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EXAMINATION OF VARIOUS ROLES FOR COVARIANCE MATRICES IN THE DEVELOPMENT, EVALUATION, AND APPLICATION OF NUCLEAR DATA

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The last decade has been a period of rapid development in the implementation of covariance-matrix methodology in nuclear data research. This paper offers some perspective on the progress which has been made, on some of the unresolved problems, and on the potential yet to be realized. These discussions address a variety of issues related to the development of nuclear data, the evaluation of nuclear data, and the applications for nuclear data. Topics examined are: the importance of designing and conducting experiments so that error information is conveniently generated; the procedures for identifying error sources and quantifying their magnitudes and correlations; the combination of errors; the importance of consistent and well-characterized measurement standards; the role of covariances in data parameterization (fitting); the estimation of covariances for values calculated from mathematical models; the identification of abnormalities in covariance matrices and the analysis of their consequences; the problems encountered in representing covariance information in evaluated files; the role of covariances in the weighting of diverse data sets; the comparison of various evaluation procedures involving covariance matrices; the role of covariances in updating existing evaluations; the influence of primary-data covariances in the analysis of covariances for derived quantities (sensitivity); and the role of covariances in the merging of diverse nuclear data information.

[Statistics, covariance matrices, error propagation, sensitivity, fitting, evaluation]

Introduction

A strong interest in the subject of nuclear data uncertainties began to emerge in the early 1970's, primarily in response to an important need within the reactor physics community for the development of rigorous methods of nuclear data manipulation, applicable to cross-section evaluations, to the analysis of results from various reactor benchmark experiments, and to reactor sensitivity studies. During the past decade there has also been substantial growth in the development and application of covariance methods in other areas of nuclear data research. The scope of this work has become so extensive that it is now virtually impossible for any one individual to master all of the details, let alone to address them in a review of this nature. The growth of activity in this field is reflected in Table 1.

Table 1: Numbers of papers dealing with covariance matrices, as presented at earlier conferences in the present series "Nuclear Data for Science and Technology."

Conference	Papers Dealing with Covariances
Washington (1975)	6
Harwell (1978)	6
Knoxville (1979)	23
Antwerp (1982)	17
Santa Fe (1985)	20

However, there are some less encouraging aspects of this story which are not evident in such numbers. It is a fact that the nuclear data community and many applied users of nuclear data have not demonstrated universal enthusiasm, or even compliance, concerning the implementation of covariance methodology. Responses have ranged from guarded, "Experience should be gained over the next few years to establish whether it is a practical approach" (D.L. Smith [Smi80]), to ambivalent, " ... widespread use of correlated uncertainty information is unlikely to cause a major upheaval in the nuclear world ... (though) in certain cases it can make a significant contribution ..." (A.K. McCracken [McC78]), to supportive, "Covariance ... methods are versatile and elegant analytical tools. ... The usefulness of these methods for routine data fitting applications ... would alone justify expending effort to learn the techniques." (D.L. Smith [Smi81]). These particular quotes do show that attitudes are changing toward a more favorable posture. Nevertheless, it is apparent that quite a few areas of applied nuclear research (and most basic nuclear studies) are largely untouched by the issue of covariance matrices.

Interest in nuclear data uncertainties is linked to the rational conviction that researchers ought to embrace procedures which yield a credible, and quantitatively accurate, foundation of basic physical information to guide the development of safe, reliable, and economically viable nuclear energy systems. Covariance methods are indeed playing a very important role in this context, and their impact on applications is likely to broaden. It is therefore essential that workers in this field become familiar with these methods and apply them whenever it appears that significant benefits might accrue.

Space limitations, and the broad scope of the subject, preclude this paper from being technically detailed. I have chosen to give a narrative overview, with the intent of appealing to a wide audience. Included are: a brief review of fundamental concepts, an examination of the role of covariance methods in several areas of applied nuclear science, and comments on the future potential of these methods and on some of the unresolved problems. An extensive list of references is included, thereby providing a representative (and, hopefully, not too biased) "sampling" of the literature on this subject.

Fundamental Principles

Covariance matrices originate from set and probability theories and statistics. Many textbooks treat these subjects [e.g., Ayr62, Abb69, Ash70, Bee58, Bro58, Bro60, Bra63, Bas66, Bur68, Bev69, Bra70, Cra70, Fel50, Fre62, Fis63, Hil52, Hau57, KM76, Men67, Mah68, Mar71, Ney50, Par60, Tuc67, Zeh70]. Furthermore, several tutorial documents exist to serve the needs of the nuclear data community [e.g., Per78a, All80, Pet80, Man81, Smi81, Sta81, Pee82, Smi82a, Smi83, Fro86, Szo86].

