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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

COVARIANCE METHODS AND PRACTICES IN THE FIELD OF NUCLEAR DATA

Proceedings of a IAEA Specialists' Meeting on
Covariance Methods and Practices in the Field of Nuclear Data
held in Rome, Italy, 17-19 November 1986
(in co-operation with NEA/OECD)

Edited by V. Piksaikin

January 1988

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

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I. SUMMARY OF THE MEETING

Abstract

This document contains the 14 invited papers presented at the quoted meeting and summarizes the conclusions and recommendations that arose from the discussions during this meeting. Special emphasis was given to the treatment of correlated neutron nuclear data in fission and fusion reactor applications including computations related to neutron dosimetry and neutron spectra, fission-product yield data, and evaluated nuclear data files.

1. INTRODUCTION

The IAEA Specialist's Meeting was organized by the IAEA Nuclear Data Section, with the co-operation of NEA/OECD.

The objectives of the meeting were to review the status of contemporary covariance information for standard reference neutron fields and evaluated nuclear data files, as well as to discuss the methodologies used for generating covariance data from experimental information, and to review existing and planned computer codes for processing covariance data into multigroup structure form.

The meeting was attended by 15 specialists from seven countries and three international organisations.

Over a decade ago, the development of comprehensive sensitivity analysis pointed to the possibility of estimating the uncertainties in fission reactor performance parameters that are induced by uncertainties in nuclear data. This possibility, however, also depended on detailed evaluation of nuclear data variance and covariance components. The same developments would make formally possible the implementation of a proper scheme for the adjustment of cross sections to take into account integral experiment results. The quality-conscious reactor physics discipline was attracted by the promised capability to assess uncertainty independent of integral experiments, as well as by the prospect of being able to include integral experiment results in a logical way when it was desired to do so. Attention turned to how one might represent evaluated nuclear data covariance information. The main difficulties were related to the development of an appropriate format in which evaluated files of covariance and variance quantities could be structured to permit processing to multigroup cross-section covariance matrices. Over the intervening years such covariance formats were accepted, evaluated covariance files were included in ENDF-V format for a number of important reactions. These files were processed at various laboratories, and numerous complete calculations have been performed using codes that combine these multigroup matrices with sensitivity coefficients for macroscopic system parameters.

However, in developing the covariance formats and files for the ENDF/B-V library, a number of approximations were made that were expected to be refined before the covariance propagation technology would be considered complete. Thus one of the objectives of this meeting was to review some of these areas and consider which improvements seem important and achievable.

The current status of the covariance information was presented in 14 papers and discussed in workshop sessions. As outcome of the discussions during the workshops the participants of the meeting worked out the list of covariance information needs in the field of fusion dosimetry, core physics applications for fast, thermal and intermediate spectrum reactors, as well as for power reactor surveillance programmes. Special attention was drawn to the information needed from experimentalists in order to be able to generate the covariances needed for evaluations. It was pointed out that the EXFOR system and EXFOR nuclear data library (maintained by the IAEA Nuclear Data Section) could play an important role in accumulating such information.

2. AGENDA

Monday, 17 November, morning

Session 1: Status of Covariance Data Related to Evaluated Nuclear Data Files and Standard Neutron Fields.

Chairman : R. Peelle

1. Covariance Data and Processing Codes Available from the OECD NEA Data Bank.
   E. Sartori

2. Covariance Files for Neutron Spectra and Fission Yield Evaluation with Notes on Monte Carlos Sensitivity Calculations.
   D.R. Weaver

3. Covariance Data in the REAL-84 Exercise
   W.L. Zijp

4. Nuclear Data Needs for the Covariance Information Used in the Neutron Spectrum Adjustment.
   E.J. Szondi

5. Evaluating Nuclear Data Uncertainty: Progress, Pitfalls and Prospects.
   R.W. Peelle

Monday, 17 November, afternoon

Session 2: Review of Methodologies Used for Generating Covariance Data on the Basis of Experimental Information

Chairman : D.L. Smith

1. Covariances of Evaluated Nuclear Data Based on Experimental Data Uncertainties and Nuclear Models.
   W.P. Poenitz

2. Covariances for Measured Activation and Fission-Ratios Data.
   D.L. Smith and J.W. Meadows

3. A Method to Evaluated Covariances for Correlated Nuclear Data.
   Y. Kanda

4. Covariances Generated in Simultaneous Evaluation of Fission and Capture Cross Sections for Heavy Nuclides.
   Y. Kanda

5. An Interactive Facility for Multiparametric Covariant Evaluation.
   C. Bastian.

6. Covariances of Nuclear Model Parameters Generated from Experimental Information.
   Y. Kanda

7. Covariance Data Impact on Experimental Planning.
   M. Salvatores

Session 3: Review of Methodologies and Computer Codes involved in Processing ENDF/B Format Uncertainty Data into Multigroup Covariance Matrices

Chairman : D.W. Muir

1. A Program for Deriving Covariance Matrices from ENDF-B/V Information.
   W.L. Zijp

2. Parameter Covariances for the Adjustment of Derived Quantities.
   W.P. Poenitz

3. Covariance Formats and Multigroup Processing Issues.
   D.W. Muir

Working group status, needs and future developments in the field of covariance information

Chairman : R.W. Peelle
Secretary: D.W. Muir

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4. CONCLUSIONS AND RECOMMENDATIONS

AVAILABILITY OF SENSITIVITY AND UNCERTAINTY ANALYSIS TECHNIQUES TO UTILIZE EVALUATED COVARIANCE FILES

There was general consensus that capabilities to propagate uncertainties and otherwise employ nuclear data covariance libraries are far advanced relative to our knowledge of the covariance data themselves. The needed techniques have been demonstrated except possibly for neutronics calculations performed using "continuous energy" Monte Carlo techniques.

AVAILABILITY OF FORMATS TO REPRESENT EVALUATED COVARIANCE DATA

The European effort, JEF, will use ENDF formats. Distributions by the NEA Data Bank have been entirely concerned with multigroup processed data. JENDL has not yet defined formats, but will consider the ENDF ones.

It was noted that ENDF-V formats were incapable of including the correlation between 2200 m/s ν and σ_f, a weakness expected to be removed in the ENDF-VI formats. Uncertainties and correlations of Westcott g-factors also cannot be represented because they are not ENDF cross-section parameters. Otherwise, the main gaps noted in ENDF-V were covariance formats for secondary energy and angle distributions.

Some general concern was expressed about the clumsiness of handling covariance data within the ENDF file structure. Specific concern was expressed that covariance file processing was made unnecessarily complex by the restrictions of the FORTRAN language.

AVAILABILITY OF COVARIANCE FILE PROCESSING CODES

Code systems exist in several centres for processing data in the existing ENDF-V covariance file formats to multigroup form. These systems typically provide plotting facilities. At the initial level, the NNDC checking codes perform certain tests on evaluated covariance files. However, it was generally agreed that a more complete system of widely available test codes is needed, including a minimum capability to plot and tabulate the data on the evaluators's energy grid and a desired capability to show that the matrix is positive. Since in the ENDF covariance formats some components are absolute and some are relative, a complete covariance matrix even for a specific reaction cannot be developed without processing cross section as well as covariance files.

AVAILABILITY OF METHODS FOR EVALUATING NUCLEAR DATA COVARIANCE QUANTITIES

Whenever an evaluation of neutron cross sections is performed using one of the least-squares techniques, and if the input data are weighted with the inverse of their covariance matrix, covariance data are available of the output cross sections. These data should be valid when there is consistency among the input data and, if curve fitting is involved, with the family of fitting functions employed. When consistency among input data is not

achieved, either ignoring or compensating this inconsistency by expanding all estimated errors invokes a challenge to the validity of the whole data combination.

At this meeting, papers demonstrated how to obtain output covariance data both for evaluations involving combinations of pointwise data and for those requiring adjustment of nuclear model parameters to match experimental cross sections. The final step, placing the results of large data combination efforts into ENDF or related formats, has not been well demonstrated.

All these techniques for logical data combination require that covariance information be available for the individual underlying experiments. Most experimental cross-section papers do not provide sufficient information to allow the evaluator to construct the covariance matrix of the results. However, some experimenters are recognizing that such information is required if their results are to be fully used.

ROLE OF INTERNATIONAL COOPERATION IN IMPROVING COVARIANCE DATA AND USAGE

Several recommendations came from the workshop sessions beyond those inherent in the above text:

(a) Covariance data in standard formats should be developed for evaluated cross sections as required for the several technologies (see above).

(b) Since such covariance files from any two sources would be based on essentially the same sets of experimental data, they should be comparable.Therefore, interchange and comparison of covariance data is encouraged. In particular, it is recommended that a detailed comparison on a suitable energy grid be performed between the results obtained by Kanda et al., and the CSEWG standards subcommittee, Carlson et al. The fission cross sections of ^{235}U, ^{238}U, and ^{239}Pu would be a suitable data subset for this comparison. If the results of the initial comparison do not agree, it is suggested that the degree of significance of the differences be explored and the source of the differences be sought.

(c) When data centres distribute multigroup data sets corresponding to evaluations for which covariance files exist, multigroup covariance data on a compatible but coarser grid should be included.

(d) When experimental data sets are offered to a data centre, the staff should ask for further detail if the correlation pattern for each component of the systematic uncertainty is not indicated. Similarly, the staff should question the experimenter if no breakdown of experimental uncertainties is given. It is asked that this recommendation be included on the agenda of the next meeting of the nuclear data centres.

(e) It is suggested that the importance of covariance information be brought to the attention of the participants in the IAEA CRP on Level Densities and Particle Emission Processes. In particular, the idea should be introduced that covariances for the fundamental nuclear model parameters can be deduced from model/data comparisons (e.g., Dr. Kanda in this meeting), and that such information would be extremely useful for applications.

(f) For dosimetry reaction products, the compilations of decay scheme data such as ENSDF should include covariance data for the emissions useful in determining activation rates.

(g) A file 36 covariance data format should be developed for ENDF-VI that deemphasizes the reaction in which a secondary neutron is generated but allows the covariance data for double-differential spectra to be represented in modest detail.

(h) Since evaluated cross sections are now often computed from nuclear models, a covariance data format for ENDF-VI should be strongly considered that would contain the covariance matrix of the nuclear model parameters and, for each reaction type, the energy-dependent derivatives of the computed cross sections with respect to these parameters. This approach would avoid the intermediate step of placing covariance data into a complex file structure that would require further approximation in processing.

(i) The values of using the APL computer language for covariance file manipulation should be considered because of its flexibility in defining data structures.

(j) When a covariance component in an ENDF file is indicated to depend in part on that for a standard cross section, all the other reaction types and materials for which data covariances are implied should be listed. It is recognized that this recommendation is inconsistent with the sequential development of nuclear data files. For this reason it would be acceptable for this information to be given in the documentation rather than in the data file itself.

(k) The IAEA is asked to organize another meeting in cooperation with the NEA Data Bank in about three years to discuss status and progress in the covariance data area. Meanwhile, it would be helpful if the NEA Data Bank newsletter would highlight progress in the area of covariance data evaluation and utilization.

(l) It would be helpful to nuclear data evaluators if the program committees of international nuclear data meetings could ask invited speakers on data needs to consider for which cases covariance data are needed.

COVARIANCE DATA NEEDS FOR FUSION DOSIMETRY

There is strong overlap in the needs for dosimetry data as expressed by the fusion energy community with those of concern for fission reactor dosimetry. The major difference is a reduced emphasis on non-threshold dosimeters with very low energy response, for obvious reasons. The stated requests for uncertainty information for fusion dosimetry applications are not very detailed. They generally amount to a blanket accuracy request, generally of the order of 5%. Realistically, the uncertainty information needs are more extensive. No particular difficulty is forseen from a format point of view in accommodating these needs. That is, an energy range up to 20 MeV, and provision of pointwise differential cross section information (with contemporary detail) and covariances (with improved detail) in ENDF/B or equivalent format, should be adequate. It is planned to enlarge the ENDF/B-V Dosimetry File (which is widely used in this field) to include several

additional reactions for version VI. This argumentation reflects the influence of the fusion community as well as other considerations.

Some requests have been received from the fusion community for specialized reactions of interest for plasma diagnostics. Since it is not evident whether a consensus exists on these selections, it is probably premature to consider them for the evaluated files for this purpose only.

The general experience of analysts who apply the existing dosimetry files for unfolding applications in the several - MeV energy range is that there are unacceptable deficiencies in several of the evaluated cross section sets, and in the covariances. In the latter case, the inadequacy of the correlation information may be of more serious consequence than the variances. However, there are situations where the given variances are so large that the influence of the corresponding dosimeter reaction on the unfolding process is either too small or too uncertain (e.g., the $^{93}Nb(n,n')^{93m}Nb$ reaction).

Many of these issues were raised at a recent meeting on the Coordinated Fusion Nuclear Data Programs of the Division of Basis Energy Sciences, held at Argone National Laboratory, 17-19 September 1986. A data needs list from the fusion community was compiled and reviewed in conjunction with this meeting. Dosimetry needs were also included. Currently, the emphasis within the fusion community is mainly on neutron dosimetry for tritium fuel breeding, radiation damage assessment and for prediction of the build up of long-lived activities in reactor structural materials.

COVARIANCE DATA NEEDS FOR CORE PHYSICS APPLICATIONS IN FISSION REACTORS

For core physics applications (fast, thermal or intermediate spectrum reactors) the covariance data are needed for smooth data, for the parameters of a few major low energy resonances, for thermal energy data (e.g. Axton type), and eventually in the epithermal range to prescribe shapes in energy (e.g. for η). Concerning inelastic scattering the higher priority is for covariance data on the total inelastic cross sections; secondary energy distribution uncertainties are needed with a lower priority. In the resonance range (10keV ÷ few eV) the need is mostly for average information.

The last statement concerns the form which will be preferable for the data (and for which the needs are more urgent). The data are needed by fairly large energy bands (10 ÷ 15), e.g.: 10 - 5 MeV, 5 - 1,35 MeV, 1.35 - 0.5 MeV, 500 - 100 keV, 100 - 30 keV, 30 keV - 10 keV, 10 keV - 3 keV, 3 keV - 1 keV, 1 keV - 300 eV, 300 eV - 100 eV. The detail between 30 keV and 100 eV can be sufficient to represent a meaningful energy grid by means of which users and evaluators can "exchange" informations (e.g. results of adjustments which can be further used to finalize evaluations).

Below 100 eV down to thermal, 4 to 5 energy bands can be sufficient and in these bands some specific resonance parameters uncertainties and correlations are needed (e.g. the first three resonances of U-238, the Pu-240 first resonance).

The isotopes and reactions concerned are the following:

- the major actinides (U-238, Pu-239, U-235, Pu-241, Pu-240); fission and capture cross sections (and ν, when applicable). U-238 total inelastic cross section can be valuable.

- the structural materials (Fe, Ni, Cr); capture, inelastic and total cross-sections.

- the light elements (oxygen, Na, H_2O); elastic (total) cross sections.

For thermal data, the Axton type of data should be used.

Cross correlations are considered as very important both among reactions and isotopes and should be systematically made available. Simple "diagonal" terms can be of interest for some minor isotopes like Am-241, U-236.

It was pointed out that completeness and ready availability should have priority over sophistication. Evaluators should be encouraged to provide very simple, quantitative estimates, even reducing drastically the number of points given in the appropriate files, together with reasonable interpolation rules to help processing.

β_{eff} related uncertainities (spectra, yields), which are available on a fine (experimental) level, should be organized in a standard user-oriented format (according to current schemes).

COVARIANCE DATA NEEDS FOR FUEL CYCLE STUDIES

In fuel cycle studies the main interest of the data users is the prediction of the amounts of materials (or isotopes) in the various parts of the fuel cycle. Of particular interest are the actinides, fission products and the radiations (α, β, γ and neutrons) emanating from them. The production of Pu-236 (a precursor of Th C"- a strong γ-emitter) and Cm-244 and Cm-242 (spontaneous fission neutron emitters) are particularly important. The correct description of the branching ratios in the (n,2n) reaction of Np-237 and the (n, γ) reactions of Am-241 (and Am-243) are of the highest priority.

The calculation of fission products is relevant to many aspects, such as:

- decay heat (or afterheat);

- reactivity loss with burn-up;

- reactor control and kinetics through the delayed neutron emission;

- fuel burn-up determination; and

- fuel reprocessing.

The evaluated fission yields are necessarily correlated as a result of the way they are measured and evaluated, and these correlations will probably need to be represented in the files. However, it may be premature to define the necessary format at this stage as the form and extent of the correlations will only become available when the evaluations currently in progress have been completed.

INFORMATION REQUESTED FOR THE FISSION POWER REACTOR SURVEILLANCE PROGRAMS

The following conclusions are based on the outcome of the IAEA REAL84 exercise and the discussions in this meeting:

1) The a-priori neutron spectrum should be generated in a medium-five energy group structure together with its covariance matrix. (The number of groups lies within the limits 50 to 100, mainly 50 to 60). This job requires the availability of:

   a) the absorption, fission, elastic and inelastic scattering cross sections and their covariance matrices of all the surrounding materials (NB for the moderators: light and heavy water, graphite),

   b) information on the energy distributions of the scattered neutrons (e.g. iron, U-238) and the covariance matrices of these spectra,

   c) data on the angular distribution of the scattered neutrons in P1 approximation (parameters and their covariance matrices),

   d) the fission spectra of the most important components (U-235, U-238, Pu-239) of the fuel and covariance matrices to them.

   It should be checked that the covariance matrices of the user's energy group structure are positive definite. In certain cases proper interpolation rules may be needed.

2) The evaluation of the dosimeter activities uses as input data the gamma ray emission probabilities (gamma abundances) as well. The covariance matrices of these should be developed with higher priority of the radionuclides having not-well-known data. (In the first phase the radionuclides characterized with 2% and more relative uncertainty of the gamma abundances should be investigated).

3) The covariance matrices of the dosimetry reaction cross sections should be available for all the reactions used in the practice. (See: W.L. Zijp, J.H. Baard: Nuclear data guide for reactor neutron metrology. Report EUR7164EN, Luxembourg, 1981). These matrices of the user's energy group structure should be positive definite.

4) The a-posteriori neutron spectrum at the surveillance position describes the source term of the extrapolation of the radiation damage exposure parameters to the LWR pressure vessel wall, etc. The extrapolation procedure may then be performed in a coarser (e.g. 20 to 30) group structure. The necessary data are similar to the ones described in paragraph 1, but the data on the angular distribution are needed in P3 approximation.

5) The users of the covariance data should be supplied with utility programs to treat the covariance files mentioned above. The IAEA is asked to support the development of these programs.

The practical benefit of the use of better quality data in the surveillance programs is the less uncertain prediction of the service life of the power reactors, therefore a longer service life might be licensed by the safety authorities.

DELAYED NEUTRON PARAMETERS FOR FISSION

Delayed neutron information is required for reactor kinetics and control, and also for safeguards and neutron assay methods. It is also of use to the nuclear physics and astrophysics communities.

Present data may be divided among two classes: (a) that for individual precursors, and (b) aggregate information where data is typically presented in a group formalism (Keepin's six groups being the most common). Spectra have been measured both for separated precursors and in an aggregate way.

