a means to find possible unknown errors of individual measurements. The problem is widely discussed in the literature [33] but procedures differ and have some subjective character. These methods range from rejection (Chauvenet's criterion) to error adjustment. It appears in the area of nuclear data more often than once that a new measurement resulted in values which were in disagreement with prior reported data sets of good consistency but were later proven to be correct or at least in the "right direction". Thus, the rejection of data, employed for example by Tagesen et al. [27] is not to be recommended. Introduction of weights based on the evaluators judgment [10] appears to introduce subjective elements. The best procedure seems to be to add an unknown error to the discrepant measurement based upon a criterion for the probability that the measurement result represents the true values. A lesser than 2.3% (2 standard deviations) probability seems to be sufficiently cautious.

A more detailed analysis may be carried out and error reassignment refined. A χ^2-test of the shape of a data set would reveal whether statistical errors were appropriately accounted for, or accidental errors occurred. It can be tested whether the unknown error was due to the normalization or energy dependent systematic effects. The reassigned error can then be accounted for as totally or partially correlated.

IV. THE USE OF AUXILIARY INFORMATION

The result obtained from the evaluation of the experimental data can be further improved by utilizing nuclear models. The first obvious benefit comes from a fit of the evaluated data with a nuclear model. The evaluated experimental data will show local fluctuations which are caused by statistical (uncorrelated) errors, data inconsistencies and an insufficient number of input data at some energy grid points. A nuclear model fit will remove these fluctuations and provide a result which is highly correlated for adjacent energies. This is shown for the capture cross section of ^{238}U in Fig. 10.

The nuclear model may also be used to obtain cross section information which is independent on the evaluated experimental cross sections, if other experimental data are available to determine the model parameters. In case of the capture cross section of ^{238}U, the major parameters are

V	The real optical potential strength,
V_E	The energy-dependence of V,
R_R	The radius of the real potential,
A_R	The diffusness of the real potential,
W	The imaginary optical potential strength,
W_E	The energy-dependence of W,

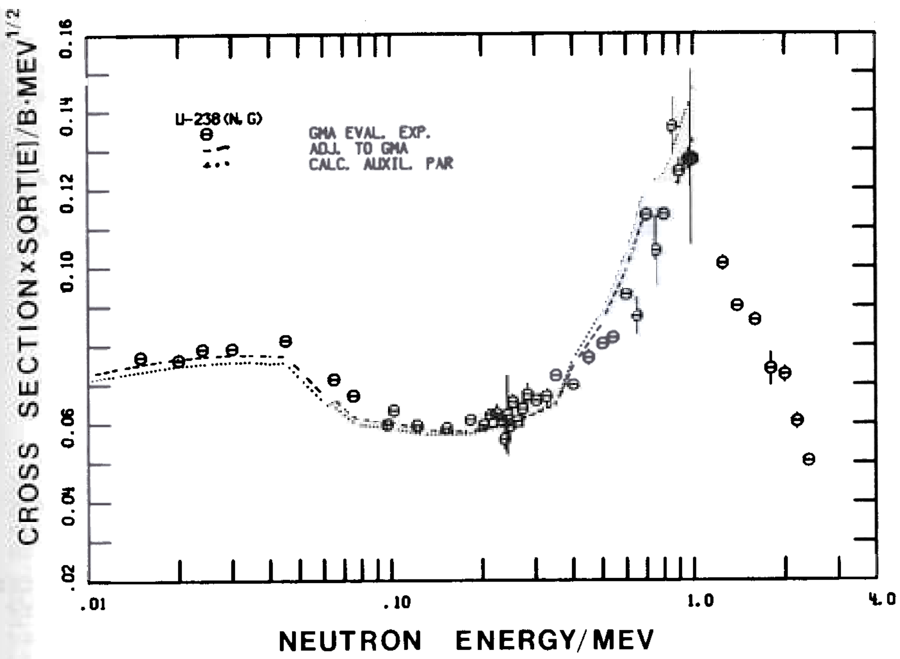

Fig. 10. Theoretical Model Calculations for $^{238}U(n,\gamma)$.