We are concerned with relationships between observable physical quantities and explicitly useful parameters which can subsequently be deduced from the observations. Let $\bar{x}$ be an array of continuous random variables which represent the observables. In Nature, the outcomes of such observations are predictable only in a statistical sense, as governed by a joint probability density function $p(\bar{x})$. It cannot be measured directly, but its lower-order moments can be estimated from acquired data. The mean value array $<\bar{x}>$ and the symmetric elements $V_{xij} = <(x_i-<x_i>)(x_j-<x_j>)>$, which form the covariance matrix $\bar{V}_x$, are the most important, with $<g> = \int g(\bar{x})p(\bar{x})d\bar{x}$ signifying statistical expectation. $<\bar{x}>$ represents the best estimate for $\bar{x}$, while $\bar{V}_x$ completely specifies all the uncertainties associated with this estimate. The V_{xii} are the variances (squares of the standard deviations or errors) and the V_{xij} $(i \neq j)$ are covariances. Correlations are given by the expression $C_{xij} = V_{xij}/(V_{xii}V_{xjj})^{1/2}$; they lie in the range -1 to +1.

A covariance matrix must be positive definite [e.g., D+79, L+79, GS88], with equal dimension and rank, and positive eigenvalues. Physically, this signifies that the information content is consistent and not redundant. For various reasons (many traceable to computer and file structure limitations) these very fundamental rules have often been violated in nuclear data covariance matrix applications [e.g., N+87, GS88].

Uncertainty information is often sought for parameters, $\bar{q}$, related to measured ones, $\bar{x}$, by the set of continuous, differentiable functions $\bar{q} = \bar{q}(\bar{x})$. This is accomplished through the "Law of Error Propagation." The formula $\bar{V}_q = \bar{T}^+ \bar{V}_x \bar{T}$ yields the covariance matrix for $\bar{q}$, with $\bar{T}$ being the matrix of partial derivatives $\partial q_i/\partial x_j$ ("+" signifies matrix transposition). Most reactor sensitivity studies are actually based on this first-order differential formalism.

Bayes' theorem offers a very powerful statistical method for refining prior knowledge through the acquisition of new information, an essential feature of nuclear data research. Suppose $\bar{x}$ is a collection of observed results, and $\bar{q}'$ is a possible choice for parameter set $\bar{q}$, drawn from a space of possibilities Q. Then the posterior conditional probability density $p(\bar{q}'|\bar{x})$, that observation of $\bar{x}$ justifies the choice $\bar{q}'$, is given by the formula $p(\bar{q}'|\bar{x}) = L(\bar{x}|\bar{q}')p(\bar{q}')/\int_Q L(\bar{x}|\bar{q})p(\bar{q})d\bar{q}$. Here $p(\bar{q})$ is the prior probability density (rational expectation) that $\bar{q}$ is the correct set, and $L(\bar{x}|\bar{q})$ is the likelihood that $\bar{q}$ would produce $\bar{x}$. Unlike likelihoods, reasonable prior probabilities are quite difficult to establish. Nevertheless, this method provides a valuable procedure for statistical inference, namely "learning by accumulated experience."

Measurement is equivalent to statistical sampling. From the samples (which often involve redundant information) one must construct estimators. In order to obtain the best values for the desired parameters which can be generated from the available sampling results, these estimators should be unbiased and of minimum variance. According to the Gauss-Markov theorem, the method of least squares offers an appropriate algorithm for generating these estimators in those instances where the joint probability density function for the observables is normal or nearly normal (true for most situations of interest in the present context). Generally, the problem involves minimizing the quadratic form (known as the chi-square) $\chi^2(\bar{q}) = [\bar{x}-\bar{x}(\bar{q}_0)]^+\bar{V}_x{}^{-1}[\bar{x}-\bar{x}(\bar{q}_0)] + [\bar{q}-\bar{q}_0]^+\bar{V}_{q0}{}^{-1}[\bar{q}-\bar{q}_0]$. In the Bayesian interpretation, a data set $\bar{x}$, with covariance matrix $\bar{V}_x$, is used to deduce the best (minimum chi-square) revised estimate of the parameter set $\bar{q}$, given prior knowledge $\bar{q}_0$, its covariance matrix $\bar{V}_{q0}$, and an assumed functional relationship between $\bar{x}$ and $\bar{q}$. Here the new and old information are treated as independent. Applications of the least-squares method range from the fitting of linearly parameterized models to complicated non-linear formulations.

The integrity and worth of all statistical procedures depend strongly on the elimination of bias. Bias can result from use of improper estimators, from analyses that encompass limited subsets of those possibilities which should be considered, and from the presence of unidentified systematic errors. Avoidance of bias involves much more than the blind application of "rigorous" mathematical methodology. There are subjective considerations which can never be completely avoided. Thus considerable experience and good judgement are essential for success.