1. For separated precursors, P_n values have been evaluated for approximately 86 nuclides, and some correlations exist between different nuclides because common experimental techniques were employed. These values are combined with fission yield data in order to produce parameters required for reactor use; this implies the requirement for corresponding uncertainty information for the yields file. Currently, additional information is added on the basis of nuclear physics models for a further ~190 precursors for which no P_n values have been measured. While this procedure opens the possibility of propagating the effect of uncertainty of model parameters, this refinement would be unlikely to add much to the understanding of the final desired parameters because the precursors for which measured data have been evaluated represent the vast majority of delayed neutron emissions in typical fissioning systems.

2. Aggregate information. Total yields: evaluation efforts such as that being undertaken by Tuttle, which combine variation with energy with systematics among fissioning nuclides, will produce output which is correlated between energy groups and between nuclides. The resultant correlation information should be made available to users.

   Group yields and decay constants: there is some study of the significance of using another number of groups to represent delayed neutron emission; however, it is unlikely that the user community will move rapidly away from the traditional six groups of Keepin. The evaluation of group parameters, either from summation of individual precursors or from aggregate yield measurements, leads to fractional yields and decay parameters which are very highly correlated. This correlation information must be made available in the data files.

   Spectra: experimental groups measuring separated precursor or aggregate spectra are using covariance techniques, and the capability exists for producing covariance information on derived group spectra.

INFORMATION NEEDED FROM EXPERIMENTALISTS IN ORDER TO BE ABLE TO GENERATE THE COVARIANCES NEEDED FOR EVALUATIONS

It is widely agreed by evaluators that experimenters should make available the following information on the uncertainties in their experiments:

1) A list of the sources of experimental uncertainties in the experiment should be provided, with a brief description which will serve to clarify what the author has done.

2) The partial error values corresponding to each of these error sources should be explicitly tabulated.

3) Critical information on the nonlinear sensitivity of the experimental results to parameters which are uncertain (above) should be provided along with the actual values of the parameters used. (e.g., half lives and other important standards information).

4) For uncertainty components which are either partially or fully correlated (systematic), specific information on the nature of the correlation (in the range -1 to +1) and the explicit data points involved should be given. Information on correlations to previous data is also very important.

5) Provision of the final data set covariance matrix by the experimenter is not required. By no means should the experimenter provide *only* the final covariance matrix and <u>not</u> provide the component information indicated in item nos. 1 to 4 above.

5. REPORT OF THE WORKING GROUP

SPECIALIST'S MEETING ON METHODS AND PRACTICES IN THE FIELD OF NUCLEAR DATA COVARIANCE

The Working Group portion of this Specialist's Meeting was asked to assess the status of the field, needs, and what future actions by international organizations might be helpful. International cooperation is facilitated by the commonality of formats, terminology, and approaches that was apparent at the meeting.

The group approached its task starting from expressions of needs for covariance files in the various fields. The effort was to identify the materials and reactions for which covariance data are needed, and the desired level of detail as a function of energy. Differences among the types of data required for the various applications were to be noted.

In the meeting it was apparent that uncertainty analysis for complex neutronic systems has become very sophisticated, and that would-be users of covariance information have had to use preliminary and hypothetical covariance data to estimate the effects of uncertainty; the need was evident to obtain and distribute well-founded nuclear data covariance evaluations.

Most of the paragraphs below were written by working group participants expert in the various fields, and these are credited. The chairman also acknowledges the corrections and revisions offered by the participants on reviewing the draft report.

I. NEEDS FOR NUCLEAR DATA COVARIANCE FILES

A. Fission Reactor Core Physics

1. For core physics applications (fast, thermal, or intermediate spectrum reactors) the covariance data are needed for smooth data, for the parameters of a few major low energy resonances, for thermal energy data (Axton type), and eventually in the epithermal range to prescribe shapes in energy (*e.g.* for η). Concerning inelastic scattering the priority is for covariance data on the total inelastic cross sections; secondary energy distribution uncertainties are needed with a lower priority. In the resonance range (~10 keV to a few eV), the need is mostly for information relating to the average cross sections.

2. The data are preferred and more urgently needed for 10 to 15 fairly large energy bands, *e.g.*: 10 to 5 MeV, 5 to 1.35 MeV, 1.35 to 0.5 MeV, 500 to 100 keV, 100 to 30 keV, 30 keV to 10 keV, 10 keV to 3 keV, 3 keV to 1 keV, 1 keV to 300 eV, 300 eV to 100 eV. The detail between 30 keV and 100 eV can be sufficient to represent a meaningful energy grid by which users and evaluators can exchange information, *e.g.* results of adjustments which can be further used to finalize evaluations. Below 100 eV down to thermal, 4 to 5 energy bands can be sufficient and in these bands some specific resonance parameter uncertainties and correlations are needed (*e.g.* the first three resonances of ^{238}U, the ^{240}Pu first resonance).

3. The nuclides and reactions of interest are:

   - The major actinides (^{238}U, ^{235}U, ^{239}Pu, ^{240}Pu, ^{241}Pu) fission and capture cross sections, and ν with emphasis on the fissile nuclides. The ^{238}U, ^{235}U, and ^{239}Pu inelastic cross sections, and ^{235}U and ^{239}Pu fission spectra can be valuable.

   - The structural materials (Fe, Cr, Ni) capture, inelastic,and total cross sections.

   - The light elements (oxygen, sodium, water) elastic (total) cross sections

   For thermal data, the Axton-type of data should be used.

4. Cross correlations are considered very important (between reactions and between nuclides) and should systematically be made available.

5. Simple "diagonal" terms can be of interest for some minor isotopes, like ^{241}Am or ^{236}U.

6. It is worthwhile to stress that completeness and ready availability should have priority over sophistication. Evaluators should be encouraged to provide very simple quantitative estimates, even reducing drastically the number of points given in the appropriate files, together with reasonable interpolation rules to help processing. The evaluation of covariances should be mandatory, but should not increase the effort involved in an evaluation in an excessive way.

7. A comment on the needed accuracy of covariance data: Correlation coefficients are probably needed with an accuracy of ~20%. Coefficients below, say, 0.10, are probably unnecessary on the coarse energy grid indicated above unless the values are consistent over a very large energy range. Diagonal elements ("main" uncertainties) are needed to about 10% accuracy (*i.e.* 2% or 2.2% are equivalent from a user's point of view), with some notable exceptions such as covariance data in the thermal range.

8. Finally, β_{eff}-related uncertainties (delayed neutron spectra and yields), which are available on a fine (experimental) level, should be organized in a standard user-oriented format according to current schemes.

Max Salvatores

B. Fast Reactor Shielding

The main need in fast reactor shielding is to have covariance data applicable to iron shields. In the keV range, the energy grid structure should be sufficiently tight in the "window" regions to allow their effects to be considered. The "vitamin" cross section libraries contain some narrow groups for this purpose, and this energy grid structure might be adopted for covariance analysis. (Note that this application is quite different from those for core physics in that here the applicable spectrum weighting function has very strong structure.)

In the MeV incident neutron energy region there may be need for covariance data for shield materials covering inelastic scattering and the secondary neutron energy distribution.

C. Fission Reactor Fuel Cycle

In fuel cycle studies the main interest of the data users is the prediction of the amounts of the several materials or nuclides in the various parts of the fuel cycle. Of particular interest are the actinides and fission products and the radiations (α, β, γ, and neutrons) emanating from them. The production of ^{236}Pu (a precursor of ThC'' - a strong γ-emitter) and ^{242}Cm and ^{244}Cm (spontaneous fission neutron emitters) are particularly important. The correct description of the branching ratios and their covariances in the (n,2n) reaction of ^{237}Np and the (n,γ) reactions of ^{241}Am (and to a lesser extent ^{243}Am) are of the highest priority.

The calculation of fission product arisings is relevant to many aspects such as

a. decay heat (or afterheat),

b. reactivity loss with fuel burn up,

c. reactor control and kinetics through the delayed neutron emission (see E below),

d. fuel burn-up determination, and

e. fuel reprocessing.

The evaluated fission yields are necessarily correlated as a result of the way they are measured and evaluated, and these correlations will probably need to be represented in the files. However, it may be premature to define the necessary format at this stage as the form and extent of the correlations will only become available when the evaluation(s) currently in progress has been completed.

Mike Sowerby

D. Fission Power Reactor Pressure Vessel Surveillance

The following conclusions are based on the outcome of the IAEA REAL84 exercise and the discussions in this meeting.

1. The *a-priori* neutron spectrum should be generated in a medium-fine energy group structure together with its covariance matrix. (The number of groups lies within the limits 50 to 100, mainly 50 to 60.) This job requires the availability of

    a. the absorption, fission, elastic and inelastic scattering cross sections and their covariance matrices for all the surrounding materials (*N.B.* for the moderators: light and heavy water, graphite),

b. information on the energy distributions of the scattered neutrons (*e.g.* from iron, ^{238}U) and the covariance matrices of these spectra, .LI data on the angular distribution of the scattered neutrons in P1 approximation (parameters and their covariance matrices),

c. the fission spectra of the most important components (^{235}U, ^{238}U, ^{239}Pu) of the fuel and their covariance matrices. It should be checked that all the covariance matrices on the user's energy group structure are positive semidefinite.* In certain cases proper interpolation rules may be needed.

2. The evaluation of the dosimeter activities uses as input data the gamma-ray emission probabilities (gamma abundances). The covariance matrices of these should be developed with higher priority for the radionuclides having not-well-known data. (In the first phase the radionuclides having gamma abundances characterized with 2% and more relative uncertainty should be investigated.) This judgement is based on the idea that other uncertainties will tend to dominate if the decay scheme is very well known.

3. The covariance matrices of the dosimetry reaction cross sections should be available for all the reactions used in practice. (See: W. L. Zijp and T. H. Baard, "Nuclear Data Guide for Reactor Neutron Metrology," Report EUR7164EN, Luxenbourg, 1981.) These matrices on the user's energy group structure should be positive semidefinite.*

4. The *a-posteriori* neutron spectrum at the surveillance position describes the source term of the extrapolation of the radiation damage exposure parameters to the LWR pressure vessel wall, etc. The extrapolation procedure may then be performed in a coarser (*e.g.*, 20 to 30) group structure. The necessary data are similar to the ones described in paragraph 1, but the data on the angular distribution are needed in P3 approximation.

5. The users of the covariance data should be supplied with utility programs to treat the covariance files mentioned above. The workshop participants propose that the IAEA support the development of these programs.

The practical benefit of the use of better quality data in the surveillance programs would be less-uncertain prediction of the service life of power reactors; therefore, a longer service life might be licensed by the safety authorities.

Egon Szondi

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* Such positive semidefinite matrices are only approximations to the correct positive definite ones not likely to be available on a medium-fine group structure. The consequences of these approximations are of concern. (See proceedings of the September 1986 IAEA Consultant's Meeting on results of the REAL84 exercise.)

E. Delayed Neutron Parameters for Fission

Delayed neutron information is required for reactor kinetics and control, and also for safeguards and neutron assay methods. It is also of use to the nuclear physics and astrophysics communities.

Present data may be divided among two classes: (a) that for individual precursors, and (b) aggregate information where data is typically presented in a group formalism (Keepin's six groups being the most common). Spectra have been measured both for separated precursors and in an aggregate way.

1. For separated precursors, P_n values have been evaluated for approximately 85 nuclides, and some correlations exist between different nuclides because common experimental techniques were employed. These values are combined with fission yield data in order to produce parameters required for reactor use; this implies the requirement for corresponding uncertainty information for the yields file. Currently, additional information is added on the basis of nuclear physics models for a further ~190 precursors for which no P_n values have been measured. While this procedure opens the possibility of propagating the effect of uncertainty of model parameters, this refinement would be unlikely to add much to the understanding of the final desired parameters because the precursors for which measured data have been evaluated represent the vast majority of delayed neutron emissions in typical fissioning systems.

2. Aggregate information. Total yields: evaluation efforts such as that being undertaken by Tuttle, which combine variation with energy with systematics among fissioning nuclides, will produce output which is correlated between energy groups and between nuclides. The resultant correlation information should be made available to users.

   Group yields and decay constants: there is some study of the significance of using another number of groups to represent delayed neutron emission; however, it is unlikely that the user community will move rapidly away from the traditional six groups of Keepin. The evaluation of group parameters, either from summation of individual precursors or from aggregate yield measurements, leads to fractional yields and decay parameters which are very highly correlated. This correlation information must be made available in the data files.

   Spectra: experimental groups measuring separated precursor or aggregate spectra are using covariance techniques, and the capability exists for producing covariance information on derived group spectra. It is not yet clear what degree of detail is required by the user community.

David Weaver

F. Fusion Reactor Blanket and Shielding

Fusion-reactor operation will involve many of the same phenomena as fission reactors and will thus benefit from files assembled for fission systems studies. Because of the long time scale foreseen for fusion development, the near-term accuracy requirements will, in general, be less demanding for fusion wherever the needs overlap.

Even so, fusion reactors will place certain additional requirements on data and covariance files for four main reasons:

1. The fusion neutron source rate per watt will be about ten times higher.

2. The average neutron energy is much higher.

3. The number of different materials present in a "typical" fusion blanket will be larger.

4. The blanket geometry will be more complicated, because of design features such as large vacuum ports and plasma divertors.

For several of these reasons, it is essential to have complete covariance information on the secondary-neutron angle and energy distributions, especially those from neutron interactions above 10 MeV. By "complete," we mean that the evaluator should provide reaction angle energy correlation information in sufficient detail that the user can reasonably estimate the covariance between one double-differential cross section and another,

$$\mathrm{cov}[\sigma_{n,Xn}(E'_i,\theta_j),\ \sigma_{n,Xn}(E'_k,\theta_l)]\ ,$$

where $\sigma_{n,Xn}(E',\theta)$ is the differential neutron emission spectrum at secondary neutron energy E′ and angle θ from the incident neutron direction.

Because of the greater material complexity, fusion uncertainty analysis will frequently require cross-material covariances between different construction materials (the various components of steel, aluminum, lead, tungsten, etc.)

It is also important to have covariances for various neutron effects, especially tritium-production cross sections and data related to heat deposition.

D. W. Muir and D. Weaver

G. Fusion Reactor Dosimetry

There is a strong overlap between the needs for dosimetry data expressed by the fusion energy community and the needs for fission reactor dosimetry. The major difference is a reduced emphasis on non-threshold dosimeters with very low energy response, for obvious reasons. The stated requests for uncertainty information for fusion dosimetry applications are not very detailed. They typically amount to a blanket accuracy request, generally of the order of 5%. Realistically, the uncertainty information needs are more extensive. No particular difficulty is foreseen from a format point of view in accommodating these needs. That is, an energy range up to 20 MeV and provision of pointwise differential cross-section information (with contemporary detail) and covariances (with improved detail) in ENDF/B or equivalent format should be adequate. It is planned for Version VI to enlarge the ENDF/B-V Dosimetry File (which is widely used in this field) to include several additional reactions.

Some requests have been received from the fusion community for data on specialized reactions of interest for plasma diagnostics. Since it is not evident whether a consensus exists on these selections, it is probably premature to consider them for the evaluated files for this purpose only.

The general experience of analysts who use the existing dosimetry files for unfolding applications in the several-MeV energy range is that there are unacceptable deficiencies in several of the evaluated cross-section sets, and in the covariances. In the latter case, the inadequacy of the correlation information may be of more serious consequence than the variances. However, there are situations where the given variances are so large that the influence of the corresponding dosimeter activities on the unfolding process is either too small or too uncertain (*e.g.*, the $^{93}Nb(n,n')^{93m}Nb$ reaction).

Many of these issues were raised at a recent meeting held at Argonne National Laboratory.* A data needs list from the fusion community was compiled and reviewed in conjunction with this meeting. Dosimetry needs were included. Currently, the emphasis within the fusion community is mainly on neutron dosimetry for tritium fuel breeding, for radiation damage assessment, and for prediction of the buildup of long-lived activities in reactor structural materials.

It seems advisable to emphasize improvement of the intrinsic quality of the contemporary evaluated dosimetry cross-section data files, including covariances, for those reactions which have been widely used in the past and will continue to be used for fast-neutron spectrum adjustment and damage assessment. Careful attention ought to be given to the matter of correlations. In principle, cross-reaction correlation information would be useful, but it is probably unrealistic to anticipate significant progress in this area for the near term.

D. L. Smith

H. Chairman's Summary on Needs

In comparing the categories of need for covariance data outlined above, several points stand out:

a. Only for pressure vessel surveillance and fast reactor shielding is need apparent for a fine energy grid (>15 energy regions) in the processed covariance data. In the first case, most present nuclear power plants employ pressure vessels subject to radiation effects surveillance, so covariance evaluators have good reason to satisfy needs for pressure vessel dosimetry. In the second case, the sensitivity profiles in some instances have large magnitude in limited energy regions.

b. The need for covariance data for secondary energy and angle distributions is mentioned only for fusion blanket performance and perhaps for shield design.

c. For the one area in which enough analysis has been performed to allow assessment, fission core physics, the energy group structure for processed multigroup covariance matrices may be rather coarse (10 to 15 groups), but the covariance elements are believed to be needed to some precision. When the covariance evaluator's energy grid includes

* Meeting of the Coordinated Fusion Nuclear Data Programs of the Division of Basic Energy Sciences, U.S. Department of Energy, Argonne National Laboratory, September 17-19, 1986. The Proceedings will be issued as an Ohio University report early in 1987. Copies can be obtained from the meeting secretary, Dr. Harold Knox, Accelerator Laboratory, Physics Department, Ohio University, Athens, Ohio, U.S.A.

values that differ from the energy group boundaries used in neutronics analysis, the covariance data processing introduces some reduction of processed covariance values. The requested precision therefore gives covariance evaluators the incentive to provide data with a finer energy structure than would otherwise be warranted, or to select energy grid values likely to be coincident with processed cross-section group boundaries.

II. AVAILABILITY OF SENSITIVITY AND UNCERTAINTY ANALYSIS TECHNIQUES TO UTILIZE EVALUATED COVARIANCE FILES

There was general consensus that capabilities to propagate uncertainties and otherwise employ nuclear data covariance libraries are far advanced relative to our knowledge of the covariance data itself. The needed techniques have been demonstrated except possibly for the application of sensitivity techniques to certain neutronics calculations performed using "continuous energy" Monte Carlo.

III. AVAILABILITY OF FORMATS TO REPRESENT EVALUATED COVARIANCE DATA

The European Community effort EFF (European Fusion File) and the Nuclear Energy Agency Data Bank project JEF (Joint Evaluated File) will both use ENDF formats. Distributions by the NEA data bank have been entirely of multigroup processed data. JENDL has not yet defined formats, but will consider the ENDF ones.

It was noted that ENDF/B-V formats were incapable of including the correlation between 2200 m/s ν and σ_f, a weakness expected to be removed in the ENDF-VI formats. Uncertainties and correlations of Westcott g-factors cannot be represented because they are not ENDF/B cross-section parameters. Otherwise, the main lacks noted in ENDF/B-V were covariance formats for secondary energy and angle distributions.

Some general concern was expressed about the clumsiness of handling covariance data within the ENDF file structure. Specific concern was expressed that covariance file processing was made unnecessarily complex by the restrictions of Fortran.