R_I	The radius of the imaginary potential,
A_I	The diffusness of the imaginary potential,
V_{SO}	The spin-orbit potential strength,
a	The level density parameter related to nuclear temperature,
σ	The spin-cut-off parameter of the level density,
E_G	The energy of the giant dipole resonance,
Γ_G	The width of the giant dipole resonance,
E_i, J_i, π_i	Parameters of low lying levels of the target nucleus,
Γ_γ/D	The gamma width over the average level spacing near the binding energy.

More refined models require the introduction of more parameters. The optical model parameters, V through V_{SO}, can be determined with total and scattering cross section measurements. Values for the level density parameters are known from a variety of sources. Γ_γ/D may be calculated from the level density formula and the giant dipole resonance, however, the resulting values are in substantial discrepancies with measured values. Thus, one prefers to use Γ_γ/D as determined experimentally close to the neutron binding energy.

In order to combine the cross section obtained from the nuclear model calculation with the directly evaluated data, its uncertainty has to be known. It consists of several components:

i) The data uncertainties used to derive the model parameters cause uncertainties of these parameters

ii) The model approximations cause uncertainties of the predictions.

The former can be quantitatively determined, however, the latter are much more difficult to assess. The next step is the determination of the sensitivity of the calculated cross section to the model parameters and to obtain its uncertainty.

The cross sections obtained from the fit of the evaluated experimental data can now be combined with the cross section obtained from the nuclear model calculation which is based upon other auxiliary data information by obtaining a weighted average. This is shown in Fig. 10 using again $^{238}U(n,\gamma)$ as an example. Another approach would be to include the model prediciton with its uncertainty in the original least-squares fit as an input set.

V. COMPARISON OF VARIOUS EVALUATIONS

The least-squares fitting program used in 1970 [9] which based on Eq. 23 was modified in order to include correctly correlations according to Eq. 20. This program is called GMA (for Gauss-Markov-Aitken) and follows the outline given in Sections III.1 and III.3. Results obtained with this program may be compared with other evaluations for which approximations were used. A first run was made using as input only data for $^{235}U(n,f)$ and ratios to H(n,n) above 100 keV. This permits to compare the GMA result with the evaluations by Konshin et al. [34], Poenitz [12], and Bhat [35]. The data base used by Konshin et al. was somewhat different from the one used by Poenitz and by Bhat. Konshin et al [34] included correlations in the determination of weights for the experimental data. Their procedure differs from the commonly used method which was summarized in Section III.1, however, should be expected to lead to similar results. Poenitz [12] used approximations

to handle correlations as outlined in Section III.2. Bhat [35] employed a technique of data fitting which was developed by Forsythe [36], neglecting correlations. Fission spectrum average cross sections were used by Poenitz but not by Konshin et al. nor Bhat. The results from these evaluations are compared in Fig. 11 with the result from GMA. Interative steps (see Section III.5) and nuclear model smoothening were not yet applied in GMA.