Uncertainties and Covariance Matrices

It can be anticipated that the quality of results arising from the use of covariance techniques can be no better than that of the underlying uncertainty information. Many attempts to apply covariance methods to nuclear data problems have been hampered by serious deficiencies in the quality of the available covariance matrices, sometimes tarnishing the reputations of the methods themselves [e.g., Pee83, Pee87]. It is therefore important to know how to properly estimate errors and how to generate covariance matrices from them.

"For decades there has been but little contact between experimental physics and statistics ... both parties have been the losers for giving up so easily." (W.J. Youden [You61]). In reality, much has been written about the nature of error in physics [e.g., You61, You72, Mue79, Poe81, PB83, C+83a, Hol86]. The most important issue appears to be that of distinguishing between random error and systematic error, while at the same time establishing procedures which enable the latter to be embraced within the framework of statistical theory. Some believe that an error is random or systematic depending upon the context (and the nature of the correlations) and that they can often be treated similarly [e.g., Mue79]. Others feel that one should perhaps consider as random errors only those which can be deduced from statistical sampling, while identified systematic errors are those which must be subjectively estimated [e.g., Hol86]. All agree that unidentified and/or improperly corrected systematic effects thwart the successful application of statistical methods. Another important concern is that of interpreting errors in terms of confidence limits. So long as the underlying distributions are nearly normal, all 1σ errors imply identical confidence, and error propagation preserves confidence. Otherwise, problems can arise which confound interpretation of the results.

Here, we focus mainly on practical matters. Experimenters and evaluators both face the same task in assessing experimental errors. The job should be simpler for experimenters because they are in a position to benefit from an intimate knowledge of their experiment, while, for evaluators, "achaeological" skills are usually demanded. Evaluators may also be faced with the need to estimate covariances for priors in order to be able to apply modern Bayesian techniques, frequently resorting to information derived from nuclear models in the process [e.g., TV78, Pee83, SG83, Pee87, Von87]. What is basically involved here is the identification of all major error sources for an experiment, and careful tabulation of the corresponding error components, as indicated in Table 2.

Table 2: Schematic tabulation of specific error components for an hypothetical data set $x_1, x_2, \ldots, x_i, \ldots, x_n$.

Data Point	Error Component						Total Error
	1	2	...	l	...	L	
1	e_{11}	e_{12}	...	e_{1l}	...	e_{1L}	E_{x1}
2	e_{21}	e_{22}	...	e_{2l}	...	e_{2L}	E_{x2}
i	e_{i1}	e_{i2}	...	e_{il}	...	e_{iL}	E_{xi}
n	e_{n1}	e_{n2}	...	e_{nl}	...	e_{nL}	E_{xn}

Experience has shown that it is important to deal with error sources at the most elementary level, thereby minimizing complexity and increasing the reliability of the estimation process [e.g., Smi82a, SMW87]. In this context, covariance methods can be extremely useful in the analysis of data and in the assessment of associated errors. Procedures for estimating these errors are described in the literature [e.g., Pee75, Pet80, Smi81, VT81, Col82, O+82, Smi82a, L+83a, LLH84, ESL85, L+85, Bas87, Smi87b, SMW87]. These discussions emphasize the need for detailed examination of the measurement processes, making it apparent why evaluators, who often must cope with poor documentation and inexperience, are at such a disadvantage.

Referring to Table 2, it is assumed that the error components (columns, l) correspond to distinct error sources which are uncorrelated, while non-vanishing correlations between data points (rows, i) may very well exist, depending on l. The formula $V_{xij} = \sum_{l=1}^{L} S_{lij} e_{il} e_{jl}$ yields the elements of the covariance matrix. Here, the "microcorrelation" matrix $\bar{S}_l$ specifies all those correlations for the l-th error source. While it can be difficult to estimate these individual correlations, it often happens that composite "macrocorrelations" C_{xij} are not very sensitive to the exact details of the microcorrelations, provided that L is sufficiently large (L > 10). This result follows as a consequence of the Central Limit Theorem [Smi87b]. The formalism above underscores the importance of accurately determined standards in this context [Pee75]. Errors in standards are often strongly correlated, and these correlations are seen to be propagated across a wide range of otherwise unrelated nuclear measurements and processes. However, if the errors in the standards are relatively small, and if the correlations are well known, then the problems associated with such wide-ranging correlations are manageable.