IV. AVAILABILITY OF COVARIANCE FILE PROCESSING CODES

Code systems exist in several centers for processing data in the existing ENDF/B-V covariance file formats to multigroup form. These systems typically provide plotting facilities. At the initial level, the NNDC checking codes perform certain tests on evaluated covariance files. However, it was generally agreed that a more complete system of widely available test codes is needed, including a minimum capability to plot and tabulate the data on the evaluator's energy grid and a desired capability to show that the matrix is positive semidefinite. Since in the ENDF covariance formats some components are absolute and some are relative, a complete covariance matrix even for a specific reaction cannot be developed without processing cross section as well as covariance files.

V. AVAILABILITY OF METHODS FOR EVALUATING NUCLEAR DATA COVARIANCE QUANTITI

Whenever an evaluation of neutron cross sections is performed using one of the least-squares techniques, and if the input data are weighted with the inverse of their covariance matrix, the covariance matrix for the output parameters is obtained. This data should be valid when there is consistency among the input data and, if curve fitting is involved, with the family of fitting functions employed. When consistency among input data is not achieved, either (a) use of the propagated uncertainties implied by the input data covariance matrix or (b) compensating this inconsistency by expanding all estimated errors invokes a challenge to the validity of the whole data combination. Evaluators may find preferable the expansion of those input uncertainties that have not been well justified by experimenters.

At this meeting, papers demonstrated how to obtain output covariance data both for evaluations involving combinations of pointwise data and for those requiring adjustment of nuclear model parameters to match experimental cross sections. The final step, placing the results of large data combination efforts into ENDF or related formats, has not been well demonstrated.

All these techniques for logical data combination require that covariance information be available for the individual underlying experiments. Most experimental cross-section papers do not provide sufficient information to allow the evaluator to construct the covariance matrix of the results. However, some experimenters are recognizing that such information is required if their results are to be fully and properly utilized in subsequent cross section evaluations.

VI. INFORMATION NEEDED FROM EXPERIMENTALISTS IN ORDER TO BE ABLE TO GENERATE THE COVARIANCES NEEDED FOR EVALUATIONS

It is widely agreed by evaluators that experimenters should make available the following information on the uncertainties in their experiments:

1. A list of the sources of uncertainty in the experiment should be provided, with a brief description which will serve to clarify what the author has done.

2. The partial uncertainty values corresponding to each of these uncertainty sources should be explicitly tabulated, including energy uncertainty and resolution.

3. Critical information on the sensitivity of the experimental results to parameters which are uncertain (above) should be provided along with the actual values of the parameters used (*e.g.*, half lives and other important standards information).

4. For (systematic) uncertainty components which are either partially or fully correlated, specific information on the nature of these correlations should be provided. That is, the degree of correlation (in the range -1 to +1) and the explicit data points involved should be specified. Information on correlations to previous data is also very important.

5. Provision of the final data set covariance matrix by the experimenter is not required. By no means should be experimenter provide only the final covariance matrix and not provide the component information indicated in items 1 to 4 above.

D. L. Smith and W. P. Poenitz

It is generally felt that tools are available to the careful experimenter to enable the necessary covariance data to be obtained. Moreover, it is believed that similar analysis is required if improved experiment designs are to be developed. In some cases, covariance data on inputs used by the experimenter, such as for branching ratios required to fully analyze activation data, need to be provided by the evaluators of that data.

VII. ROLE OF INTERNATIONAL COOPERATION IN IMPROVING COVARIANCE DATA AND USAGE

Several recommendations came from the workshop sessions beyond those inherent in the above text:

a. Covariance data in standard formats should be developed for evaluated cross sections as required for the several technologies (see I above).

b. Since such covariance files from any two sources would be based on essentially the same sets of experimental data, they should be comparable. Therefore, interchange and comparison of covariance data is encouraged. In particular, it is recommended that a detailed comparison on a suitable energy grid be performed between the results shown by Kanda *et al.* at this meeting and those by the CSEWG standards subcommittee, referred to here in the papers of Poenitz and of Peelle. The fission cross sections of ^{235}U, ^{238}U, and ^{239}Pu would be a suitable data subset for this comparison. If the results initially compared do not agree, it is suggested that the degree of significance of the differences be explored and the sources of the differences be sought.

c. When data centers distribute multigroup data sets corresponding to evaluations for which covariance files exist, multigroup covariance data should be included.

d. When experimental data sets are offered to a data center, the staff should ask for further detail if the correlation pattern for each component of the systematic uncertainty is not indicated. Similarly, the staff should question the experimenter if no breakdown of experimental uncertainties is given. It is asked that this recommendation be included on the agenda of the next meeting of the nuclear data centers.

e. It is suggested that the importance of covariance information be brought to the attention of the participants in the IAEA CRP on Level Densities and Particle Emission Processes. In particular, the idea should be introduced that covariances for the fundamental nuclear model parameters can be deduced from model/data comparisons (*e.g.*, Drs. Kanda and Poenitz in this meeting), and that such information would be extremely useful for applications.

f. For dosimetry reaction products, the compilations of decay scheme data such as ENSDF should include covariance data for the emissions useful in determining activation rates.

g. A File 36 covariance data format should be developed for ENDF-VI that deemphasizes the reaction in which a secondary neutron is generated but allows the covariance data for double-differential spectra to be represented in modest detail.

h. Since evaluated cross sections are now often computed from nuclear models, a covariance data format for ENDF-VI should be strongly considered that would contain the covariance matrix of the nuclear model parameters and, for each reaction type, the energy-dependent derivatives of the computed cross sections with respect to these parameters. This approach would avoid the intermediate step of placing covariance data into a complex file structure that would require further approximation in processing.

i. The values of using the APL computer language for covariance file manipulation should be considered because of its flexibility in defining data structures.

j. When a covariance component in an ENDF file is indicated to depend in part on that for a standard cross section, all the other reaction types and materials for which data covariance are implied should be listed. It is recognized that this recommendation is inconsistent with the sequential development of nuclear data files. For this reason it would be acceptable for this information to be given in the documentation rather than in the data file itself.

k. The IAEA is asked to organize another meeting in cooperation with the NEA Data Bank in about three years to discuss status and progress in the covariance data area. Meanwhile, it would be helpful if the NEA Data Bank newsletter (NNDEN) would highlight progress in the area of covariance data evaluation and utilization.

l. It would be helpful to nuclear data evaluators if the program committees of international nuclear data meetings could ask invited speakers on data needs to consider for which cases covariance data are needed.

CONCLUDING REMARKS

The Workshop Chairman again thanks the ENEA and Maria Petilli in particular for so much help in carrying out the agenda and making the participants comfortable, the IAEA and NEA for their roles in bringing about the meeting, Dr. Piksaikin for his key role in these arrangements, and all the participants for their earnest efforts in these discussions.

The chairman believes the proceedings of this meeting will be a significant increment to the literature on covariances among nuclear data. A good start has been made toward defining for which portions of the nuclear data file we should seek quantitatively evaluated covariance files.

R. W. Peelle, Chairman

6. SUMMARY REPORT OF WORKING GROUP 3 ON AN INTERNATIONAL FUSION NUCLEAR DATA FILE

(IAEA Advisory Group Meeting on Nuclear Data for Fusion Reactor Technology)

1. Introduction

The main task of WG3 was to investigate the possibility for creating an international nuclear data file for use in fusion-reactor technology and to indicate how such a file could be organised. The current evaluations for nuclear data for fusion reactors are connected to the fission-reactor programmes of the various countries or regions. The newest versions of these evaluations will be completed in the period 1987 to 1989. At present some of these regional evaluations are still restricted with respect to their distribution, but it is expected that these restrictions will disappear in the near future, certainly for the materials important in fusion-reactor design. Within two years further evaluation work could perhaps be organised with world-wide participation. However, there is already now a need for one joint file, in particular for the design of the international Engineering Test Reactor (ETR). The presently available INTOR file (INDL-F) is not adequate for this purpose and therefore this file should be updated to form an international ETR-file consisting of the best evaluations that could be obtained within one or at most two years. This short-term goal could also be the start of a fully international cooperation in the field of nuclear data, certainly after the completion of the current regional data files.

2. Availability of current evaluations

The availability of the current evaluations is shown in Table 1. Some comments are added in the last column.

Table 1. Availability of current evaluations

Library	Availability	Remarks
ENDF/B-IV	Available	Not adequate for fusion applications
ENDF/B-V	Only parts available	Fusion material evls. less restricted
ENDF/B-VI	Expected to become available	Completed mid 1989; released element by element
EFF-1,2	Largely unavailable at present	Part of JEF 2, except for Li, Al, Si, Pb
JENDL-2	Available	Not adequate for fusion applications
JENDL-3	Available by March'88	Preliminary evaluations are JENDL-3-PR1,2
BROND	Available by Jan.'87	USSR + Dresden (56 nuclides)
ENDL	Available	Not strictly ENDF-V format; large number of materials
CENDL	Available (INDL-V)	China, 14 materials
IRDF	Available	International Reactor Dosimetry File (ENDF/B-V + 10 evaluations from IRK, Vienna)

The completion date of ENDF/B-VI, EFF-2, JEF-2 and JENDL-3 is in the period 1988 to 1989. Until that time most of the evaluators are involved in these regional evaluations. However, there are already at present a number of recent evaluations for fusion materials that have been released or could be made available for the purpose of an international fusion file.

3. Status of the present international (INDL-F) fusion file

The International Nuclear Data Library for Fusion (INDL-F) was completed in 1983. It is a collection of evaluations mainly from ENDF/B-IV with parts of ENDF/B-V (some standards and some dosimetry cross sections) and ENDL. The format is ENDF-5.

This data file is not adequate for the design calculations for ETR. However, it could be used as a "starter file" for the ETR-project. The first step would be to translate this file into ENDF-VI format (there should also be an option to translate files in ENDF-VI format into ENDF-V format to serve users with version-V processing codes). As information becomes available the data on this starter file could be replaced material by material.

4. Need for an international fusion file

At the last Kyoto meeting it was stated that a joint numerical file with Atomic and Nuclear Data is wanted for the ETR-project. The Nuclear Data Section of IAEA could play a role in the nuclear data part of this file. A pre-condition for the success of setting up an ETR file is that both users and evaluators agree on this initiative. Therefore the proposal for a joint nuclear data file for fusion needs to be discussed with the ETR-team. This team should support the project of setting up an international nuclear data file.

5. Requirements for an international fusion file

The detailed requirements for the ETR nuclear data file should be specified by the ETR-team. The working group has made the following comments. First of all, the format of the file should be ENDF-VI. The file should be made to facilitate neutron and photon transport calculations, e.g. to obtain the tritium breeding ratio and the (magnet) shielding properties. For activation and dosimetry calculations a separate file is needed (see also section 7).
The file should be specific for fusion applications, with no information on fissile materials. The materials listed in EFF are used as a basis, and these are shown in Table 2 with two addional materials. If possible the evaluations should be isotopic rather than elemental where the elements are not mono-isotopic. Only about a few of these materials are design-dependent.

Table 2. Materials in ETR file

H, D, T, ^{6}Li, ^{7}Li, Be, ^{10}B, ^{11}B, C, O, N
Al, Si, Ti, V, Cr, Mn, Fe, Ni, Co, Cu, Zr
Nb, Mo, Ba, W, Pb, Bi.

To develope this file an "evaluation of the existing evaluation" could be carried out. It is hoped and expected that for this purpose some new evaluations (as yet not widely distributed) will be made available. By mid 1988 the starter file should have had each material examined and the preferred evaluation should be selected. This library will require testing

and checking prior to distribution, and this is expected to take about one year to be completed. Therefore by mid 1989 a useful version of the file could perhaps be distributed. A further phase where new evaluations (where required) can be carried out can then follow.

6. Organisation create and maintain an international fusion file

A similar method of organisation to that used for JEF-1 could also be employed for the ETR file. The details will need to be specified by IAEA but the following ideas may be useful. An "expert committee" comprising evaluators, users and experimentalists would oversee the project. This will need technical support of approximately 1 to 2 amy, e.g. to cover the production of "review kits" in the initial phase. Once the library exists it will require a similar level of support to cover maintenance etc. The details of where the technical support will be based (at IAEA or at one of the data centres) will need further study. A small subcommittee of evaluators for each material (or a set of materials) should be formed by the expert committee. A typical example is: Pb evaluation - Oak Ridge, Japan, ECN and TUD. The subcommittee would act as a group of referees on the existing evaluations and would be supplied with a "review kit" with possible contains shown in Table 3.

Table 3. Contains of review kit to be produced by IAEA

Numerical data for each evaluation
Graph of data for individual evaluations
Comparative graphs
Documentation
Summary of integral quantities
14 MeV data points
Multigroup Data (3 groups per decade)
Results of runs of checker codes (both format & physical)

The referee reports from the subcommittee should also contain recommendations about parts of the chosen evaluation that need revisions in the second phase of the project.

Data arising from several of the new Coordinated Research Programmes (e.g. on 14 MeV Double Differential Cross Sections, Structural Materials and Methods of Evaluations) should be used as it arises by the subcommittees. Also new CRP's could be suggested.
The first meeting of the expert committee should be held early in 1987. This could be linked with the first ETR project meeting and should contain members of the INTOR design team so as to facilitate a two-way flow of information. Following meetings should be held every six months.

7. Other evaluated data

A new activation file (from Dr. F. Mann) is freely available. This contains approximately 6000 reactions and is already being used for activation calculations. Improvements are being made by Hanford, ECN and Harwell. A slight change in format will be agreed by January 1987 before a copy is sent to IAEA.

For dosimetry there is already an international file (IRDF) that could be further extended and updated to satisfy the data needs for ETR.

H. Gruppelaar (chairman)

R.A. Forrest (secretary)

Report of Working Group 4

Summary

IAEA SPONSORED INTERNATIONAL COMPARISON OF BENCHMARK MEASUREMENTS

Chairman: P.K. Sumita
Secretary: R. Jones

Introduction

The role of the working group was to decide what benchmarks should be included in the intercomparison and what the responsibilities of the IAEA should be. Two types of benchmark were discussed: a calculational benchmark intended to intercompare and validate different neutron transport codes, and an experimental benchmark that would allow comparison of the experimental techniques used in different laboratories. The role of the IAEA was expected to be in the publication of the specifications, assisting with the provision and exchange of data files, and in sponsoring a meeting for the discussion of results.

Calculational Benchmark

It was proposed that this should be a fairly simple benchmark to begin with and that it could be expanded later. It is proposed that the calculations be for single material (Pb) in a simple geometry (sphere). The size of the sphere should be the same as that used in measurements by the Dresden group which are to be published early in 1987 in Atomkern-energie. The data for the calculation should be the ECN file for lead (from Gruppelaar). The proposed geometry and the parameters to be calculated are summarized below.

(1) Size of sphere: Outer diameter 50 cm
Thickness 22.5 cm

(2) Source spectrum: As given in Dresden report

(3) Parameters to calculate:

a) Leakage spectrum per source neutron
(energy group structure to be defined)

b) Spatial distribution of reaction rates, at least of
U-238, Cu-65 and Al-27 (using ENDF/B-V for dosimetry file)

c) Neutron multiplication as a function of energy

This is a minimum set of parameters, the calculation of others and the use of other data files would be welcomed.

Experimental Benchmark

The intention here is to provide the specifications of a benchmark assembly that can be set up in any laboratory so that measurements made on it can be compared with the same set-up elsewhere. It was decided to propose the same size lead sphere as that described in the calculational bencmark.

It was felt that the most useful measurements that could be made would be of the low energy part of the neutron spectrum ($\lesssim$ 1 MeV) inside the sphere (scalar flux), normalized to the source strength.

Role of the IAEA

This should be as follows:

1) Publish the benchmark specifications and invite participation.

2) Provide participants in the calculational benchmark with the ECN Pb file and a suitable processing code to enable group averaged data to be produced.

3) It is recommended to arrange a Specialists' Meeting in 1988 (fall) for communication and discussion of the results obtained.

II. INVITED PAPERS

Neutron Interaction Cross-Section Covariance Data and their Processing Codes Available from the NEA Data Bank

E. Sartori*

NEA Data Bank

November 1986

Abstract

The current status of computer codes for uncertainty analysis in neutron transport problems, covariance data and their processing codes, data consistency and adjustment codes using covariance data that are available from the NEA Data Bank are described.

Introduction

The NEA Data Bank is providing a service in computer codes and data of importance to the nuclear power programme.

The quality of the neutron cross section data bases has been improved considerably over the years and recently, in addition to the estimated "best" values, their uncertainty and correlation have become generally available at least for a number of materials. Also computer codes for carrying out uncertainty analysis of calculated neutron transport quantities have been developed and made available.

Interest in covariance data and processing codes has been shown mainly for neutron dosimetry and neutron shielding applications. In particular, it is for the analysis of shielding benchmark experiments that the most sophisticated tools have been developed.

The covariance data and processing programs available from the NEA Data Bank are described in the sections that follow.

* Staff member of the I.A.E.A.

Relation Between Sensitivities and Covariances

Given a set of computed quantities $\bar{q}$ which depend on the set of parameters $\bar{p}$, a variation $d\bar{p}$ of the parameters causes a variation $d\bar{q}$ of the quantities which in the linear perturbation approximation can be expressed by:

$$d\bar{q} = sens(\bar{q}) \cdot d\bar{p}$$

where $sens(\bar{q})$ is the sensitivity matrix of $\bar{q}$ with respect to $\bar{p}$.

The covariance of $\bar{q}$ is then given by:

$$cov(\bar{q}) = sens(\bar{q}) \cdot cov(\bar{p}) \cdot sens(\bar{q})^T$$

where $cov(\bar{p})$ is the covariance matrix relative to all parameters used in the calculation of $\bar{q}$. The diagonal elements $diag(cov(\bar{q}))$ represent the variance of the set $\bar{q}$ due to the uncertainty of the parameters $\bar{p}$.

In order to estimate the uncertainties of the calculated quantities in neutron transport the following is required:

- The sensitivity matrix which can be calculated through deterministic or Monte Carlo neutron tranaport codes.
- The covariance matrix which contains information on uncertainties and correlations in the neutron source strengh and shape, in the detector response functions and in the material cross sections describing the interaction of the neutron with matter. This information is stored in data libraries.
- When experimental values corresponding to $\bar{q}$ exist, consistency analyses between the observations and the parameters used together with parameter adjustments can be carried out with the help of the covariance information. In the adjustment procedure in addition to the adjusted parameters, new covariance information is produced containing the new variances and correlations.

Covariance Data

Covariance data is available in two forms:

- energy dependent covariances in ENDF/B format
- multigroup covariances

The second type is normally derived from the first one.

Table 1 lists the generally available covariance data in evaluated form. ENDF/B-V contains the most comprehensive set of covariances; however only part of it is generally available.

The first multigroup covariance library was established by Drischler and Weisbin /2/ ten years ago and has become generally available. As this in-

formation is rather coarse, improved group covariances have been produced based on recent evaluations.

The ENDF/B-V dosimetry file was processed to a multigroup covariance library for LWR dosimetry (DOSCOV) /1/ by ORNL and EPRI and released worldwide.

Work for producing improved group covariance sets for shielding applications was carried out at CEA Cadarache and IKE Stuttgart /3/, /4/; at LANL a multigroup covariance file for fusion studies (COVFILS) /6/ and at ORNL for fast reactor studies (COVERV) /7/ was produced. The restrictions on the distribution of COVERV and COVFILS have not yet been removed at present. However, the report describing COVFILS /6/ displays the information in great detail in graphical form.