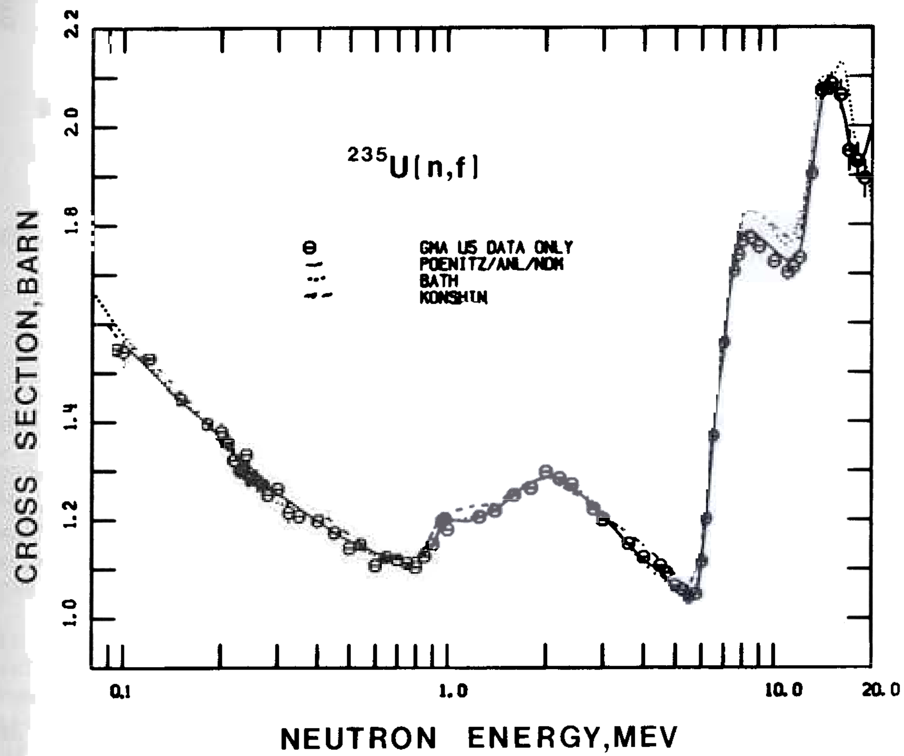

Fig. 11. Comparison of Several $^{235}U(n,f)$ Evaluations.

The agreement between the evaluations by Poenitz [12] and by Bhat [35] is very good in the energy range from 100 keV to 6 MeV and confirmed by the present GMA result. The evaluation by Konshin et al. [34] differs by 2-3% in the energy ranges 0.8-1.5 MeV and 3.5-6 MeV. The difference appears to be due to several factors: i) one particular data set has an excessively high weight between 1 and 6 MeV, ii) the cross section uncertainties due to energy uncertainties were not taken into account, and iii) the data base was lacking some of the newer sets included by Poenitz [12] and by Bhat [35].

Konshin et al. [34] obtained between 8 and 12 MeV ~2.5% higher values as a consequence of their higher values between 3.5 and 6 MeV, this means that they agree in shape with the evaluation by Poenitz [12], a result also confirmed by GMA. The evaluation by Bhat [35] differs above 8 MeV by ~2.5% and more than 4% at 16 MeV. This appears to be the consequence of not taking into account the correlated errors.

A more direct comparison can be made by consideration of the ratio between values in the 8.0-8.5 MeV range vs. the 5.0-5.5 MeV range:

Experimental values	
Kari [37]	1.687 ± .028
Czirr and Sidhu [39]	1.688 ± .019
Poenitz [40]	1.745 ± .061
Smith et al. [41]	1.625 ± .036
Average	1.681 ± .015
Ratios from Evaluations	
Konshin et al. [34]	1.703 ± .029
Poenitz [12]	1.710
Bhat [35]	1.736
GMA (present)	1.680 ± .016

Correlated errors were taken into account in the calculation of the experimental ratio values.

The least-squares consistency fit of data for $^{235}U(n,f)$, $^{197}Au(n,\gamma)$, $^{238}U(n,\gamma)$ and $^{6}Li(n,\alpha)$ resulted 10 years ago in substantially lower $^{235}U(n,f)$ cross section values than the direct measurements would have indicated (Poenitz [9]). This difference appears to be much less for the present data base, e.g. the consistency of the experimental data has greatly improved. Figure 12 shows the difference between the GMA result for $^{235}U(n,f)$, using $^{235}U(n,f)$ data alone and using data on $^{235}U(n,f)$, $^{238}U(n,\gamma)$, $^{197}Au(n,\gamma)$, H(n,n), $^{6}Li(n,\alpha)$, $^{6}Li(n,n)$, $^{10}B(n,\alpha)$, $^{10}B(n,\alpha\gamma)$, and $^{10}B(n,n)$, and ratios as well as total cross sections for these reactions. This result may somewhat change as all data were not yet included in the fit.