Evaluators debate whether experimenters should be asked to provide explicit covariance matrices or only tables of errors, along with accompanying correlation information, from which covariances can be readily derived. Since information is indeed lost in the generation of covariance matrices, tabulation of error and correlation information is surely essential; however, supplemental provision of explicit covariance matrices by the experimenters can sometimes be quite beneficial. Whenever data sets are quite large (e.g., white source transmission data and differential scattering data), it may be necessary to collapse such matrices to ones of lower rank by averaging processes [Smi87a], or, in certain other instances, it may very well be impractical to provide explicit matrices at all. In these situations, since the true ranks of microcorrelation matrices are often smaller than the size of the data set, the uncertainty information can best be represented by judiciously tabulating the distinct error components and providing the associated correlation information separately.

Fortunately, more and more experimenters are rising to the challenge of providing reasonable covariance information for their experimental results. Evidence of this is seen in papers dealing with monoenergetic differential [e.g., WSM80, SM82, D+83, R+83, W+83, KMS84, Mea87, M+87], white-source differential [e.g., Lar86, S+87] and integral [e.g., O+82, PG85, SMB85, W+87] cross section and reaction rate studies; in neutron spectrum investigations [e.g., CKS83, Man83b, OWW81, WWO83, PG85, W+86]; in thermal-neutron parameter determinations [e.g., ARR86]; and in calibrations involving standards [e.g., C+83b, PM83], to mention a few. More investigators need to be encouraged to cooperate in this regard, because there is still a considerable need for improvement.

Covariances in Experimental Design and Analysis

Two serious objections have been voiced by various experimenters against providing detailed uncertainty information: First, it demands time, labor, and other scarce resources. Second, error estimation for complex experiments often appears to be such a subjective activity that it may amount to no more than an empty exercise. It is argued that time is better spent obtaining new results. However, "the need for ... covariance information rests on the simple but powerful proposition that there would be little sense in evaluating a million (new) ... quantities if no ... information were recorded on how well the numbers are known." (R.W. Peelle, [Pee87]).

Fortunately, covariance methods themselves seem to offer opportunities for resolving this dilemma. The solution lies in including such concepts into the design of experimental and data analysis procedures. Covariances provide approaches for assessing the impact which new experiments, at certain anticipated accuracy levels, might be expected to have on refining the knowledge of important physical processes, thereby establishing whether such experiments are worth the effort before they are undertaken. Once new experiments commence, these methods can also provide algorithms for optimizing the experimental procedures. Such an approach would seem to be very appealing, and there is evidence that the possibilities are being aggressively exploited by the nuclear data community. A group at PTB, FRG, has employed a covariance formalism in the analysis of calibration data for a Van de Graaff accelerator [SS85]. Covariance methods have been utilized in fission-ratio and activation cross section measurements at the Argonne FNG [e.g., Smi81, Smi82a, SMW87]. Several codes employing covariance techniques are used there to establish calibrations, to assess their errors (through curve fitting), and to combine partial errors from diverse origins, yielding total errors and their correlations. This group, in collaboration with CBNM, Geel, Belgium, is also investigating procedures which employ both monoenergetic and broad spectrum techniques to improve knowledge of various standard and dosimetry activation cross sections, through the identification and elimination of integral-differential discrepancies [e.g., SL82, L+83b, SMB85, Smi87d]. One goal of this program is to develop, test, and implement a specific procedure for improving knowledge of differential cross sections through the merging of data acquired from measurements in diverse neutron fields, based on a novel application of the method of Bayesian refinement of prior information [Smi82b]. This concept has been tested experimentally [WSQ85], and it appears to offer promise. A very elaborate computer-intensive covariance procedure is being pursued by the Oak Ridge ORELA group in the analysis of neutron resonance experiments [e.g., L+83a, LLH84, L+85]. Using the Bayesian code SAMMY and the error propagation code ALEX [e.g., Lar84, Lar86], detailed error information is propagated through to final resonance-parameter results, including detailed consideration of all the elementary features of the experiments. A group at CEA-Cadarache, France, is employing covariance methods in the optimization of various reactor-physics experiments [PS87]. Muir [Mui87] has developed a general formalism which is also intended for use in planning and analyzing integral experiments. Other examples of the application of covariance procedures in experimental design and analysis are described in the literature [e.g., Nak83, WP83, N+85, Ito86, Szo86]. It is apparent that the exploitation of covariance matrices in the design and analysis of experiments is coming of age, and the potential benefits are enormous. This is definitely an area that merits considerable attention by the nuclear data community in the immediate future!