Recently Zijp from ECN, Petten, has processed covariance information from the ENDF/B-V and IRDF-85 dosimetry files to 3, 26 and 37 groups /13/.

Covariance Data for the JEF-1 Project

The amount of covariance data in JEF-1 is limited as can be observed in Table 1.

In order to complement the reduced amount of this information, the covariance matrices produced at CEA Cadarsche and IKE Stuttgart have been made available to the NEA Data Bank within the JEF-1 project.

Recently a 175 group neutron cross section library based on JEF-1 for shielding benchmark calculations has been produced at the NEA Data Bank (VITAMIN-J) /5/. Also covariance matrices for the same group structure have been produced using evaluated and group covariance information available to the JEF-1 project.

Due to the heterogeneity of the available information (different group structures and formats) a special procedure has been used which is graphically outlined in Fig. 1.

Evaluated covariances are processed here through the ERRORR module of NJOY (Appendix I) /12/.

The variety of group averaged cross section covariance data had to be transformed to a uniform group structure. The VITAMIN-J group structure contains a higher number of energy groups than all available covariance data. In order to achieve this transformation at first an interpolation-extrapolation algorithm given in Ref. /8/ was used; however, its author has recently clarified the limitations of this procedure. A revised transformation algorithm has therefore been introduced in a computer code ANGELO /9/. Uncertainties (relative standard deviations) and correlation matrices are kept separate in the transformation. As no new information on data correlations is used in the transformation, a correlation "conservation" algorithm is adopted. Account is therefore taken so that the transformation will not "increase" the original information content (increase of structure in the covariances).

When interpolation in an energy range is carried out where data correlation is constant, the values are simply copied over from the original matrix. Whenever a new energy group intersects the old group boundaries, the integral of the correlation over the group-lethargy domain is kept constant in establishing the new correlation value.

In addition, extrapolations imply complete correlation with the contiguous energy space from which the extrapolation is carried out. A similar procedure is used for the variances. No flux weighting is carried out in the present version but it may be introduced in a later development.

The covariance matrices in VITAMIN-J group structure are listed in Table 2.

The first criticism to which this covariance information is subjected is that it is not completely homogeneous with the cross section data. In fact the source of the covariance data is only in part identical to the one for cross sections. However, most of the recent evaluations are based approximatively on the same bulk of experimental data. Therefore to a relative high degree of precision a new estimation of covariance data where it is inexistent in JEF-1 would lead to essentially the same covariance information used in the VITAMIN-J library. It is for this reason also that no strong necessity is felt for producing new covariance data specific to JEF-1.

Codes for Processing Covariance Data from Evaluated Files to Multigroup Form

Formats for storing covariance information in evaluated files have been designed in the U.S. within the ENDF/B project /11/.

The program PUFF-2 developed at ORNL /10/ (Appendix I), the NJOY module ERRORR /12/ developed at LANL and UNC32/33 developed at ECN, Petten /13/ process covariance information from the ENDF/B form to a multigroup structure.

PUFF-2 produces multigroup covariance matrices in the standard COVERX format /14/ and has been used for generating the COVERV library. Multigroup cross sections and fluxes must be provided in the input.

The ERRORR module is capable of producing both group cross sections and their covariance matrices. Group cross sections already produced by another NJOY module (GROUPR) can also be used in the input. The output follows the module interface file formats of NJOY. This format can be processed by the module COVR to a very compact form called BOXR. The COVR module in addition produces plots which give a clear insight into the structure of the produced covariance information /6/.

Codes for Sensitivity and Uncertainty Analysis

The most popular and widely used code for determining the sensitivity of a calculated quantity to microscopic cross section data so far has been SWANLAKE, developed at ORNL (Appendix I). It has been used in connection with the one-dimensional discrete ordinates code ANISN. Through an interface

code VIP, which translates two-dimensional angular flux and adjoint moments from DOT to a form suitable for SWANLAKE, two-dimensional sensitivity analyses had also become possible.

The capabilities of this code were expanded and generalized in the FORSS system /15/ for carrying out a complete sensitivity and uncertainty analysis. This system also contains modules for data adjustment.

A more comprehensive code than SWANLAKE was developed at LANL: SENSIT (Appendix I). It carries out both sensitivity and uncertainty analysis and accepts in part angular fluxes and adjoints produced both by the ORNL and LANL discrete ordinates codes. A two-dimensional version SENSIT-2D was developed recently.

ANL has developed a sensitivity analysis code VARI-1D to be used in connection with one-dimensional diffusion theory (Appendix I).

Several Monte Carlo codes have been developed for calculating sensitivity profiles in shields with complicated geometries. The code TIMOC /16/ and PEST /17/ use a correlated tracking method; however, DUCKPOND /18/ uses a differentiation technique for scoring probabilities.

Two sensitivity and uncertainty analysis codes were developed recently based on the generalized perturbation theory: HOPES at CEA Cadarache, and SAGEP at Osaka University (Appendix I).

A library ZZ-SENPRO of multigroup sensitivity profiles in a standardized format for a variety of benchmark experiments has been produced with FORSS and VARI-1D. In Appendix I the different sensitivity profiles for fast reactors, thermal reactors and shielding benchmarks contained in the library are listed.

Codes for Data Consistency Analysis and Adjustment

Before data are adjusted to improve agreement with available integral observations, a data consistency analysis is required. Unphysical changes introduced in the adjustment may worsen agreement with other important unmeasured integral parameters.

The code ALVIN for carrying out sensitivity analysis data, consistency analysis and adjustments has been developed at LANL (Appendix I) using one dimensional discrete ordinates code output.

The code DATAK carries out uncertainty analysis using sensitivity profiles obtained with the Monte Carlo method and carries out consistency analysis using differential cross section data and integral observations /19/.

Data adjustments are also carried out by the program AMARA and NEUPAC (Appendix I).

Use of Uncertainty Analysis

Many reactor physics calculations aim at an accurate prediction on integral design parameters of power reactors. Confidence in the calculated results is enforced if uncertainty estimates are also produced. Uncertainty analysis therefore becomes an important tool for achieving this goal and to identify areas where the microscopic data need improvement.

When looking into the amount of requests received at the NEA Data Bank for data and codes required for uncertainty analysis one observes that there has been a certain interest in codes for calculating sensitivity profiles, little interest has, however, been shown in uncertainty analysis codes outside the research centres where the codes have been developed. Reasons for this may be the following:

- Except for dosimetry applications the covariance information available is incomplete.

- No standardized group structure has been adopted for the different applications; therefore the different users would have to produce multigroup covariances suitable for their own application.

- Available multigroup covariance data are coded in different formats which are not necessarily accepted by the different uncertainty analysis codes.

As more covariance data becomes available, it would be advisable, where possible, to complement the group cross section libraries released for specific application fields with the corresponding covariance information. Also, a computer code for translating covariance information from COVERX to BOXR format and vice versa should be developed.

The program ANGELO is being developed with the aim of making the use of available multigroup covariances more attractive. The user will need to specify only his own group structure in the input in addition to providing existing multigroup covariance matrices. It is planned to make this program available in the future together with some utility programs for format translation and for plotting the covariance information which makes the verification of the correctness of the data manipulation easy (Fig. 1). The plotting program COVA imitates the covsriance display format designed in COVR because it is the most effective one found in the literature. However, it does not use proprietary plotting software.

Table 1

EVALUATED COVARIANCE DATA

Nuclide	Reactions	Evaluated Files
H-1	total, elastic, capture	ENDF/B-V, JEF-1
Li-6	total, elastic, (n,t)	ENDF/B-V, JEF-1
B-10	total, elastic, (n,alpha)	ENDF/B-V, JEF-1
C	total, elastic, non-elastic (n,n'l)(l=1,18), (n,n'contin.) (n,gamma), (n,p), (n,d), (n,alpha)	ENDF/B-V, JEF-1
N-14	total, elastic, inelastic (n,gamma), (n,p), (n,alpha)	ENDF/B-IV
O-16	total, elastic, inelastic (n,p),(n,alpha)	ENDF/B-IV
F-19	(n,2n)	ENDF/B-V
Na-23	(n,2n), (n,p), (n,gamma) res.param.	ENDF/B-V
Al-27	(n,p), (n,alpha)	ENDF/B-V
S-32	(n,p)	ENDF/B-V
Sc-45	(n,gamma)	ENDF/B-V
Ti-45	(n,p)	
Ti-46-48	(n,p), (n,n'p)	ENDF/B-V, JEF-1
Mn-55	(n,2n)	ENDF/B-V
Fe-54	(n,p)	ENDF/B-V
Fe-56	(n,p)	
Fe-58	res.param., (n,gamma)	
Co-59	(n,2n), (n,gamma), (n,alpha)	ENDF/B-V
Ni-58	(n,2n), (n,p)	ENDF/B-V
Ni-60	(n,p)	
Cu-63	res.param., (n,gamma), (n,alpha)	ENDF/B-V
Cu-65	(n,2n)	ENDF/B-V
In-115	(n,n'1), (n,gamma)	ENDF/B-V
I-127	(n,2n)	ENDF/B-V
Au-197	(n,gamma)	ENDF/B-V, JEF-1
Th-232	fission, (n,gamma)	ENDF/B-V
U-235	$\bar{\nu}$, fission, (n,gamma)	ENDF/B-V, JEF-1
Np-237	Res.param., fission	ENDF/B-V
Pu-239	fission	ENDF/B-V
Pu-242	res.param., total, elastic, inelastic, (n,2n), (n,3n), (n,gamma)	ENDF/B-V
Am-241	res.param., total, elastic, inelastic, (n,2n), (n,3n), (n,gamma)	ENDF/B-V

Table 2

VITAMIN-J RELATIVE COVARIANCE MATRICES

Isotope	Autocorrelations	Cross Correlations With
H-1	total	elastic, (n,gamma)
	elastic	
	(n,gamma)	
C-12	total	elastic, non-elastic, inelastic, first-inelastic, continuum-inelastic, (n,gamma)
	elastic	non-elastic, inelastic, first-inelastic continuum-inelastic
	non-elastic	inelastic, first-inelastic, continuum-inelastic, (n,gamma)
	inelastic	first-inelastic, continuum-inelastic, (n,gamma), (n,p), (n,d), (n,alpha)
	first-inelastic	continuum-inelastic, (n,gamma), (n,alpha)
	2nd-18th inelastic	continuum-inelastic
	continuum-inelastic	(n,gamma), (n,p), (n,d), (n,alpha)
	(n,gamma)	
	(n,p)	
	(n,d)	
	(n,alpha)	
O-16	total	elastic, inelastic, (n,p), (n,alpha)
	elastic	inelastic, (n,p), (n,alpha)
	inelastic	(n,p), (n,alpha)
Na-23	total	
	elastic	nonelastic, inelastic
	nonelastic	inelastic
	inelastic	
	(n,2n)	
	(n,gamma)	
	(n,p)	
	(n,alpha)	
Cr	total	
	elastic	
	inelastic	
	(n,gamma)	
Fe	total	elastic
	elastic	inelastic
	nonelastic	
	inelastic	
Ni	total	
	elastic	
	inelastic	
	(n,gamma)	
	(n,p)	
	(n,alpha)	

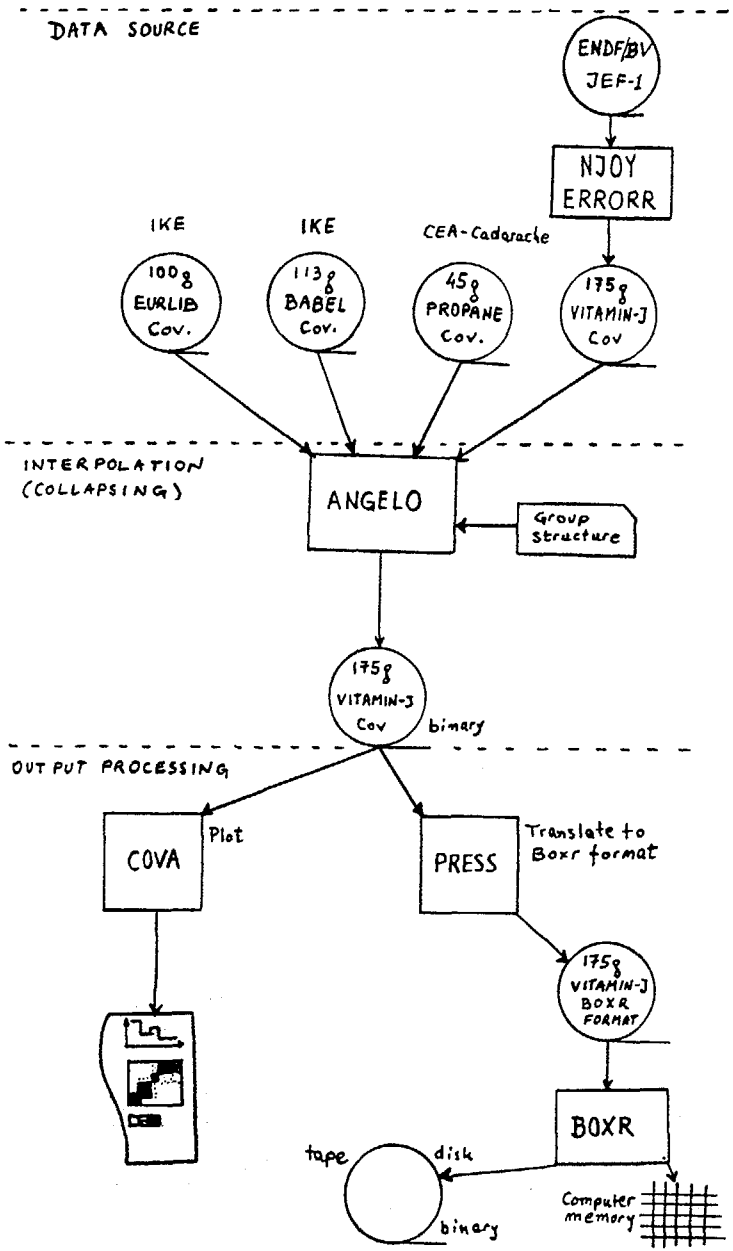

Fig. 1 Processing of Covariance Information

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Appendix I.

Short Program and Group Data Description
(Information Stored at NEA DB - October 1986)

NAME OR DESIGNATION OF PROGRAM - ALVIN

COMPUTER FOR WHICH PROGRAM IS DESIGNED AND OTHER MACHINE VERSION PACKAGES AVAILABLE -

Program-name	Package-ID	Orig. Computer	Test Computer
ALVIN	NESC0815/01	CDC 7600	CDC 7600

DESCRIPTION OF PROBLEM OR FUNCTION - ALVIN analyzes the consistency of a set of differential and integral nuclear data, adjusts the differential nuclear data to improve agreement with integral observations, and identifies inconsistent data. ALVIN also computes required sensitivities and related quantities such as sensitivity profiles.

METHOD OF SOLUTION - Linear perturbation theory is used for the sensitivity calculations. Data consistency and adjustment computations use least squares techniques.

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NAME OR DESIGNATION OF PROGRAM. AMARA.

COMPUTER FOR WHICH PROGRAM IS DESIGNED AND OTHER MACHINE VERSION PACKAGES AVAILABLE -

Program-name	Package-ID	Orig. Computer	Test Computer
AMARA	NEA 0403/01	IBM 370 series	IBM 370 series

NATURE OF PHYSICAL PROBLEM SOLVED. The program calculates corrections to nuclear data, correlating them to integral experiments. The corrections can be obtained when discrepancies between measured and calculated integral data, and sensitivites of integral data to nuclear data are known.

METHOD OF SOLUTION. Lagrange multipliers.

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NAME OR DESIGNATION OF PROGRAM - NEUPAC. Neutron Unfolding Code Package.

COMPUTER FOR WHICH PROGRAM IS DESIGNED AND OTHER MACHINE VERSION PACKAGES AVAILABLE -

Program-name	Package-ID	Orig. Computer	Test Computer
NEUPAC	NEA 0823/01	FACOM M-200	IBM 3084Q

DESCRIPTION OF PROBLEM OR FUNCTION - The code is able to determine the integral quantities and their sensitivities, together with an estimate of the unfolded spectrum and integral quantities. The code also performs a chi-square test of the input/output data, and contains many options for the calculational routines.
NEUPAC-ADJUST - performs neutron cross section adjustment using the J1-method with the standard neutron spectra.

METHOD OF SOLUTION - The code is based on the J1-type unfolding method, and the estimated neutron flux spectrum is obtained as its

solution.

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NAME OR DESIGNATION OF PROGRAM - NJOY. Nuclear Cross Section Processing System.

COMPUTER FOR WHICH PROGRAM IS DESIGNED AND OTHER MACHINE VERSION PACKAGES AVAILABLE -

Program-name	Package-ID	Orig. Computer	Test Computer
NJOY(6/83)	PSR-0171/08	IBM 370 series	IBM 3084
	PSR-0171/09	CDC 7600	CDC CYBER 740

DESCRIPTION OF PROBLEM OR FUNCTION - NJOY is a system of processing modules which convert evaluated nuclear data in ENDF/B format into forms useful in various applications. The following two modules are used for processing covariance data:

ERRORR Produces multigroup covariance matrices from ENDF/B uncertainties.
COVR Reads the output of ERRORR and performs covariance plotting and output-formatting operations.

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NAME OR DESIGNATION OF PROGRAM - PUFF-2.

COMPUTER FOR WHICH PROGRAM IS DESIGNED AND OTHER MACHINE VERSION PACKAGES AVAILABLE -

Program-name	Package-ID	Orig. Computer	Test Computer
PUFF-2	PSR-0157/01	IBM 3033	IBM 3081
	PSR-0157/02	CDC CYBER 176	

DESCRIPTION OF PROBLEM OR FUNCTION - PUFF-2 processes ENDF/B-V uncertainty data into multigroup covariance matrices calculated for an energy group structure and weighting function specified by the user. It requires as input multigroup cross sections together with their associated flux spectrum and energy group structure. PUFF-2 can also calculate the covariance matrices for ratio data, in which case uncertainty data for the 'standard' reaction must be supplied.

Covariances can then be folded with sensitivity coefficients to obtain uncertainties in selected integral parameters such as k-effective and breeding ratio.

METHOD OF SOLUTION - Cross section and flux values on a 'super energy grid', consisting of the union of the required energy group structure and the energy data points in the ENDF/B-V file, are interpolated from the input cross sections and fluxes. Covariance matrices are calculated for this grid and then collapsed to the required group structure.

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NAME OR DESIGNATION OF PROGRAM - SAGEP

COMPUTER FOR WHICH PROGRAM IS DESIGNED AND OTHER MACHINE VERSION PACKAGES AVAILABLE -

Program-name	Package-ID	Orig. Computer	Test Computer
SAGEP	NEA 1037/01	FACOM M-380	IBM 3034Q

DESCRIPTION OF PROBLEM OR FUNCTION - SAGEP computes the sensitivity coefficients of reactor parameters such as neutron multiplication factor, reactivity worth and reaction rate distribution to cross section changes in two dimensional systems.

METHOD OF SOLUTION - The generalized perturbation theory is used.

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NAME OR DESIGNATION OF PROGRAM - SENSIT.