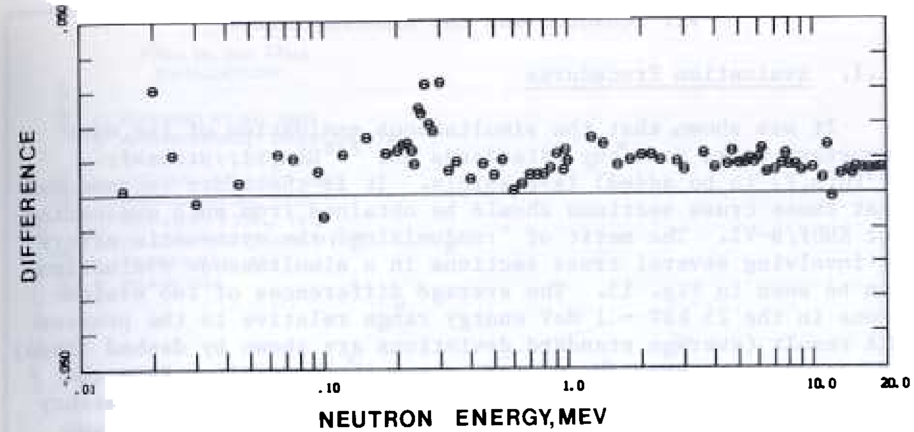

Fig. 12. The Difference for $^{235}U(n,f)$ between an Evaluation of $^{235}U(n,f)$ Data and a Simultaneous Evaluation of Several Cross Sections.

The thermal cross section of $^{235}U(n,f)$ evaluated by Leonard [37] (583.54 ± 2.92 b) was used as input for the fit. The fitting result is 588.6 ± 2.5 b, in better agreement with a value which would be obtained from a consistency fit of the 2200m sec data (Lemmel [39]). The thermal cross section for $^{6}Li(n,\alpha)$ obtained from the GMA fit is 942.4 ± 2.4 b in contrast with 935.9 B presently used on ENDF/B-V. Antoher "oddity" appears to be that the GMA evaluated value for $^{235}U(n,f)$ at ~14 MeV is lower than any of the measured values (by ~1.5%).

An interesting consideration is the H(n,n) cross section. It is sometimes pointed out that cross sections measured relative to the H(n,n) cross section should be preferred (or heavier weighted) in an evaluation because the H(n,n) cross section is so well known. This appears to be a pseudological or incomplete logical argument because the uncertainty of a cross section measurements does not depend on the uncertainty of the reference cross section alone, but on its implementation as well (besides other factors). The H(n,n) cross section is well known because it is identical to the total cross section (above thermal energies), but in cross section ratio measurements it is used as a reaction cross section and the problems associated with the determination of the reaction rate seem to have caused discrepancies up to ~30%. The present fit indicates somewhat lower cross sections for $\sigma_{n,n}(H)$ at higher energies (>3 MeV). This may be a consequence of $^{235}U(n,f)$ absolute data which are lower than those measured relative to H(n,n).

VI. CONCLUSIONS AND RECOMMENDATIONS

VI.1. Evaluation Procedures

It was shown that the simultaneous evaluation of the most important cross sections (standards and ^{238}U(n,γ), probably ^{239}Pu(n,f) to be added) is feasible. It is therefore recommended that these cross sections should be obtained from such evaluation for ENDF/B-VI. The merit of "randomizing" the systematic errors by involving several cross sections in a simultaneous evaluation can be seen in Fig. 13. The average differences of two evaluations in the 25 keV - 1 MeV energy range relative to the present GMA result (average standard deviations are shown by dashed lines) are shown. In three out of four cases the prediciton from the objective evaluation technique using a least-squares consistency fit proved better than other evaluations at that time [43] and even fall within the (somewhat optimistic) standard deviations of the GMA result. The fourth case is a standoff.