Covariances and Nuclear Models

Nuclear models play a very important role in the interpretation and evaluation of nuclear data, so it is not surprising that covariance methods are beginning to enter this domain. So far, the impact has not been very great, and the prognosis for the future is not yet clear. Nuclear models have fundamental appeal because they offer the potential for representing huge bodies of data with relatively few parameters (and, incidentally, introducing strong long-range correlations in the process [Smi87c]), and for interpolating and extrapolating parameters to regions where measurements are difficult or impossible. Models also provide the opportunity to simultaneously derive mutually consistent results for many reaction channels, with automatically imposed physical constraints (e.g., that partial cross sections must sum to the total cross section). If covariance methods can be utilized to estimate parameter errors and correlations, then error estimates can be made for all the derived quantities through error propagation. A number of papers have been written about the application of covariance methods in nuclear modeling [e.g., Pea75, Fro81, Lio81, Pee83, PP87]. Explicit mention should be made of the extensive recent work by Kanda and coworkers [e.g., U+86, KU87c], who have applied this method in the determination of nuclear model parameters and their uncertainties for various isotopes of Mn, Fe, Co, and Ni; by Smith and Guenther [SG83], who examined regional neutron optical model parameter uncertainties in the context of total and elastic scattering data; and by Vonach and coworkers [Von87], who have examined in some detail the problem of determining uncertainty estimates for theoretically calculated cross sections. These endeavors, for the most part, amount to complicated manifestations of basic "curve fitting," in which model parameter uncertainties are deduced from the fits (i.e., from scatter of the data about the model). But the models themselves introduce unavoidable bias through the imposition of a priori structure, as embodied in a variety of imposed physical conditions and simplifying assumptions [Pee87]. It is not at all clear how one should go about quantifying model bias (deficiencies), which are systematic and truly distinct from errors of a statistical nature. There is strong evidence that many of the models which are employed in nuclear data studies contain assumptions which are either physically incorrect or are excessively limiting. Furthermore, coding errors have historically been a serious problem in nuclear modeling practice. Finally, systematic errors are commonly introduced by the misuse of codes and/or their improper parameterization. In spite of these negative considerations, it is my opinion that there is merit in applying covariance methods to nuclear modeling, but only to the extent that good, experimentally well verified models are available (e.g., the spherical optical statistical model as applied to neutron scattering for certain nuclei). Primary attention for the foreseeable future should be given to understanding the basic physical principles upon which reliable nuclear modeling must ultimately be based, and to the development and validation of reliable model codes, with covariance issues relegated to secondary status.

Nuclear Data Evaluation

Covariance methods have probably had more of an impact on evaluation activities than on any other area of nuclear data research. The time was clearly favorable in the mid 1970's for the introduction of new methods. The community was embarking on a flurry of evaluation efforts (e.g., for the ENDF, JEF, JENDL, CENDL and SOKRATOR libraries), and older, inconsistent, and generally subjective methods previously employed ("Age of Archaic Evaluations" [Poe81]) no longer seemed adequate in the face of ever more stringent demands for reliable nuclear parameters and their uncertainties. Many different procedures involving covariances are now used for evaluations ("Age of Renaissance" [Poe81]); for these, the principle of least squares is almost universally incorporated. Specific methods usually fall into the following general categories: 1) simple weighted averaging; 2) nonlinear algorithms in which unweighted priors are used only to linearize the problem (permits inclusion of ratios as well as direct parameters); 3) Bayesian nonlinear algorithms in which the covariances of the priors are also included (permits the refinement of a prior evaluation by inclusion of new data uncorrelated to the old); and 4) very general Bayesian adjustment algorithms in which a diversity of new data (including differential and integral direct parameters and ratios, as well as derived parameters) and assorted prior information (including theoretical results derived from models), which is uncorrelated to the new data, can be merged to yield evaluations. Most such procedures can handle energy-dependent data, and several can tackle simultaneous (multi-process) evaluations. The literature on contemporary evaluation methods is sizeable and it is growing rapidly [e.g., Sch78, Sch79a, Sch79b, Sch80, SS80a, And81, Bha81, GD81, Mar81, Poe81, Sta82, K+83, Man83b, Pee83, Bas87, Poe87a, PP87]. Many of the procedures that have been developed are embodied in an expanding arsenal of computer codes - too extensive to review here except for mentioning a few selected examples of those bearing names: GMA (and its derivatives) [e.g., Poe81, Poe87b, Sug87], FERRET [e.g., Sch82a, Sch82b], BAYES [e.g., FHP80], GLUCS [HF80], MINUIT [e.g., JR75].