COMPUTER FOR WHICH PROGRAM IS DESIGNED AND OTHER MACHINE VERSION PACKAGES AVAILABLE -

Program-name	Package-ID	Orig. Computer	Test Computer
SENSIT	CCC-0405/01	IBM 3033	IBM 3033

DESCRIPTION OF PROBLEM OR FUNCTION - SENSIT computes the sensitivity and uncertainty of a calculated integral response (such as a dose rate) due to input cross sections and their uncertainties. Sensitivity profiles are computed for neutron and gamma-ray reaction cross sections (of standard multigroup cross-section sets) and for secondary energy distributions (SED's) of multigroup scattering matrices. In the design sensitivity mode, SENSIT computes changes in an integral response due to design changes and gives the appropriate sensitivity coefficients. Cross-section uncertainty analyses are performed for three types of input data uncertainties: (a) cross-section covariance matrices for pairs of multigroup reaction cross sections, (b) spectral shape uncertainty parameters for secondary energy distributions (integral SED uncertainties), and (c) covariance matrices for energy-dependent response functions.

METHOD OF SOLUTION - For all three types of data uncertainties, SENSIT computes the resulting variance and expected deviation in an integral response of interest, based on generalized perturbation theory.

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NAME OR DESIGNATION OF PROGRAM. SWANLAKE. Cross section sensitivity analysis code for one-dimensional discrete ordinates codes.

COMPUTER FOR WHICH PROGRAM IS DESIGNED AND OTHER MACHINE VERSION PACKAGES AVAILABLE -

Program-name	Package-ID	Orig. Computer	Test Computer
SWANLAKE	CCC-0204/03	IBM 3081	IBM 3081

NATURE OF PHYSICAL PROBLEM SOLVED. Determination of the sensitivity of a calculated quantity or result to microscopic cross section data utilized in the calculation.
SWANLAKE (CCC-0204/03): The new version of SWANLAKE contains the following changes over the original version:
1. Fission contributions are considered with an option for a mini or maxi print edit of fission sensitivities.
2. The Shortlist feature was implemented for most I/O transfers which cut execution time considerably.
3. Plotting features were eliminated and replaced by a (punch/write)

option.
4. For coupled neutron-gamma-ray problems, an output edit is printed which gives the group and zonewise contributions to the total response due to gamma-ray production.

METHOD OF SOLUTION. A particular sensitivity function, which represents an application of earlier perturbation approaches, is determined for the cross sections which were utilized in the discrete ordinates calculations.

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NAME OR DESIGNATION OF PROGRAM - VARI-1D
SUMMARY LIST:

Program-name	Package-Id	Status	Date	Establ.
VARI-1D	NESC0625/01	T	751000	NESC

COMPUTER(S).

Program-name	Package-ID	Orig. Computer	Test Computer
VARI-1D	NESC0625/01	IBM 370 series	IBM 370 series

DESCRIPTION OF PROBLEM OR FUNCTION - The VARI-1D code calculates estimates of changes in reactivity worths, keff, reaction rates, power fractions, prompt-neutron generation time, delayed neutron effectiveness, and flux integral ratios due to changes in nuclear data or composition by use of a variational formalism. The code is applicable to a wide range of reactor or critical experiment design problems and sensitivity studies.

METHOD OF SOLUTION - VARI-1D first calculates the diffusion theory flux and adjoint in the reference one-dimensional system using a standard power iteration algorithm with Chebyschev extrapolation. Next, the generalized functions GAMMA* and GAMMA are calculated using a successive approximation method with the source term appropriate to the type of estimate. These generalized functions are then used to calculate the integrals required to obtain variational and first-order perturbation theory estimates of the effect of different system alterations on the given reactivity perturbation, reaction rate ratio, etc.

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NAME OR DESIGNATION OF PROGRAM - ZZ-DOSCOV.

COMPUTER FOR WHICH PROGRAM IS DESIGNED AND OTHER MACHINE VERSION PACKAGES AVAILABLE -

Program-name	Package-ID	Orig. Computer	Test Computer
ZZ-DOSCOV	DLC-0090/01	IBM3033	IBM3084Q

DESCRIPTION OF PROBLEM OR FUNCTION - DOSCOV is a library of covariance data for the following dosimetry materials (Table I) processed into 24 group covariance matrices.

TABLE I

Material	Reaction(s) processed	Material	Reaction(s) processed
U-238	(n,f)	Ti-47	(n,p) (n,n'p)
Pu-239	(n,f)	Ti-48	(n,p) (n,n'p)
Np-237	(n,f)	Fe-56	(n,p)
U-235	(n,f)	Ni-58	(n,2n) (n,p)
Al-27	(n,p) (n,alpha)	Cu-63	(n,gamma) (n,alpha)
Mn-55	(n,2n)	Cu-65	(n,2n)
Co-59	(n,2n) (n,p) (n,alpha)	In-115	(n,n') (n,alpha)
Ti-46	(n,p)	I-127	(n,2n)

METHOD OF SOLUTION - The program PUFF-2 was used to generate the library from the ENDF/B-V General Purpose tapes or the Special Purpose Dosimetry File.

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NAME OR DESIGNATION OF PROGRAM - ZZ-SENPRO.

COMPUTER FOR WHICH PROGRAM IS DESIGNED AND OTHER MACHINE VERSION PACKAGES AVAILABLE -

Program-name	Package-ID	Orig. Computer	Test Computer
ZZ-SENPRO/45C	DLC-0045/02	IBM 370 series	IBM 370 series

DESCRIPTION OF PROBLEM OR FUNCTION - SENPRO is a package of data libraries containing multigroup sensitivity profiles for several fast reactor, thermal reactor and shielding benchmarks. Table I lists the various sensitivity profiles along with references describing the procedures used in their creation.

Table 1. Sensitivity Profile Libraries Included In DLC-45C/SENPRO

Benchmark Type	Assemblies	Number of Groups	Number of Profiles	Lab
Fast Reactor	ZPR6-7, ZPR6-6A, ZPR3-56B, ZPR3-11, Godiva, Jezebel	126	650	ORNL
Fast Reactor	ZPR3-48, ZPR6-7, ZPR6-6A, ZPR9-31	12	262	ANL
Fast Reactor	LCCEWG	32	54	ORNL
Fast Reactor	ZPR6-7	4	10	ORNL
Fast Reactor	Combination of All the Above	26	1263	ANL, ORNL
Shielding	CRBR Upper Axial Shield	171	126	ORNL
Thermal Reactor	TRX-2	131	234	ORNL
Thermal Reactor	U-L212	57	94	ORNL

SENTINEL — Calculates the percent change in a specified reponse due to given percent changes in specified reaction cross sections over specified energy regions.

METHOD OF SOLUTION - For descriptions of the procedures used in the generation of the data, see the references of the report.

NAME AND ESTABLISHMENT OF AUTHOR - Contributed by:
Oak Ridge National Laboratory
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and
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Covariance Files for Neutron Spectra and Fission Yield Evaluations with Notes on Monte Carlo Sensitivity Calculations

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ABSTRACT

Three areas of work are described: the production of covariance error files associated with the unfolding of experimental results from measurements of delayed neutrons from fission; progress in evaluation of fission yields and the implications for covariance analysis; and the production of a correlated tracking option in the Monte Carlo code MORSE and its use in the production of sensitivity matrices.

DELAYED NEUTRON SPECTRA AND THE PRODUCTION OF COVARIANCE ERROR FILES

The spectra of beta delayed neutrons from fission in fuels of interest to nuclear power technology are of significance to the behaviour of reactors as the energies are somewhat lower than those of prompt neutrons. Recent results from several experimental groups were reported at the recent Specialists' Meeting held in Birmingham (1). These represent measurements either of the emissions from separated delayed neutron precursors or of aggregate spectra where no attempt is made to separate the precursor nuclides. On the Birmingham Dynamitron and at AERE Harwell, measurements have been made by us of the aggregate spectra from fission in both 235-U and 239-Pu.

The experiments consist of cyclical irradiation of fissile samples with delayed neutron counting taking place during the beam-off period in each cycle; various timing cycles have been employed in order to emphasise different delayed neutron groups. The spectra have been measured with a pair of high resolution 3-He ionization chambers for which a typical energy response in shown in Figure 1, though in practice dual parameter (energy versus pulse rise-time) counting has been used in most measurements.

The procedure for unfolding has been described earlier (2) and in greater detail in a laboratory report (3) but essential consists of identifying the response matrix R for each spectrometer through subsidiary experiments which determine the resolution and efficiency of the counters. Ideally the knowledge of the response matrix would be complete so that the effect of the detector on an incident flux, ϕ, could be represented exactly by the matrix operation:

$$C = R \cdot \phi$$

where C is the counts spectrum.

Typically the counts spectra are taken over 100 or more channels and therefore R must be a matrix at least this size squared. The form normally assumed for the response to a monoenergetic neutron flux is a combination of two Gaussians plus a wall effect function according to the theory of Batchelor, Aves and Skyrme (4); the Gaussians have independently fitted amplitudes, means and widths and a Marquardt method non-linear least squares fitting routine (5) is used to determine the parameters. It is not realistic to attempt calibration measurements for every row of the R matrix, rather calibrations are made at a representative number of points and polynomial interpolation used to produce the appropriate values for the matrix elements in R. Thus the overall result is that around 26 parameters are sufficient to described the whole of the response matrix.

The unfolding procedure consists of finding the solution to the inverse equation:

$$\phi = \text{Rinv} \cdot C$$

where Rinv is the inverse of R and is found by an iterative process. Many other unfolding codes take account of the uncertainties in the counts spectrum C and determine the corresponding errors in the estimated flux ϕ. However R is itself uncertain, having been determined from the subsidiary calibration experiments. In our analysis, the effect of uncertainties on the 26 paramters which describe R are determined and combined with those from the counting statistics to produce a complete description of the final covariance matrix of errors for the output solution ϕ. This is done by perturbing each of the parameters used to describe R, one at a time, and re-performing the unfolding operation. In this way one obtains an estimate for the change in each of the output channels channels, $\delta\phi i$, for a small change in the R matrix parameter δPj. If one can approximate and use the ratio of $\delta\phi i/\delta Pj$ as the differential $d\phi i/dPj$ then the normal methods of error propagation can be used:

$$\text{Var}(\phi) = D^{T} \cdot \text{Var}(P) \cdot D$$

where D is the matrix of differentials and D^{T} is its transpose. The method is not as time consuming as might at first be supposed because the unperturbed case acts as a good first guess at the solution for the perturbed case and the matrix inversion usually only requires a fraction of the number of iterations required for the normal case. The method demands that the whole of the Var(P) covariance matrix be known; in practice it has been possible to determine those parts which relate to the polynomial representation of the variation with neutron energy of the parameters of the Gaussian fit, but not to fill in the portions between different parameters. The Var(P) matrix therefore becomes the combination of individual parts which are typically 3 by 3 or 5 by 5 matrices depending on the polynomial used to describe the energy variation.

$$\mathrm{Var}(P) = \begin{pmatrix} \mathrm{Var}(E1) & & & & & & \\ & \mathrm{Var}(E2) & & & 0 & & \\ & & \mathrm{Var}(P(2)) & & & & \\ & & & \mathrm{Var}(P(3)) & & & \\ & & & & \mathrm{Var}(P(4)) & & \\ & 0 & & & & \mathrm{Var}(P(5)) & \\ & & & & & & \mathrm{Var}(P(6)) \end{pmatrix}$$

where $$Y(E) = P(1) \cdot \left[\exp\left| \frac{-1}{2} \cdot \left(\frac{E-En}{P(2)} \right)^2 \right| \right.$$

$$\left. + P(3) \cdot \exp\left| \frac{-1}{2} \cdot \left(\frac{E-|En-P(4)|}{P(5)} \right)^2 \right| + P(6) \cdot \mathrm{wall\_effect}(E) \right]$$

is the Gaussian fitting function and E1 and E2 are two terms describing the variation of the counter efficiency with energy.

Ultimately it is hoped to perform the fitting for the response function terms and their variation with neutron energy in a simultaneous process so that the off-diagonal terms can be evaluated, but currently the computing facilities do not allow such large arrays to be determined.

The importance of knowing the whole covariance matrix for ϕ has been demonstrated when calculations of parameters such as average delayed neutron energy were made because then the covariance terms in Var(ϕ) are required and we have shown that to ignore the off-diagonal terms in Var(ϕ) can lead to serious miscalculation in the uncertainty of derived values.

Finally a point on estimated fluxes as a result of this procedure. The flux determined from the unfolding is an estimate based on a statistical sampling of possible input counts values and thus, for an energy group where the true value of the flux is zero but there is a finite standard deviation, the actual result ought to have a scatter about the zero mean with equal probability of being on the positive or negative side. So long as the combined spectrum does not predict negative numbers of neutrons overall, there is nothing illogical in declaring an individual group to have negative intensity. We are of the opinion that methods which force the resultant flux to be positive are bound to introduce bias in results.

FISSION PRODUCT YIELD EVALUATION

Fission yield evaluations were made in the UK during the 1970's by Crouch (6). Following his retirement, a research fellow from the University of Birmingham has been appointed to bring the evaluation up-to-date and to extend the analysis to include covariance information. Currently the programme has produced a new evaluation based on data published up to 1981 for independent yields and this has been submitted to JEF 1. Two different sets have been produced: unadjusted and adjusted. In the latter, allowance is made for physical constraints such as the conservation of nucleons, pairing between the light and heavy mass peaks etc. The operation of the constrained fit clearly makes the result correlated both within mass chains and between mass chains.

In addition, a complementary evaluation of cumulative yields is about to be completed. According to custom the independent yields have been calculated before delayed neutron emission, while the cumulative yields allow for delayed neutron emission and consequently for movement between different mass chains.

If the independent yield of the i-th fission product is given by Yi and the corresponding cumulative yield by Ci, then the decay of other precursors to form that i-th nuclide can be expressed as:

$$\sum_j \delta_{ij} C_j = C_i = Y_i + \sum_j B(j>i) \cdot C_j$$

where δ_{ij} is a Kronecker delta and B(j>i) represents the branching ratio for decay from the preceding nuclide in the decay chain or for movement from the previous mass chain through delayed neutron emission. The equation is written in this form because the branching ratios are obtained from a code such as FISPIN as a factor by which the cumulative yield of the earlier nuclide is to be multiplied.

$$\sum_j [\, \delta_{ij} - B(j>i) \,] \cdot C_j = Y_i$$

which can be expressed in matrix terms as

$$P \cdot C = Y$$

where $$P_{ij} = [\, \delta_{ij} - B(j>i) \,]$$

In order to determine the cumulative yields the inverse matrix P^{-1} must be determined. This is a very large array, but it has been calculated. From this the covariance matrix for the cumulative yields due to the covariance of the independent yields can be calculated by using the propagation of errors form:

$$\mathrm{Var}(C) = [P^{-1}] \cdot \mathrm{Var}(Y) \cdot [P^{-1}]^T$$

What is more difficult, and will require further study, is the way that the effect of uncertainties in the Pij terms can be incorporated into the calculation. Unlike the delayed neutron spectra in the first section, where only about 26 different paramters were involved, the P matrix is around 1000 by 1000 elements in size. The method of perturbing each term and recomputing the results is therefore unlikely to be applicable.

A further area for attention will be the correlations between the data values used for the evaluation. Many measurements use the same reference yield as a normalising factor, indeed many results are quoted as a ratio with respect to the reference value. Several different experimental groups may use the same

library yield value as their basis and will therefore become correlated when their values are converted into absolute terms by use of the "known" reference yield. A further complication arises in "ratio of ratio" measurements where yields in a less common fissile nuclide are compared with measurements of a reference yield, but also with the same pair of yields in a more common fissioning system, often 235-U. In this way the data for one fissile nuclide is correlated with that for the other. These points will be investigated with the aim of making some allowance for these correlations in the evaluation process (7).

DETERMINATION OF SENSITIVITY MATRICES BY MONTE CARLO METHODS

As part of a study (8)of a fusion reactor benchmark experiment performed at an earlier time in Birmingham (9), modifications have been made to the Monte Carlo code MORSE. A correlated tracking routine has been added which operates in a manner quite similar to the perturbation method applied to the delayed neutron spectral measurements described above. What is not done is a complete rerun of the MORSE code for data with and without perturbations; this would clearly require very long run times in order to reduce the random error between cases to the point where the effects of the perturbation can be seen. Rather the code simultaneously records results for the perturbed and unperturbed input data as a particular particle history is tracked. Hall et al (10) have implemented a version of this method in the Winfrith code McBEND by calculating the first derivative of the probability functions; this implementation is known as DUCKPOND. The method chosen here was to apply equal and opposite finite perturbations about the normal value. This approach has the advantage that calculations may be undertaken where large perturbations are present, but anyway the user has the freedom to vary the size of the perturbation applied to match expected cross section uncertainties. Because the calculation of the sensitivity S from:

$$S = \frac{\phi_{pos} - \phi_{neg}}{2\ \Delta\Sigma}$$

demands the subtraction of two nearly equal quantities, there must be a concern for the possibility of rounding errors affecting the results. In the study of the fusion reactor benchmark, this did not appear to be a problem for perturbations of greater than about 1%.

During a Monte Carlo random walk the following probability density functions are used:

1. Exponential transform for distance to next collision
2. Angular probability density function for direction of emission
3. Probability of downscatter into the relevant group
4. Probability of absorption at each collision site

Each of these may be sensitive to perturbations in cross sections.

The first is taken into account by accepting the distance to next collision from the unperturbed case, but adjusting the subsequent particle weight according to the perturbed total cross section. In this way the positions of interactions of the perturbed and unperturbed cases are kept the same.

The code has not been altered to account for the second and third effects because these both depend only on the partial probability of scattering into a particular direction. As the perturbations to scattering cross sections are assumed to act only on the total scattering cross section and not on the angular variations, these two effects will give zero contribution under the assumption made.

Because MORSE never terminates particle histories as a result of absorption, but regards every event as a scatter and allows for the probability of absorption by downweighting the history at each collision, the fourth effect, involving absorption, is taken into account in the correlated tracking algorithm by further altering the particle weight at each collision.

A further possible mechanism for perturbation arises if point estimators are being used as opposed to tracklength, collision density or surface crossing routines. This is because the point estimator method employs a calculation to determine the possibility of each collision event contributing to the "result" at the required detector position. Thus the point estimator stage is subject to the same series of alterations as the main particle history tracking as just described.

Thus, in principle, correlated tracking can be used to determine sensitivities for any alteration in partial cross section and any group response. In practice there are two major factors to be borne in mind.

Firstly, it is impractical to calculate all sensitivities to all group responses in one Monte Carlo run since this would require many tens of thousands of results to be stored and manipulated withn the code.

Secondly, the problem of statistical uncertainty will limit the degree to which phase space can be subdivided within the assembly being modelled. If the sensitivity of a response to too small a region of phase space is required then the problem of achieving sufficient sampling within that phase space region will be the limiting factor in achieving the required accuracy.

The method has been compared with results from two alternative methods: (i) ANISN/SWANLAKE and (ii) first order perturbation results fom adjoint MORSE runs.

Comparisons of both methods are shown in Figures 2 and 3 and indicate the good agreement found between the results, though the first order perturbation method tends to show lower results than the correlated tracking (FISHTANK) version.