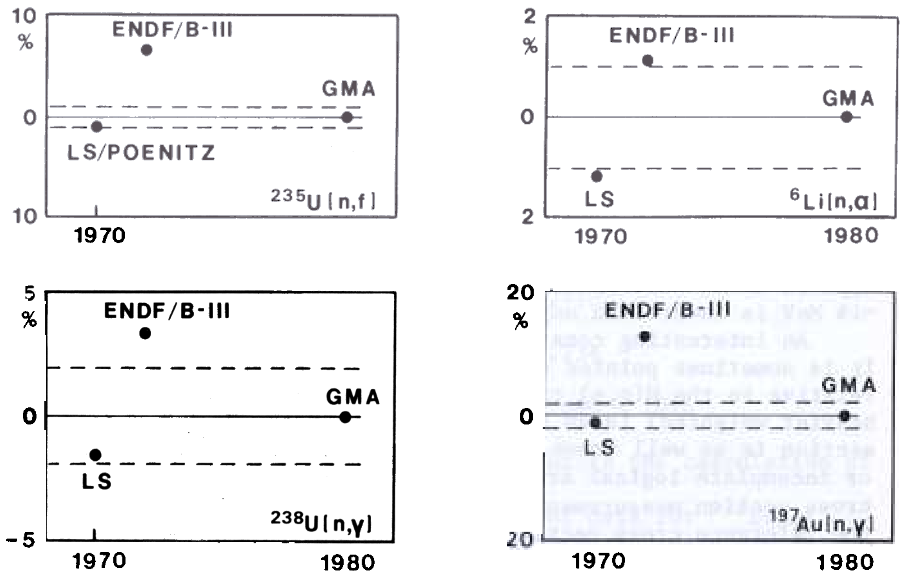

Fig. 13. Comparison of ENDF/B-III and a Least-Squares Evaluation with Present GMA Results. The Average Differences are Shown in Chronological Order.

Subjective evaluation might be very tempting, specifically if the data base is very poor. An example is shown in Fig. 14. Available data for the ^{23}Na(n,2n) cross section are discrepant and some evaluators choose one data set above all the others. The evaluation shown in the graph was based upon all available data (Adamski et al. [44]). Which evaluated result will prove

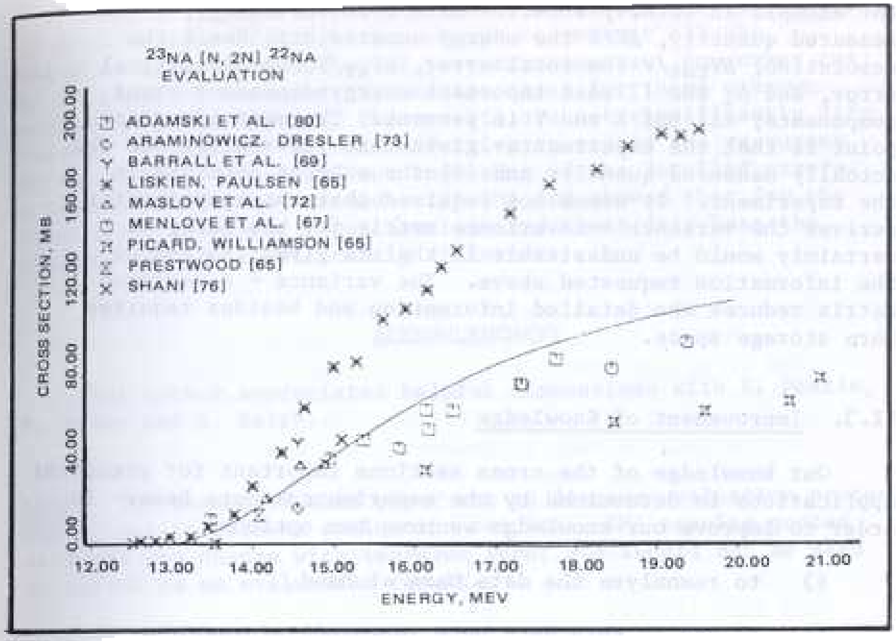

Fig. 14. ^{23}Na(n,2n). A Sore Data Base and an Objective Evaluation.