Success or failure in the practice of computer-based, statistical evaluation rests more on the quality and scope of the data base and error information, and on the judicious application of the methods and codes (e.g., the use of various techniques to reduce the size of matrices which must be inverted, to transform data points to appropriate group or grid values, to smooth the least-squares solutions, etc.), than on the merits of the codes themselves. Effective use of these codes demands extensive data compilation effort and the implementation of sophisticated data-base management systems [e.g., Poe81]. The relevant data bases available in the literature for evaluations are often sparse and of mixed quality. Serious discrepancies which confound statistical treatment abound. Since underlying "constants" which affect experimental results (e.g., decay parameters, neutron fluence standards, etc.) undergo periodic revision, and undetected systematic errors lurk in many experimental data sets, values employed in evaluations cannot be accepted at "face value" [e.g., ESL85]. Detailed scrutiny of experimental details, with the object of avoiding bias, while eliminating or down-weighting apparently discrepant values, is an absolute necessity [e.g., VT81]. Equally important is the exercise of good judgment in the use of Bayesian priors, especially when faced with a sparsity of experimental data [e.g., Smi87c]. There is abundant evidence of misuse of the codes (usually by individuals other than the code authors), and of subjectivity and bias (supposedly absent in these methods) which are found to creep into evaluations through the means by which input data are selected and manipulated, through the choice of priors, etc. Controversy continues (though somewhat abated from former times) over the now hoary issue of what constitutes acceptable information to include in evaluations (e.g., as manifested in the long-standing conflict between "differential" and "integral" viewpoints). The availability of powerful evaluation codes, which permit inclusion of every conceivable piece of related data, acerbates this issue. A positive development is the fact that many recent experimental results of a derived nature are high in quality, well documented, linked to reliable standards, and reasonably divorced from obscure "facility dependent" complications, thereby meriting their serious consideration for applications independent differential evaluations. In view of all of these complexities, it is not surprising that the quality of results obtained from "machine" evaluations varies widely.

Nevertheless, the scope of accomplishments resulting from the use of covariance methods during the last decade is impressive. Included are many differential evaluations, several of which encompass both differential and integral data, and/or involve simultaneous treatment of multiple processes [e.g., G+75, TV78, SE79, AHS80, FHP80, RA80, SSM80, HR81, FH82, You81, UK83, ESL85, A+86, K+86, MSC86, KU87a, KU87b, M+87, Ryv87, You87]. Of particular note is the recent simultaneous evaluation of the primary ENDF cross section standards [e.g., Poe84, C+86, PP87], a set which, when formally released, will very likely be incorporated into most of the major evaluated data libraries in the world. Considerable attention has been devoted to the evaluation of purely integral data [e.g., Man82b, Z+82, Man83a, Man85, ZRN83]. Benefits have resulted from this effort, particularly in the area of dosimetry cross sections, through the identification and elimination of some long-standing integral-differential discrepancies. Evaluation efforts focused on precisely defining a representation for the Cf-252 spontaneous fission neutron spectrum have been very productive in this regard [e.g., Man87a, Man87b]. Evaluations which employ covariances have also been undertaken for thermal and resonance-parameter data [e.g., A+82a, J+83, K+87], for fission-product yield data [e.g., Wea87], for beta and gamma decay heat parameters [e.g., SS79, SS80b], and for nu-bar of various fissionable isotopes [e.g., MTK86].

Evaluated Covariance Files and Their Processing

The advent of covariances for evaluated nuclear parameters created a need to represent them in files. This task was faced early [Pee75, Per75], but it remains a concern to this day [e.g., Pee83, Pee87]. The widely adopted [e.g., RT86] ENDF covariance formats [e.g., Kin79, KM83] are the product of numerous compromises [e.g., Pee82, Pee83]. In this system, the evaluated parameters are represented pointwise (with interpolation rules) while their covariances are expressed in terms of additive components involving various interval (group-like) structures. Although this asymmetric approach works reasonably well, there are unresolved difficulties. One of these is that non-positive definite matrices are generated from the files when unrealistic 100% error correlations are unavoidably imposed for closely spaced evaluated data points [e.g., Pee87]. Some format refinements (e.g., for the case just mentioned, possibly the addition of a "zero-range" error component [GS88]) are still required to eliminate the possibility of encountering non-physical artifacts when using the covariance files.

Evaluated information, including covariances, is ultimately processed into multi-group libraries tailored for particular applications (e.g., shielding, dosimetry, fission-reactor design, fusion-blanket studies, etc.). A lot of effort has been directed toward this activity, including attention to methods [e.g., BNZ80, Man83b, WY86, LS87], processing codes [e.g., Nol87, Sar87], like the NJOY system [e.g., MMB82, MM85]), and special application libraries (e.g, VITAMIN-E [e.g., WBM80], the Argonne library of Liaw and Schmidt [e.g., LS87], and CARNIVAL IV [e.g., Sal86]). These special application libraries are often adjusted to achieve consistency within particular application "loops" [e.g., Row81, H+83], a pragmatic approach with engineering benefits but dubious merit from a fundamental point of view. One risk is that libraries tailored for a particular application (e.g., shielding) will end up being used in another application (e.g., dosimetry), leading to incorrect results. Another risk is that non-physical features will be introduced into processed libraries by transformations from one group structure to another [e.g., Man83b]. Physicists who produce evaluated nuclear data should gain some familiarity with the various ways in which this information is ultimately used in applications, and then accept some responsibility (in cooperation with the data users) for insuring that these technological applications of evaluated data conform to mathematically and physically valid practices.