The production of the sensitivity matrices allows the user to determine the overall response to a perturbation in any particular combination of data channels. A secondary code SENSMIX has been produced to facilitate the production of the required mixing of perturbations (6).

POSTSCRIPT

Having made some use of covariance matrices through the group of projects described, it has become clear that the frequent assumption that "most parameters are independent" and thus covariance terms can be ignored (to make error propagation more simple) is to say the least unwise. In the educational environment we do our students an injustice if we train them only to calculate the standard deviations on the gradient and intercept of a straight line fit. At Birmingham we attempt to ensure that all first year undergraduate physicists are given some contact with the theory associated with covariance techniques, together with practical examples, so that they will neither receive a rude shock when first attempting to manipulate data which are highly correlated nor, more significantly, fail to appreciate the consequences of ignoring the correlations.

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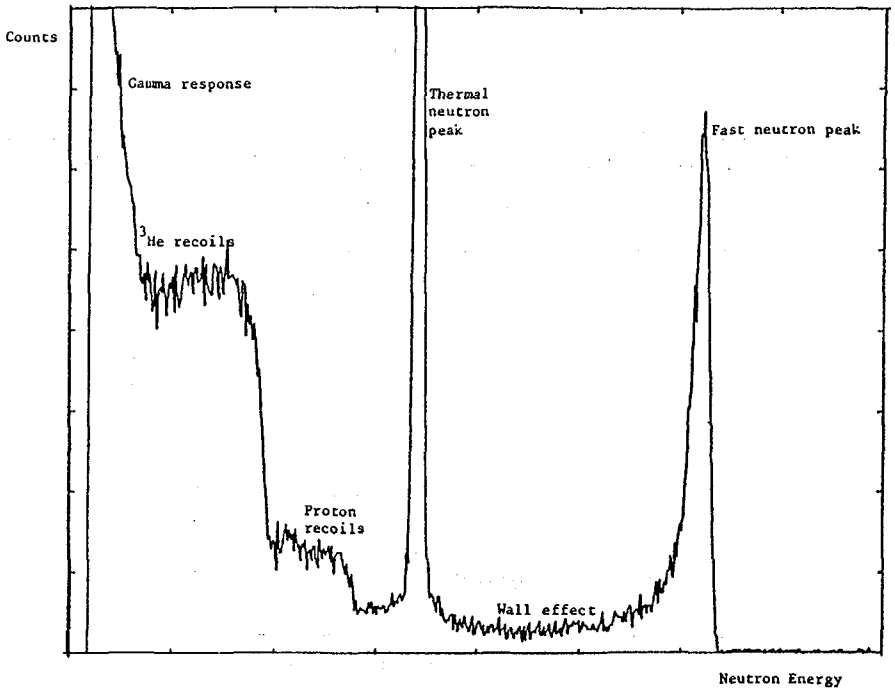
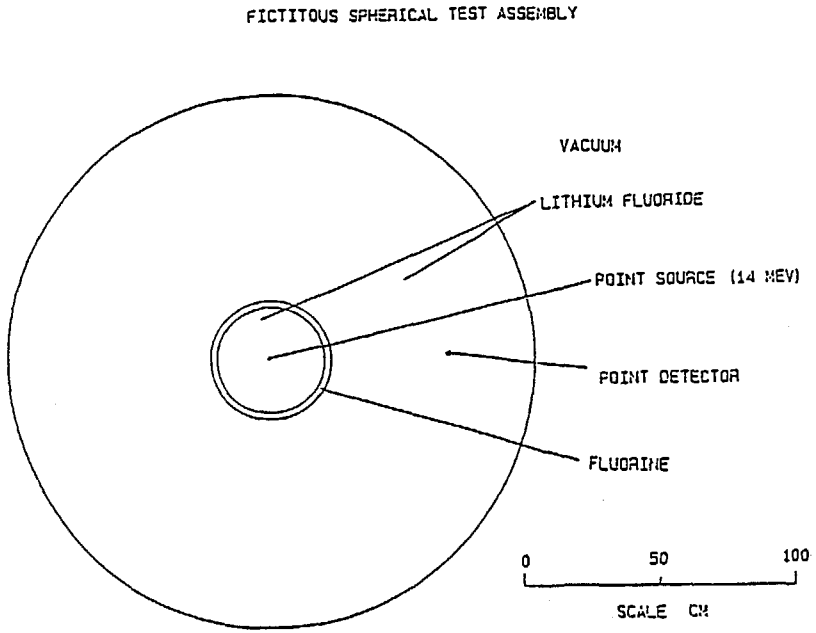


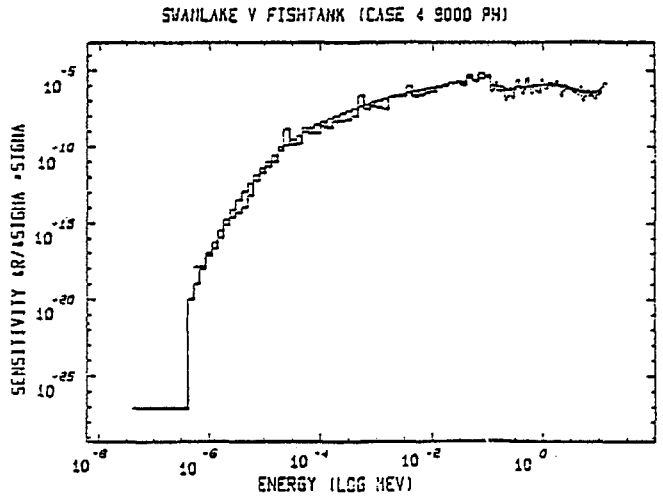
The response of the 3-He spectrometer to a monoenergetic flux of 626 keV neutrons.

FIGURE 1.

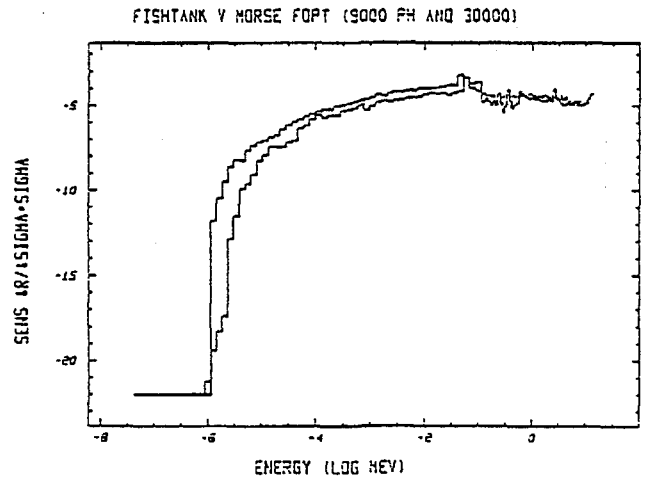


Fictitious assembly modelled exactly by MORSE and approximated by ANISN.

FIGURE 2.



3a. Comparison of SWANLAKE and FISHTANK (SWANLAKE results are smooth) - change in total flux response of detector as a function of the fractional change ot total cross section in each energy group.



3b. Comparison of MORSE first order perturbation theory and FISHTANK - change in total flux due to changes in total cross section of fluorine in each

FIGURE 3.

Covariances in the REAL-84 exercise

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SUMMARY

After an introduction on the contents and scope of the REAL-84 exercise the role of covariance information in this exercise was discussed. Covariance matrices can be singular, and the positive definite character is not guaranteed. The effective rank (according to some slightly different definitions) could be much lower than the number of groups determining the dimensions of the matrix.
Owing to reasons of numerical precision in the calculations correlation matrices are preferred to covariance matrices.

1. INTRODUCTION

The REAL-84 exercise is a follow-up of the REAL-80 exercise [1] and is organized by the Nuclear Data Section of the International Atomic Energy Agency. The aim of the exercise is to improve the assessment of accuracies in radiation damage predictions by various laboratories using good quality input data and proper calculation methods. The emphasis lies on radiation damage to reactor pressure vessels and related nuclear technology. Therefore, the neutron energy range of interest is below 20 MeV. The long term aim of REAL-84 is to strive towards establishment of standardized metrology procedures and recommended nuclear data for use in spectrum adjustments and damage parameter calculations. The short term aim is the improvement of the information. In addition, the exercise will allow to assess and validate the accuracy of the methods and computer codes used. The joint effort of the participants of the exercise will contribute in solving some basic mathematical and physical problems that occur in neutron spectrum adjustment procedures for radiation damage purposes.

2. INPUT DATA

In frame of the exercise 7 different neutron spectra (see figure 1) were investigated:

1. ANO - Pressure-vessel cavity of the Arkansas Power and Light Reactor (Arkansas Nuclear One - 1);
2. PS1 - Oak Ridge Research Reactor Poolside Facility in the metallurgical irradiation experiment (Position simulated surveillance capsule);
3. PS2 - Oak Ridge Research Reactor Poolside Facility in the metallurgical irradiation experiment (1/4 T position in the simulated pressure vessel capsule);
4. RTN - Fusion simulation spectrum measured at the RTNS-II, a 14 MeV neutron source at Lawrence Livermore Laboratory (the spectrum is a pretty fair simulation of a fusion first wall spectrum);
5. TAN - Accelerator spectrum Be(d,n) with deuteron energies of 16 MeV;
6. U35 - Fission spectrum of U235;
7. CFR - Neutron spectrum in the centre of the coupled fast reactivity measurement facility (CFRMF).

A magnetic tape was distributed to participants comprising the input data sets, such as

. measured reaction rates
. calculated input spectra
. cross-section values

accompanied by their covariance information. Also utility programs to perform data treatment were supplied.
The reaction cross-section data and their covariance information for the exercise were derived from the best available up-to-date (1985) derived compilations, such as ENDF/B-V and IRDF85 files.

The participants were asked to use adjustment codes which explicitly can treat covariance matrices, in order

a) to perform good neutron spectrum adjustments,
b) to evaluate displacement rates and gas production rates for steel,
c) to provide uncertainty and correlation data,
s) to specify the procedures followed.

Since it was required to treat the given covariance information, the number of participants was limited.

In the preparation of the input set for the magnetic tape of the exercise it was tried to obtain data of good quality for the various spectra.

A survey of participating laboratories and supplied solutions is given in table 1.

Table 2 shows the amount of the input information and its structure.

Three progress reports on the REAL-84 exercise have been prepared by a joint evaluation team of scientists from BME Budapest and ECN Petten. The final report is expected to be ready before summer 1987. A summary of the final results will be presented at the 6th ASTM-EURATOM Symposium on Reactor Dosimetry (Jackson Hole, Wyoming, May 31-June 5, 1987).

In the present document the experience with covariance matrices in reactor neutron spectrum adjustment is summarized.

INPUT COVARIANCE INFORMATION

It turned out that all input spectrum covariance matrices were singular. From a mathematical point of view this means that they cannot be inverted. Physically it indicates inadequacy of information needed to describe the relations between the different variables (e.g. fluence rate values) involved in the adjustment. In case of STAY'SL type codes the calculation procedure for the χ^2-parameter is done by a linearized model. Therefore, in this case no inversion of the input spectrum covariance matrix is needed. For the future it is necessary to investigate the quality and condition of the input spectrum covariance both from physics and mathematics points of view.

The reaction rate covariance matrices available in the exercise obviously originate from different methods. It seems to be necessary to reach agreement on the best method to determine these data.

CROSS-SECTION COVARIANCES

Cross-section covariance information is now available for the metrology reactions in the IRDF85 and ENDF/B-V libraries. For several cases the variance values are so large, that the reaction has a small statistical weight in the adjustment procedure (see table 3).

Experimental uncertainty information for the damage producing reactions is not available. Uncertainty values have been arbitrarily chosen for the gas production and displacement cross-sections, so that they have only meaning for comparison purposes. The uncertainty values chosen are 10% for Fe, 12% for Ni, and 18% for Cr. It has been assumed that the correlation between the group damage cross-sections can be described by means of a special Gaussian function with a specified width parameter.

NUMERICAL RANK

Because of the singularity of the spectrum covariance matrix an investigation was made of the rank of these matrices. It is convenient, however, not to study the covariance matrices themselves, but the corresponding correlation matrices.

In principle, covariances matrices and correlation matrices are positive definite, but it turned out that often nearly zero and/or negative eigenvalues are present.

For a positive definite matrix one has the property that the sum of the eigenvalues λ_i is equal to the trace of the matrix. For a correlation matrix this sum is equal to the dimension of the matrix (i.e. equal to m, the number of energy groups involved).

The numerical (or effective) rank of a constructed correlation matrix (which, owing to its construction, is not guaranteed positive definite) can then be an integer smaller than the trace. It is determined by the number of positive eigenvalues which are significantly different from zero.

We consider the ordered eigenvalues, such that

$$\lambda_1 \geq \lambda_2 \geq \lambda_3 \text{ , etc.}$$

and introduce a normalization, such that

$$\lambda_i^* = \lambda_i / m \ .$$

Then $\Sigma \lambda_i^* = 1.00$.

There are several choices for the definition of the numerical rank, e.g.

- the number of eigenvalues λ_i which are larger than unity;
- the number of ordered and normalized eigenvalues, for which the sum is smaller than 0.95 (or 0.98 or 0.99);
- the number of ordered and normalized eigenvalues which are larger than 0.01.

Table 4, based on data supplied by Matzke, shows values for the rank of the correlation matrices, involved in the REAL-84 exercise. It shows that the rank is much smaller than the number of energy groups in which the covariance matrix is reported in literature. For instance, the covariance matrix for the ^{235}U fission neutron spectrum has been published in 24 groups, while the underlying formula for the spectrum corresponds to [2]

$$\chi(E) = (4/\pi\, a^3 b)^{\frac{1}{2}} \sinh(\sqrt{bE}) \cdot \exp(ab/4) \cdot \exp(-E/a)$$

where $a = 0.988$ MeV and $b = 2.249$ MeV^{-1}.

Further input data are

$$v(a) = 1.2\%; \quad v(b) = 5.9\%; \quad r(a,b) = -0.21.$$

This explains why the numerical rank is 2.

The precision of the computer calculations has a non-negligible influence on the numerical precision of some characteristic values for matrices, such as rank and condition number.

The condition number, defined as the ratio of the largest positive eigenvalue and the smallest (positive) eigenvalue, is a measure for the influence which perturbations in the matrix elements have on the eigenvalues. Ill-conditioned matrices have large condition numbers. The data collected in table 5 (based on work by Szondi, [3]) show that the characteristic values can better be obtained from correlation matrices than from covariance matrices.

The IAEA Consultants' Meeting on the Assessment of the Results of the REAL84 exercise (Budapest, September 1986) advised therefore to work with correlation matrices rather than with covariance matrices.

Summarizing, it was stated that correlation matrices are preferred above covariance matrices, since correlation matrices

- have elements between -1 and +1. These elements represent dimensionless physical quantities;
- show better numerical precision in computer calculations;
- have more favourable condition numbers;
- give often with single precision results which are comparable to results which can be obtained with covariance matrices with double precision;
- facilitate calculation of effective rank.

Also during this Consultants' Meeting the following points were recognized:

a. The rank of a covariance matrix equals the number of independent "statistical" variables involved;
b. The rank of a group fluence rate spectrum covariance matrix or of a group cross-section covariance matrix should not change going from a coarse group structure to a fine group structure;
c. The rank of an output covariance matrix for group fluence rates in an adjustment procedure is lower than or equal to that of the covariance matrices of the input least-squares adjustment;
d. Least-squares adjustment with covariance matrices with deficient rank ($r<m$) corresponds to an adjustment in a certain subspace (dimension r) of the whole space (dimension m). The lower the rank of the spectrum covariance matrix, the smaller the possibility of modifying the spectrum shape.

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Table 1. Survey of participating laboratories and supplied solutions

Laboratory code	Participant	Ident of solution	Adjustment code	Spectrum
NRMI	U. Ueda, M. Nakazawa, A. Sekiguchi	SET 1	NEUPAC-JLOG	ANO
ORNL	R.E. Maerker	SET 2	LEPRICON	ANO*
ANL	L.R. Greenwood	SET 3	STAY'SL	ANO, PS1, PS2, TAN*, RTN*, U35, CFR
IJS	M.Najzer, I. Remec	SET 4	STAY'SL	ANO
KFKI	J. Végh	SET 5	STAY'SL	ANO, PS1, PS2, U35, CFR
ECN	H.J. Nolthenius	SET 6	STAYNL	ANO, PS1, PS2, TAN, RTN, U35, CFR
PTB	M. Matzke, W. Mannhart	SET 7	STAY'SL	RTN, U35
BME	É.M. Zsolnay, E.J. Szondi	SET 8 SET 9	STAYNL SANDBP	ANO, U35 ANO, PS2, U35
IPM	A. Hrabovcova	SET 10	SANDMX	ANO, TAN, RTN
ORNL	F.W. Stallmann	SET 11	LSL-M2	PS1, PS2

* More than one solution

Table 2. Physics information of input.

	ANO	PSF-1	PSF-2	RTN	TAN	U235	CFRMF
REACTION RATES							
NUMBER	6	10	6	12	18	22	23
VARIANCES PRESENT?	+	+	+	+	+	+	+
CORRELATIONS PRESENT?	+	-	-	+	+	+	-
SPECTRUM							
NUMBER OF GROUPS	55	37	37	60	39	24	26
NUMBER OF VARIANCE GROUPS	16	37	37	60	39	24	26
CORRELATIONS PRESENT?	+	+	+	-	-	+	+

Table 3. Role of cross-section uncertainties.

	ANO	PS1	PS2	TAN	RTN	U35	CFR	ϕ_{th}	$\phi_{1/E}$	ϕ_{fiss}
^{6}Li(n,α)							o	o	o	o
^{10}B (n,α)							o	o	o	-
^{27}Al(n,p)						-	-			-
^{27}Al(n,α)					o	o	-	-		-
^{45}Sc(n,γ)		o	o	-	o		o	o	o	o
^{46}Ti(n,p)	--	--	--	--	--	--	--			--
^{47}Ti(n,p)				--	--	--	--		--	--
^{48}Ti(n,p)				--	--	--	--			--
^{54}Fe(n,p)	o	o	o	o	-	o	o		-	o
^{55}Mn(n,2n)						--				--
^{56}Fe(n,p)				o		o				o
^{58}Fe(n,γ)		--	--				--	-	--	--
^{58}Ni(n,p)		-	-	-	--	-	-		-	-
^{58}Ni(n,2n)	-			--	--	--				--
^{59}Co(n,γ)		o	o	-	o		o	o	o	o
^{59}Co(n,α)				o		o				o
^{59}Co(n,2n)				-	-					--
^{60}Ni(n,p)				-	-					-
^{63}Cu(n,γ)						--	-	o	o	--
^{63}Cu(n,α)	-	-				-				-
^{115}In(n,γ)						o	o	-	-	o
^{115}In(n,n')				--		--	--		--	--
^{127}I (n,n')						--				--
^{197}Au(n,γ)				--	o	-	o	o	o	-
^{232}Th(n,γ)							--	--	--	--
^{232}Th(n,f)						-	-		-	-
^{235}U (n,f)		o		o		o	o	o	o	o
^{237}Np(n,f)		-				-	-	--	--	-
^{238}U (n,γ)				--			o	o	o	--
^{238}U (n,f)	o	o		o		o	o	--	-	o
^{239}U (n,f)	-					o	o	o	-	o

o : uncertainty 0 - 5%
- : uncertainty 5 -10%
--: uncertainty > 10%

Table 4. Numerical rank of correlation matrices.