correct remains to be seen, but for now it may be noted that the evaluation which used all the available data appears to agree better with a prediction by Pearlstein's method for calculating these cross sections.

VI.2. Data Reporting and Data Files

Past data reporting has been insufficient, specifically when larger amounts of data were involved. The information needed from the experimenter is, besides the values E, ΔE, Res, $\Delta\sigma$, $\Delta\sigma_{st}$ (see Section III.3), the error components for each data point. This could be stored in a standard format on a data file, for example

$\Delta\sigma_R$ (normalization uncertainty, in percent)

$$(E,\ V,\ \Delta E/E,\ Res/E,\ \Delta V_{tot}/V,\ \Delta V_{st}/V,\ \Delta_i,\ i \quad 1 \ldots k)_\ell,$$

$$\ell = 1 \qquad n$$

for example in 2E10.4, 15F4.1. Here E is the energy, V the measured quantity, $\Delta E/E$ the energy uncertainty, Res/E the resolution, $\Delta V_{tot}/V$ the total error, $\Delta V_{st}/V$ the statistical error, and Δ_i the 11 most important energy-dependent error components; all but E and V in percent. The most important point is that the experimenter gives this information for the actually measured quantity and all the subsets obtained in the experiment. It seems not required that the experimenter derives the variance - covariance matrix for his data, it certainly would be undesirable if that is given instead of the information requested above. The variance - covariance matrix reduces the detailed information and besides requires more storage space.

VI.3. Improvement of Knowledge

Our knowledge of the cross sections important for practical applications is determined by the experimental data base. In order to improve our knowledge we have two options:

i) to reanalyze the data base at hand

ii) to add to this data base improved information.

A decision which choice to make will depend on the cost-efficiency much more than anything else. A recent study of past measurements of $\bar{\nu}$ of ^{252}Cf cost about one man year [45]. Ten measured values are in that data base of which four were re-analyzed. We have to deal with $\sim10^4-10^5$ data values in several hundred data sets. This suggests an expenditure of ~100 man years and we suggest that this will not be cost-effective. Past data give us a standard deviation of ~1% for the evaluated cross section of $^{235}U(n,f)$ and ~2-3% for $^{238}U(n,\gamma)$. Working these data over which have at best 2-3% uncertainties and differ by up to 10% for $^{235}U(n,f)$, and have uncertainties of ~3-5% and differ up to 20% for $^{238}U(n,\gamma)$ will not improve our knowledge significantly. It is suggested that instead of reshuffling the same old data, a new generation of measurements should be made. These new measurements must be usable to test the significance of our prior kowledge. For $^{235}U(n,f)$ and $^{238}U(n,\gamma)$ this means that only measurements with $\lesssim1\%$ and $\lesssim2\%$, respectively, will have any significance.

Another important question which should be ask is whether it will be cost-effective to attempt to recover all the detailed error information of past experiments. An answer can be obtained by assuming the extreme cases for these unknown errors (see Fig. 3). If the results are not significantly different, it will not be cost-effective to expend the resources on the task of improving our knowledge of the detailed errors. A test of this kind was made with GMA and showed that for the presently considered cross sections and their data base the results are not significantly different.

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Note: The intent of this paper was to discuss evaluation procedures, not to present evaluation results. GMA results quoted or shown may change with improved input and should not be used or quoted as an evaluation result.

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