Neutron Dosimetry Applications

Neutron dosimetry basically involves the determination of spectral shapes and fluences in fission and fusion energy systems, with subsequent prediction of system response parameters (e.g., radiation damage) and their uncertainties. A 1979 review of this field [Smi80] mentioned covariances briefly; however, since then there have been significant developments in this area. The introduction of covariances [e.g., Gre81] has permitted dosimetry practice to mature from a chaotic state of empiricism, in which neutron spectra were "unfolded" from "trial" spectra by various indeterminate methods, to one where rigorous conditions, such as the least-squares principle, govern spectrum adjustments, and consequently the prediction of system response. Numerous statistical adjustment procedures [e.g., Per77, Per78b, WBM80, Sta81, A+82a, Sta82, Nak83, Sta85, Ito86, K+86, KU87b, Mat87] have evolved, and several of these have been subjected to a series of interlab "methods" comparisons (i.e., the IAEA-sponsored REAL-80 and REAL-84 exercises [e.g., Z+82, PZ85, Z+85a, Z+85b, Szo86, N+87, Zij87a, Zij87b]) in which participants applied various dosimetry techniques to standardized test problems and compared results. These exercises have identified both method and evaluated nuclear data deficiencies (especially relating to covariances), but, on the whole, current dosimetry practice is in much better shape than in earlier times. The dosimetry community generally remains committed to the notion that primary evaluated cross section files (e.g., ENDF/B) need to be adjusted, by C/E comparisons in benchmark fields, to eliminate discrepancies [e.g., Y+80, A+82b, Man82a, Z+82, Wag83, ZRN83, Man85, SOF86, WY86] before generating group cross section dosimetry libraries that are acceptable for full-scale system applications [e.g., LM82]. The general paucity of coupled activity and multiple reaction cross-section covariance information for important dosimeter processes is a serious limitation [e.g., FHP80, FH82, KU87c, SZ87]. These deficiencies should be remedied by performing comprehensive simultaneous evaluations, modeled after that undertaken for the ENDF standards (see above).

Armed with powerful new analytical tools, and an improved evaluated data base, the dosimetry community has addressed several important technological issues during the last decade, including methods for examining PWR pressure vessel damage parameters, in order to better predict power-plant life expectancies [e.g., WMB82, Gut85, M+85, T+85], and the investigation of radiation damage mechanisms in fusion materials, with the aim of providing radiation-resistant fusion-energy system designs [e.g., Gre80, Gre81, Gre82, T+82, GS85]. In some instances, these investigations have moved beyond the laboratory testing phase into field studies involving realistic systems (e.g., applications of the LEPRICON methodology [e.g., W+85, M+86, Mae87] and other similar procedures [e.g., Pet82] to commercial power reactors). Continued progress is assured, but it may come more slowly as the dosimetry community struggles to eliminate the remaining problems which afflict both the methodologies and the data libraries. This effort will clearly benefit from various improved evaluated data libraries (e.g., ENDF/B-VI, JEF-2, JENDL-3, etc.).

Fission Reactor Applications

Considerable effort has been devoted to estimating the uncertainties of reactor core design parameters, due to both methods and to nuclear data (sensitivity analysis). Analytical procedures which incorporate covariances have been established [e.g., Gan79, Col82, PS84], and these have led to the development of codes to implement them (e.g., the Oak Ridge FORSS system [e.g., W+76] and the Argonne code GMADJ [Poe87b]). Benchmark tests have been conducted (e.g, air transport [W+75], the simple integral assemblies GODIVA and JEZEBEL [WP77] and zero-power mockups of reactor cores [e.g., Col82]) to verify both methods and the processed nuclear data libraries (often leading to adjustments of the latter [e.g., Mar81, MWS82, Sal86]). The application of these procedures in full-scale sensitivity studies for the design of LMFBR systems [e.g., MWS80, PS84] has produced some successes. Since the integral adjustment of differential data libraries is a controversial issue (see above), Poenitz [Poe87b] has suggested an approach which completely avoids direct adjustment of data libraries on the basis of integral (benchmark) measurements, focusing instead on the adjustment of final derived quantities (e.g., the reactor design parameters). Conceptually, this method differs little from adjusting the libraries, but it does avoid creating a plethora of "tampered" data libraries which might later be misused.