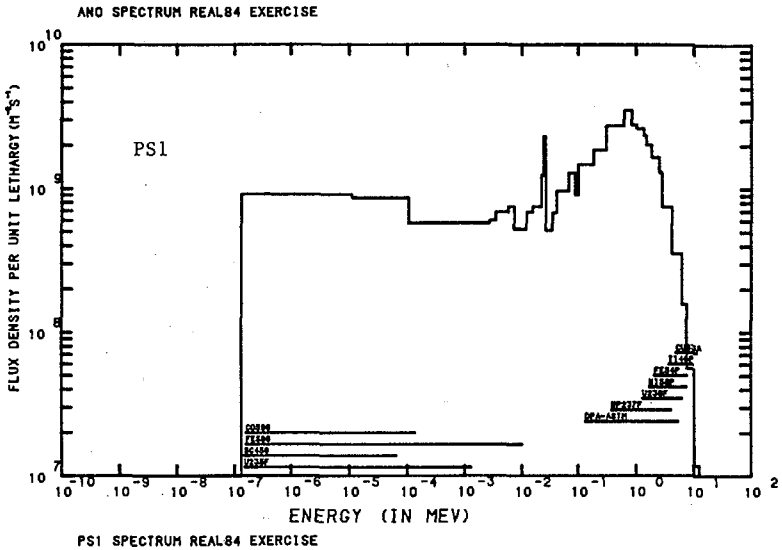
spectrum	m	number of λ_i with $\lambda_i > 1$	number of λ_i^* for which $\Sigma\lambda_i^* = 0.95$	$\Sigma\lambda_i^* = 0.99$	$\Sigma\lambda_i^* > 0.01$
ANO	16	3	6	12	6
PS1=PS2	37	4	8	21	8
TAN	39	5	4	6	6
RTN	60	10	11	15	12
U35	24	2	2	2	2
CFR	26	6	6	10	6

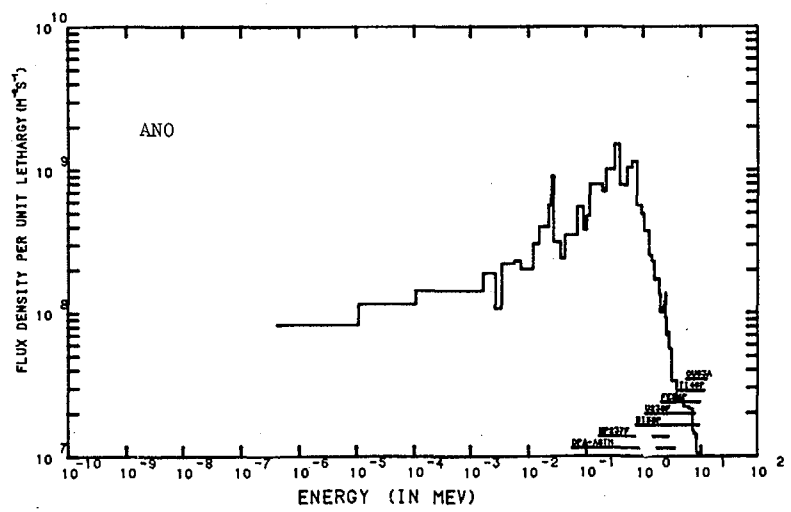
Table 5. Covariance matrix ⟷ correlation matrix.

	covariance matrix	correlation matrix
ANO - 16 groups		
non-negative λ's	16	16
$\lambda_{max}/\lambda_{min}$	67×10^{6}	545
rank, single prec.	14	16
rank, double prec.	16	16
effective rank		9
PS1 - 37 groups		
non-negative λ's	37	37
$\lambda_{max}/\lambda_{min}$	844×10^{12}	2230
rank, single prec.	29	37
rank, double prec.	37	37
effective rank		14
PS2 - 37 groups		
non-negative λ's	37	37
$\lambda_{max}/\lambda_{min}$	254×10^{12}	2200
rank, single prec.	31	37
rank, double prec.	37	37
effective rank		14
RTN - 60 groups		
non-negative λ's	49	40
$\lambda_{max}/\lambda_{min}$	8.67×10^{42}	139×10^{3}
rank, single prec.	1	60
rank, double prec.	25	60
effective rank		12

Table 5 cont.

TAN - 39 groups		
non-negative λ's	29	25
$\lambda_{max}/\lambda_{min}$	8.33×10^{21}	781×10^{3}
rank, single prec.		39
rank, double prec.		39
effective rank		6
U35 - 24 groups		
non-negative λ's	12	13
$\lambda_{max}/\lambda_{min}$	9.8×10^{92}	2.61×10^{3}
rank, single prec.	5	22
rank, double prec.	23	24
effective rank		2
CFR - 26 groups		
non-negative λ's	20	20
$\lambda_{max}/\lambda_{min}$	279×10^{12}	2.2×10^{3}
rank, single prec.	22	26
rank, double prec.	26	26
effective rank		6





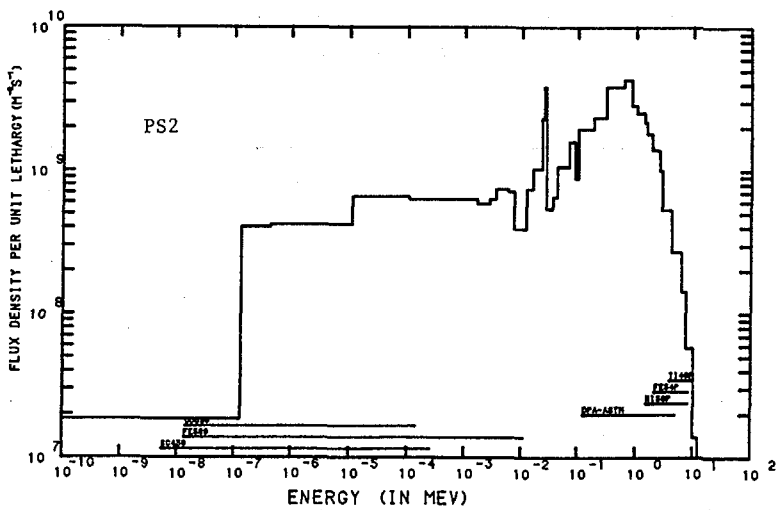
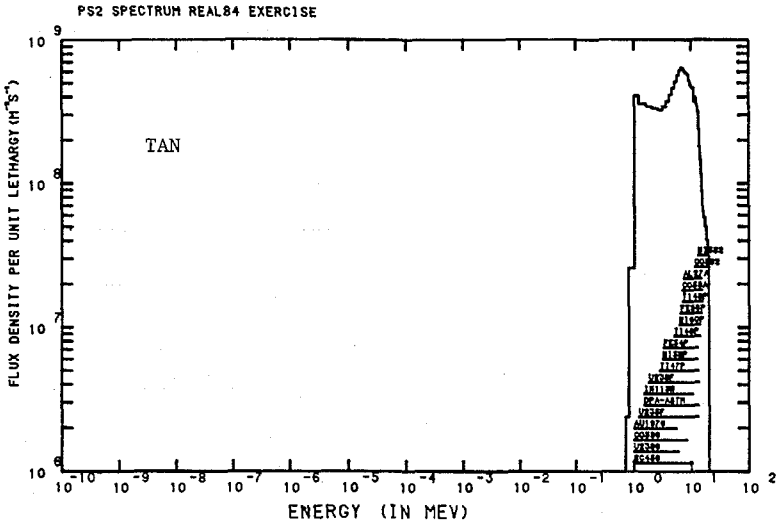


Fig. 1. Input neutron spectra.



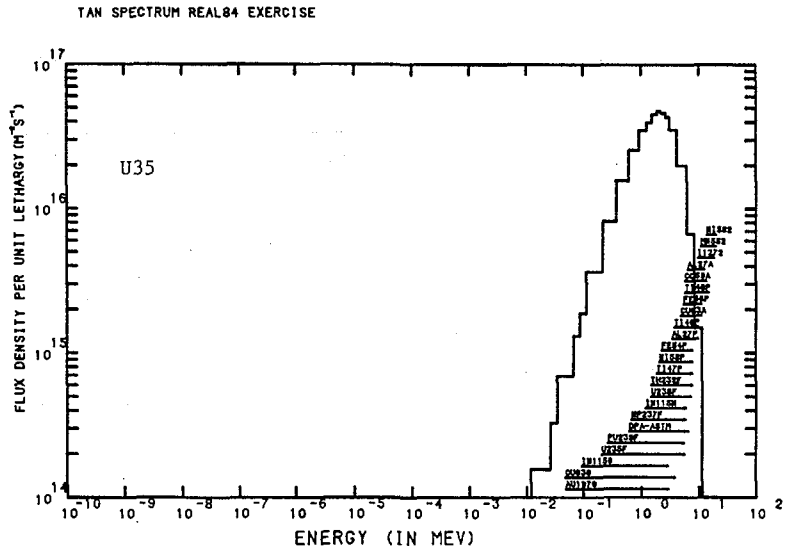
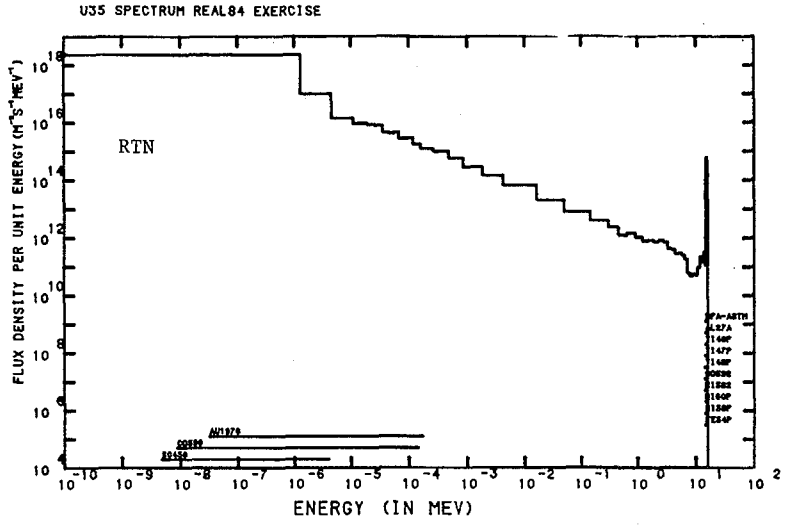
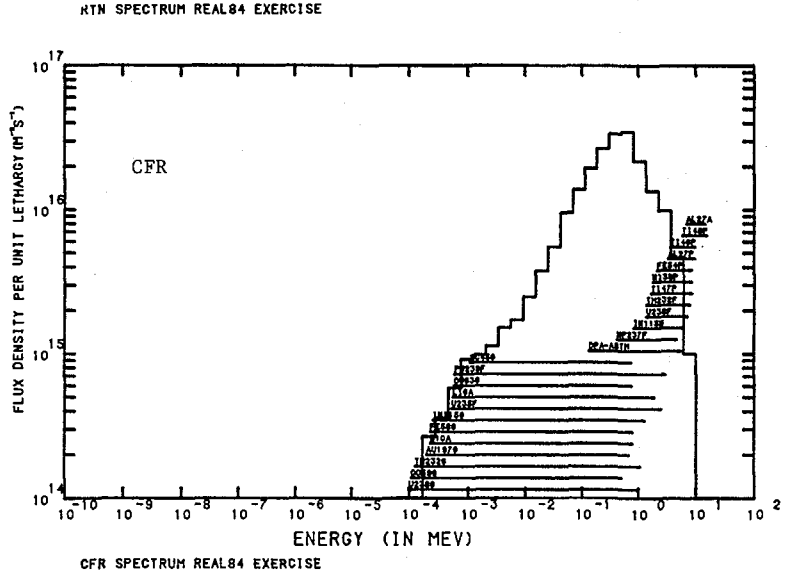


Fig. 1 (continued).





Note: In the last figure the quantity along the vertical axis is the flux density per unit energy (instead of per unit lethargy); in this way the presence of low energy neutrons is shown.

NUCLEAR DATA NEED FOR THE COVARIANCE INFORMATION USED IN THE NEUTRON SPECTRUM ADJUSTMENT

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The aim of the reactor dosimetry investigations is to provide integral damage exposure parameters (eg neutron fluence above 1 MeV) together with their covariance matrix for the service life prediction of reactor pressure vessels. One important part of this work is the neutron spectrum adjustment. The results of the IAEA REAL80 exercise have shown that the values of the damage exposure parameters determined by the different participating laboratories had a relatively small (generally some per cent) spread while the accompanying uncertainty values showed rather large (sometimes several hundred of per cents) deviations /1/.

The calculation of damage exposure parameters is based on the neutron spectrum available in multigroup form as a result of the solution of the following minimizing problem:

$$\chi^2 = \begin{bmatrix} A-A_r \\ P-P_r \end{bmatrix}^T \begin{bmatrix} cov(A_r) & 0 \\ 0 & cov(P_r) \end{bmatrix}^{-1} \begin{bmatrix} A-A_r \\ P-P_r \end{bmatrix} \longrightarrow min$$

where the formalism of the commonly used STAY'SL code is applied /2/:

- A vector, containing the saturation activities of the activation detectors,
- P vector, containing the neutron spectrum (ϕ) and the cross sections (σ):

$$P^T = [\phi^T, \sigma_1^T, \sigma_2^T, \cdots] \qquad \text{and} \quad A = [\sigma_1, \sigma_2, \cdots]^T \phi$$

and the suffix 'r' signes the referene (eg measured) values.

The predicted uncertainty of the damage exposure parameter is the outcome of a correct uncertainty propagation calculation, the basic data of which are the matrices $cov(A_r)$ and $cov(P_r)$.

Covariance matrices of nuclear data are needed to determine the uncertainties in the input - and consequently in output - data of the neutron spectrum adjustment. Performing these calculations one encounters lots of difficulties due to the lack of the necessary information.

The covariance matrix of the measured activities /3/

The activity of the activation detectors is obtained by evaluating the gamma spectrum of the radionuclides produced:

$$A = \frac{T}{t \eta \gamma}$$

where:

- T area of the total energy peak,
- t measuring time,
- η counting efficiency of the semiconductor detector for the gamma radiation of interest,
- γ gamma abundance.

One can write in a symbolic way: A=A(x), where the vector x represents all the parameter vectors present in the last equation. The matrix cov(a) is then determined using the methods of the sensitivity theory /4/:

$$cov(A) = D\ cov(x)\ D^T$$

where the matrix D consists of the partial derivatives:

$$D = \frac{\partial A}{\partial x}$$

The cov(x) matrix contains the submatrix $cov(\gamma)$, the elements of which are nuclear data.

In case if the uncertainty of the gamma abundances is comparable in order of magnitude with the one of the peak areas and/or gamma counting efficiencies, its contribution to the total uncertainty of the activity can play an important role. In general, the uncertainty of the total energy peak area and gamma counting efficiencies is in the vicinity of 1 per cent. Similar (or larger) values for the gamma abundances of activation and fission detectors listed in Tables 1 and 2 can be found. At the same time, the covariance information for these abundance is completely missing. The data available in the literatue are not sufficient to calculate the covariance matrices of interest, eg in case of the radionuclide Sc-48 one can get a 'correlation coefficient' equal to 1.92 /3/ by using the data of Ref. /5/.

The covariance matrix of the input spectrum /6/

The calculation of the reference ('input') neutron spectrum for the adjustment is based on the solution of the neutron transport equation or an approximation of this equation. Considering the multigroup diffusion equation system one can write /7/:

$$\nabla D_i \nabla \phi_i - (\Sigma_{ai} + \Sigma_{si})\phi_i + \sum_j \Sigma_{sji}\phi_j + \nu \chi_i \sum_j \Sigma_{fj}\phi_j = 0$$

where:

- D diffusion coefficient
- Σ macroscopic cross section
- ν fission yield
- χ fission spectrum
- a suffix for absorbtion
- s suffix for scattering
- f suffix for fission

In this equation all the parameters are calculated by multiplying the nuclear data (cross sections, fission yield, &c) by facility-dependent constants.

The covariance data for the pertinent cross sections should be used in generating the input spectrum covariance matrix. IAEA NDS distributes two cross section files for general use. One of them is the 'general purpose file' of ENDF/B-IV which does not contain any covariance information. The other one is the IROF85 /8/. Table 3. shows the availability of covariance data in this library. No covariance information for the scattering cross sections is present in it. As a result, the calculation of a correct input spectrum covariance matrix is rarely supported.

The covariance matrix of the detector cross sections

The covariance matrices of the IRDF85 library are usually given only in few groups. Therefore, the maximum number of the energy groups used in the neutron spectrum adjustment is limited by the rank of these matrices. More detailed analysis of this problem can be found in /9/. For increasing the energy group number of the neutron spectrum in the calculations more detailed covariance information on the cross sections is needed. Furthermore, covariance matrices for a number of dosimetry reactions should be made available, otherwise several activation neutron detectors - commonly used in the practice - are excluded from the adjustment procedure /10/.

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Table 1. Uncertainty of gamma abundances for fission detectors

Measured	Energy (keV)/Uncertainty(%)			
Zr-97	507.6/11.8	1147.9/11.5	355.4/10.6	602.4/10.1
Ru-103	497.1/ 0.8	610.3/ 1.2		
I-131	364.5/ 1.5	637.0/ 1.5	284.3/ 1.5	
Te-132	228.2/ 1.1	49.7/ 6.9		
I-132	667.7/ 0.1	772.6/ 2.4	954.6/ 3.3	522.7/ 3.7
La-140	1596.2/ 0.8	487.0/ 0.9	815.8/ 0.7	328.8/ 0.9
Ce-143	293.3/ 5.1	45.4/ 7.7	664.6/ 6.9	721.9/ 5.5

Table 2. Uncentainty of gamma abundances for activation detectors

Reaction	Energy(keV)/Uncertainty(%)			
AL27P	843.8/0.6	1014.4/1.4		
TI48P *	893.5/0.5	1312.1/0.5	1037.5/0.5	175.4/1.1
MN55G	846.8/0.3	1810.7/2.7	2113.1/2.8	
FE58G	1099.2/2.1	1291.6/1.8	192.3/2.3	
CU632	1173.0/?	875.7/4.5	2302.0/5.0	1129.0/5.3
ZN642	669.6/?	962.1/5.1	1412.1/4.4	449.9/6.9
ZR90P	202.5/0.2	479.5/0.1	1760.7/?	2319.1/?
ZR902	1712.9/9.1	1744.5/0.8	1657.3/1.0	1620.8/9.9
AG109G	657.7/?	884.7/1.1	937.5/1.2	1384.3/1.0
IN115G	1293.5/2.1	1097.3/2.1	416.9/5.1	2112.1/3.2
I1272	666.3/7.6	388.6/8.8	491.2/7.7	
TA181G	1121.3/0.9	1221.4/0.9	1189.0/0.9	1231.0/0.9
W186G	685.8/4.1	479.5/4.3	72.1/4.2	134.2/4.3
TH232G	311.9/?	300.1/5.2	340.5/5.4	86.6/?
U238G	106.1/5.7	277.6/2.8	228.2/6.5	209.8/7.7

* Ti-48(n,p)Sc-48; see Text

Table 3. Availability of cros section covariance data in the IRDF85

Material	Reactions				
3-Li	LI6A	LI7P	LI7D	LI7T	LI7A
5-B	B5A				
9-F	F92				
11-Na	NA232				
12-Mg	MG24P				
13-Al	AL27P	AL27A			
15-P	P31P				
16-S	S32P				
21-Sc	SC45G				
22-Ti	TI46P	TI47P	TI47PN	TI48P	TI48PN
25-Mn	MN552				
26-Fe	FE54P	FE56P	FE58G		
27-Co	CO592	CO59G	CO59A		
28-Ni	NI582	NI58P	NI60P		
29-Cu	CU632	CU63G	CU63A	CU652	
30-Zn	ZN64P				
40-Zr	ZR902				
41-Nb	N893N				
45-Rh	RH103N				
49-In	IN115N	IN115G			
53-I	I1272				
79-Au	AU197G				
90-Th	TH232F	TH232G			
92-U	U235F	U238F	U238G		
93-Np	NP237F				
94-Pu	PU239F				

EVALUATING NUCLEAR DATA UNCERTAINTY: PROGRESS, PITFALLS, AND PROSPECTS*

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The reasons for including variance-covariance information in evaluated nuclear data files are reviewed. Accomplishments and obstacles in meeting these needs are identified. The capability to develop and utilize evaluated cross-section covariance files has been largely demonstrated, but comprehensive files of soundly based covariance data remain to be evaluated and not all types of cross-section data have yet been included. The status of the ENDF-VI covariance formats is discussed. Priorities are suggested for further development. Most effort should be concentrated to fully develop the capability to estimate the nuclear data uncertainties in quantities calculated for a broad energy spectrum.