Shielding design has also benefitted to some extent from covariance methods [e.g., But78]. Systematic method errors are often more problematic here than are data uncertainties, because shielding geometries are generally quite complex. Uncertainties in shielding calculations can apparently be reduced by employing data libraries which are carefully optimized (weighting, choice of group structure, etc.) and adjusted using representative integral experiments [e.g., E+78, H+83]. Benchmark studies, comparable to those for core physics (see above), have also been carried out for shielding [e.g., E+80].

The analysis of decay heat in fission reactors is a crucial safety issue. Covariance methods have proved to be very useful in addressing this problem [e.g., SS75, Sch76, SS80b]. In this context, it would appear that the entire process of compilation and evaluation of nuclear radioactivity parameters (A-Chain program), upon which the analysis of decay heat rests, would benefit from the application of rigorous statistical procedures. However, only recently has evidence emerged that this is being considered [e.g., Bro86, Bro88].

Fusion Reactor Applications

Space limitations prevent a discussion of the many fusion reactor design concepts and the tritium breeding blanket performance studies that have been undertaken. For guidance in this area, review articles [e.g., Jar81, Abd83, Goh86] are suggested. Scant evidence appears in the literature to indicate that covariance procedures are being widely used in examining the non-dosimetry nuclear aspects of fusion technology. This field is apparently not as attuned to covariances as is fission technology. This could be due partly to immaturity of the field (fusion reactors have not been built yet), partly to the poorly developed state of substantial portions of the nuclear data base needed for fusion (actually identification of specific data needs is quite tentative owing to continuous evolution of the design concepts), and partly to the apparent emphasis in the fusion community on plasma physics and fuel cycle issues rather than on neutronics. Studies of sensitivity to computational methods and nuclear data (akin to those described above for fission reactors) have been performed [e.g., GDM75, G+77, EUD83], but effort in this area is likely to remain modest until controlled fusion is demonstrated. Over the near term, the only nuclear issues which are likely to attract much attention of a precise quantitative nature (and therefore interest in data covariances) are the matters of neutron multiplication and of tritium breeding potential for various conceptual design fusion reactor blankets [e.g., Abd83].

Summary and Conclusions

The nuclear data community is now firmly committed to the proposition that it must raise the overall quality of its research endeavors through implementation of scientifically rigorous procedures. Statistical methods and covariance matrices provide an important framework for this effort. Experimenters, for the most part, are striving to better document the sources of error in their measurements. The methods now employed in data evaluation, neutron dosimetry, and various other fission and fusion reactor physics investigations are generally much improved relative to what they were a mere decade ago. During the next several years, significant progress will surely be made toward the resolution of several specific problems which presently afflict this field, particularly those related to raising the quality of nuclear data covariance matrices, to the representation of covariance information in evaluated files, and to the utilization of covariances in analyses. Uncertainty estimates provided with new data sets, and techniques for resurrecting this information from older work, will inevitably improve, thereby aiding the process of evaluation. Furthermore, modern database management techniques will offer solutions for manipulating the large quantities of numerical information inevitably involved in applications.

However, three fundamental problems are likely to continue to bother the nuclear data community for the foreseeable future. The first is the broad technical issue of identifying and dealing with systematic errors. Contemporary covariance practice is based on statistical theory, and it is clear that serious systematic errors simply cannot be properly handled by such ad hoc ploys as re-scaling all the errors to guarantee that χ^2/(degrees of freedom) = 1 [e.g., Man81, Smi81]. Perey [e.g., Per81, Per82] has stressed that powerful new techniques, e.g., those based on group theory, will probably be needed in the long run to deal with systematic errors in the application of logical inference methods. To date, little progress has been made in this area. The second problem has to do with avoidance of bias that is introduced through the analysis, interpretation, and supplementation of experimental data by means of nuclear models. The tasks of gaining a good fundamental understanding of essential nuclear processes, of developing corresponding models, and of parameterizing them, is likely to occupy the attention of nuclear scientists for a long time to come. This issue will continue to be closely associated with that of assessing uncertainties in nuclear parameters required for applications. The third concern is an institutional one. As the problems of nuclear data research become more complex, the available manpower to address them is shrinking in most countries. How then should precious human and financial resources be allocated between the complementary areas of measurement and analysis (particularly with respect to the matter of uncertainties)? It is recognized that only measurements can yield truly new information, but the proper interpretation and utilization of this knowledge is ultimately an analytical concern. While the rapid growth of raw computing power is helping somewhat to ameliorate these problems, the technological demands upon this field are escalating equally rapidly, so that the conflict for limited resources is likely to remain with the nuclear data community indefinitely. The determination of a proper balance between measurement and analysis in future research endeavors is a responsibility of paramount importance which cannot be shirked by those who will provide future leadership in this field.

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