1. INTRODUCTION

Over a decade ago, the development of comprehensive sensitivity analysis pointed to the possibility of estimating the uncertainties in fission reactor performance parameters that are induced by uncertainties in nuclear data.[1] This possibility, however, also depended on detailed evaluation of nuclear data variance and covariance components. The same developments would make formally possible the implementation of a proper scheme for the adjustment of cross sections to take into account integral experiment results. The quality-conscious reactor physics discipline was attracted by the promised capability to assess uncertainty independent of integral experiments, and as well by the prospect of being able at last to include integral experiment results in a logical way when it was desired to do so.

Attention turned to how one might represent evaluated nuclear data covariance information. F. G. Perey led the way with ideas on how evaluated files of covariance and variance quantities could be structured to permit unambiguous processing to multigroup cross-section covariance matrices.[2] These matrices would be combined with differential sensitivity coefficients in practical calculations. Over the intervening years such covariance formats were accepted, evaluated covariance files were included in ENDF/B-V for a number of important reactions, these files were processed at various laboratories,[3] and numerous complete calculations have been performed using codes that combine these multigroup matrices with sensitivity coefficients for system macroscopic parameters.[4]

In developing the covariance formats and files for the ENDF/B-V library, a number of approximations were made that were expected to be refined before the covariance propagation technology would be considered complete. It is appropriate now to review some of these areas and consider which improvements seem important and achievable. During the last decade many nuclear scientists and engineers have come to better understand the treatment of uncertainty, so advances are easier now and can be readily assimilated. Much of this understanding is represented in the present workshop. On the other side, in several countries the development of optimized nuclear reactor systems is given less urgency than before, and gains must be made with reduced staff. In this period of changing applied goals we can set a strong foundation for the future uncertainty analyses that will be required. It is a pleasure to join in this workshop toward that goal.

2. FOR WHAT PURPOSES ARE COVARIANCE FILES NEEDED?

The need for evaluated nuclear data variance-covariance data rests on the simple but powerful proposition that there would be little sense in evaluating a million cross-section quantities if no corresponding information were recorded on how well the numbers are known. Since the user of cross sections may have no direct contact with evaluators, without covariance files he would have no way to estimate the accuracy of his calculated results unless pertinent integral experiment results are available. Such tests are important, but their implications can be ambiguous. Figure 1 lists the main uses that have been suggested for nuclear data "covariance" files.

The first use is the one for which the ENDF/B-V uncertainty file formats were designed, since the file itself was developed to support neutronics calculations. Progress toward implementing this use is assessed in a later section.

The second use would be largely inappropriate for the ENDF/B-V covariance files, though the applicability would increase as the energy resolution of the user's interest broadens to be comparable to the energy grid used by the covariance evaluator. This is true even though the definitions of the quantities in the ENDF covariance files are phrased in terms of covariance data at energy points.

Even if the quantities given in a covariance file were intended to give values appropriate for the neutron energy band of interest, a cautious type 2 user should learn the basis for the evaluation. While the validity of this use class should increase as evaluated uncertainty files are improved, the author believes that use 2 should be encouraged only as a preliminary indicator.

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Figure 1. Uses for Nuclear Data Covariance Files

1. To permit calculation of the standard error in any quantity computed from the corresponding evaluated cross sections. (By extension, this capability also formally allows the adjustment of the cross section set using benchmark integral experiment results.)

2. To allow a user to obtain variance-covariance data for a cross section at any desired energy points.

3. To enable the evaluated cross section set to be updated by inclusion of new differential data without explicitly addressing the entire experimental data base. Similarly, to allow the likely value of a proposed experiment to be judged based on how much reduction would be expected in the evaluated uncertainties after inclusion of the new result.

The third use has been tried using ENDF files; experience has shown that serious problems can arise.

Use 3 to obtain new evaluated cross sections for general use can be tried by using the adjustment form of the least squares equations if the new data is not correlated to data on which the existing evaluation was based. In his simultaneous evaluation of a series of dosimetry cross sections using this "Bayes" approach, Fu[5] found that the existing ENDF/B-V covariance files for the prior evaluated data led in some cases to seriously unreasonable updated evaluations. The files implied 100% correlation among the existing evaluated cross sections over an extended energy region, and the efficient computer program took this approximation as literal truth. To obtain plausible results Fu had to modify the input evaluated covariance files in a reasonable but *ad hoc* manner. Indeed, evaluated cross sections are rarely 100% correlated over a broad energy region. The original evaluated files were designed for use 1, and may have been adequate for that purpose.

To me this difficulty from the discrete nature of the energy structure of the file seems fundamental. It cannot be fully overcome within the established formats for smooth cross sections. Rather than modify the ENDF formats or covariance evaluation strategy to cover the use 3, I believe evaluators who expect to update an evaluation in this way should maintain private files with covariance quantities in a form more suitable for this purpose. Nevertheless, there will be cases for which covariance files in ENDF format can be used directly in updating an evaluation.

As for trial use to estimate uncertainty quantities for a hypothetical future evaluation that would include results from a proposed experiment, the user must critically consider the basis of the input evaluated covariance values. Moreover, the value of a new experiment often lies in the use of diverse or refined techniques. The value would then be qualitative as well as quantitative, since the new experiment could confirm or call into question the whole basis of the prior evaluation. Relying entirely on the expected numerical reduction in evaluated uncertainty to judge the value of a proposed experiment would therefore be sensible only if the experiment were to be based on unchanged techniques but, say, an increased number of detected events.

3. PROGRESS TOWARD FULL IMPLEMENTATION OF USE 1

Progress toward enabling calculation of the uncertainty in quantities computed from cross section sets can be measured in two ways: (1) in terms of the capability to represent in a useful evaluated file all the covariance data of consequence to an application, and (2) in terms of the availability of evaluated covariance files having the necessary quality. Th existence of defined formats for all reaction types would not be enough to satisfy the first measure; the definitions must also permit evaluated files to be processed into forms that can be combined with sensitivity coefficients to obtain the uncertainties in macroscopic parameters. The second measure requires in practice that the evaluated covariance files for important reactions must be founded in the experiments from which the evaluated cross sections were obtained; the covariance evaluation must be part of the cross-section evaluation process.

Utility and sufficiency of covariance file formats. The ENDF/B-V covariance file formats permit reasonably general and efficient representation of covariance information for smooth cross sections. Cross sections represented by resonance parameters can be handled if only a few resonances have important self shielding.

Practical processing capability exists to obtain multigroup covariance matrices, and the results have been successfully combined with sensitivity coefficients.[4] Since ENDF/B-V covariance formats were not defined for secondary neutron angle energy distributions, a partial exception is uncertainty propagation via the uncertainties in the elements of the energy transfer matrix. However, Furuta *et al.*,[6] did perform such an uncertainty propagation using their own covariance data for secondary angle and energy distributions.

Planned ENDF-VI formats include restricted handling of secondary angle and energy distributions and a more general format for resonance parameter covariances for cases where many resonances are subject to important self shielding.[7] While these new formats resemble the existing ones, to date there has been no demonstration that covariance data represented using them can conveniently be processed to multigroup form. Some unnecessary restrictions in the older formats are also to be removed.

Capability to produce well-founded covariance data. It is argued that even qualitatively derived covariance data are worth including in formal covariance files for reactions of significance to important applications if no better information is available. The alternative is to allow the inference that the cross section data is effectively perfect. Most of the

ENDF/V uncertainty files were derived qualitatively, and for this reason evaluators generally felt that strong quantitative conclusions should not be based on numerical results propagated from these files.

Though existing covariance files have been judged more qualitative than quantitative, many neutron cross section experiments are being performed and reported with sufficient care that the covariance properties of the results are known. As more such experiments are completed and as evaluators learn to judge how to represent experimental results not so well characterized by their authors, one may expect that least-squares or related techniques can more often be used to help obtain defensible covariance data for evaluated cross section quantities.[8] Examples of this type are in the literature and are to be discussed at this meeting.

As mentioned above, some new formats are proposed for ENDF-VI. While these proposals were designed with application in mind, there has not yet been opportunity to test any of them in an evaluation of real data. The same statement could have been made about the existing formats when they were designed. However, one must note that the new capabilities were delayed because they seemed more difficult and also less certain to provide important contributions to the uncertainties in quantities calculated from cross-section sets.

Qualitative covariance evaluations will doubtless continue, at least for nuclides and reaction types less important to applications. It would be helpful if guidelines could be developed to help evaluators perform qualitative evaluations on a consistent basis.

Within the domain of evaluation techniques that yield quantitative covariance data as part of the evaluation process, there remain problems in how best to represent covariance information in ENDF formats.

4. REPRESENTING COVARIANCE DATA FROM A LEAST-SQUARES EVALUATION

Consider as an example how one might represent in an ENDF file the covariance data for the results the CSEWG Standards Subcommittee is trying to obtain.[9] For the ^{6}Li and $^{10}B(n,\alpha)$ reactions the results will be represented by R-matrix parameters via the EDA program of Hale,[10] while at present the remaining reactions ($^{197}Au(n,\gamma)$, $^{238}U(n,\gamma)$, $^{235}U(n,f)$, $^{239}Pu(n,f)$, and $^{238}U(n,f)$) have their smooth cross sections represented on an energy grid with about 100 points to 20 MeV through the GMA program of W. Poenitz.[11] As indicated by Poenitz at this meeting, it is expected that a greater share of the data will eventually be represented by model fits.[12] Assume for discussion that this global least squares problem has been properly solved with fair representation of all experimental uncertainties, that serious discrepancies in the data base have not compromised the whole concept, and that use of first order derivatives of the light element cross covariance matrix of cross sections interpolated from the R-matrix fit.[13]

Very small uncertainties are estimated for the light-element (n,α) reaction cross sections because of the broad range of quality data utilized and because the R-matrix parametrization imposes an *a priori* structure on the results. A real challenge would be to estimate how much the uncertainties from such a model fit could change if additional resonances were postulated, resonances that are not needed to fit the data and for which no specific evidence exists. One normally assumes the formulation is exact and accepts uncertainties consistent with data scatter around the fitted result, even if the resulting uncertainties seem very small. The cross sections at neighboring energy points are highly correlated, but along the diagonal the granularity of the formats inhibits correct representation of covariances that would best be computed from the covariance matrix of the R-matrix parameters. Should not formats for evaluated covariance data be defined to contain this data together with the energy dependent derivative matrices of the various partial cross sections to the model parameters? This step could provide the general capability now lacking to codify the covariance properties of nuclear model codes in a natural way.

For the pointwise cross sections, such as $^{235}U(n,f)$, somewhat different problems arise. It is necessary to greatly condense the covariance "information" available in the output. There cannot be 100,000 meaningful uncertainty quantities resulting from a fit to 10,000 data values, but to date only judgement is used to condense covariance data. Judgement is more likely to be sound if only one main class of uses is contemplated for the evaluated covariance files.

5. PRIORITIES FOR FUTURE WORK

A meeting such as this can help develop consensus on goals for future work. I have listed in Fig. 2 the most important tasks mentioned above.

6. CONCLUDING REMARKS

Since the constraints on covariance data files are complex and many compromises are necessary in the evaluation of covariance data, it will be most fruitful if that evaluation is pointed toward a single class of uses, estimation of the uncertainties in quantities that depend on a broad spectrum of neutron energies.

The whole effort in sensitivity and uncertainty analysis has been a commendable and important development in the nuclear engineering and nuclear physics disciplines. It exemplifies the drive for closure and highest-quality results that we believe characterizes most of our work. While in many countries there is currently less work than formerly in the cross section area, one may be confident that the planning and implementation of reasonably optimum nuclear programs will require the results that

we are trying to achieve. I trust that the most important goals we recognize can be met by us or by our colleagues not present, and I believe the effort will prove fruitful to the projects of concern to our sponsors. We are correct in our simple thought that a proper measure of accuracy must accompany every important estimated quantity.

Figure 2. Priority Tasks For Covariance Analysis

- Test the new resonance parameter covariance data format proposed for ENDF-VI, both for ease of use and the capability to process the resulting files.
- Similarly test the proposed ENDF-VI formats for angle and energy distributions.
- Develop logical techniques for thinning covariance data from large least-squares data combination efforts.
- Develop guidelines for qualitative covariance evaluation that will help evaluators "capture" their knowledge on a consistent basis when quantitative covariance evaluation is not possible.
- Develop and implement a general covariance format to contain a parameter covariance matrix and the energy-dependent derivatives of cross sections relative to those parameters.
- Obtain covariance matrices for the parameters of nuclear model evaluation codes.
- Develop a covariance file format for joint angle and energy distributions not obtained from model codes.

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Covariances of Evaluated Nuclear Data Based Upon Uncertainty Information of Experimental Data and Nuclear Models

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ABSTRACT

A straightforward derivation is presented for the covariance matrix of evaluated cross sections based on the covariance matrix of the experimental data and propagation through nuclear model parameters.

I. INTRODUCTION

In an evaluation of nuclear data, the evaluator would ideally attempt to utilize and preserve all valid information contained in the experimental data base, as well as utilize the knowledge available from and through nuclear models and their associated auxiliary parameter data base. In the case of neutron cross sections, this usually calls for a simultaneous evaluation of several cross sections if correlations between such cross sections exist. This is the case for the "standards", and several cross sections of importance for reactor neutronics which will be considered here as an example. The experimental data for $^{6}Li(n,\alpha)$, $^{10}B(n,\alpha)$, $^{197}Au(n,\gamma)$, $^{238}U(n,\gamma)$, $^{235}U(n,f)$, $^{238}U(n,f)$ and $^{239}Pu(n,f)$ are correlated not only because some measurements of different cross sections were carried out with the same detectors or samples, but also because cross section ratios and sums (e.g. total cross sections for the light nuclei) were measured as well. For this reason it has been decided to evaluate these cross sections simultaneously for ENDF/B-VI.[1] Such simultaneous evaluation is especially desirable in this case as covariance information for these cross sections, as well as cross material covariances are of specific importance for applications and can be derived in a natural way.

Different theoretical models would be invoked for the evaluation of these cross sections, i.e. the R-matrix theory for the light nuclei (see for example Ref. 2) and the statistical/optical model for the reaction cross sections of the heavy nuclei (see for example Ref. 3). The use of these theoretical models is desirable for various reasons. One is the use of additional data, e.g. angular distributions, polarization and inverse reaction data through R-matrix theory for the light nuclei, and to impose physical gross structure, e.g. inelastic competition cusps, on the heavy nuclei cross sections. Another is that theoretical models provide smooth cross sections where experimental data may result in unreal structure due to statistical uncertainties and data inconsistencies.

The simultaneous fitting of the correlated experimental data with a combined R-matrix and statistical/optical model computer code would provide a multi-model parameter set and its covariance which would be used for the subsequent derivation of the evaluated cross sections and their covariance by error propagation. Though this would be the most satisfying and direct approach, it can be easily guessed that it would severely tax the present computer capabilities in both running time and storage and addressing space. A stepwise approach is discussed here which has been or may be used in parts of an evaluation proposed for ENDF/B-VI.

II. GENERALIZED LEAST-SQUARES EVALUATION OF EXPERIMENTAL DATA

A first and substantial reduction of the amount of data which have to be handled by a nuclear model code can be achieved by a generalized least-squares fit of the experimental data (about 450 data sets with more than 10,000 data values). A parameter space of ~ 1000 appears desirable in order to represent thermal parameters, energy integrals below 10 KeV, and pointwise cross sections which reflect the gross structure of the cross sections above 10-20 KeV on an appropriate energy grid. From the generalized least-squares fit one obtains the refinement vector

$$\delta = (A^{T}C_{m}^{-1}A)^{-1}(A^{T}C_{m}^{-1}M) \qquad (1)$$

with covariance

$$C_{\delta} = (A^{T}C_{m}^{-1}A)^{-1} \qquad (2)$$

(see for example Ref. 4) which is to be applied to an a priori parameter vector (arbitrary, except for the applicability of the linearity approximation). The A is the design matrix with elements equal to the first coefficients of the Taylor series expansion of the measured quantities (A^{T} is its transpose), and M is the measurement vector. With appropriate transformation,[5] C_{M} is the correlation matrix of the measured data. That a parameter space of this size can be handled with today's computer capabilities has been demonstrated with the generalized least-suqares program GMA in 1980[5] and this step is now part of an evaluation proposed for ENDF/B-VI.[1]

III. THE ADDITION OF NEW OR AUXILIARY DATA

Additional data for the evaluated parameters may be available, e.g. new experimental data, integral data, or data which have been derived

from quantities which are not part of the parameter space (for example angular distributions) with the help of a nuclear model. Integral data have been excluded from the evaluation proposed for ENDF/B-VI, with the well-justified exception of the ^{252}Cf spectrum averaged fission cross sections of ^{235}U and ^{239}Pu, in order to keep the problem of differential data uncertainties and reactor modelling uncertainties a separate issue. New data could easily be accommodated by rerunning GMA. However, the cross section data obtained from a nuclear model cannot, in general, be added as an input set to the GMA data base because its covariance matrix is singular. Instead, these data can be utilized with the well-known formalism used in "adjustment" procedures (see for example Ref. 6) if they are uncorrelated with the data used in the first step of the evaluation. Using the first-step result of the parameter vector as a priori one obtains a simplified second-step adjustment vector[7]

$$\delta_2 = C_\delta A_2^T (A_2 C_\delta A_2^T + C_2)^{-1} M_2 \qquad (3)$$

with covariance

$$C_{\delta 2} = C_\delta - C_\delta A_2^T (A_2 C_\delta A_2^T + C_2)^{-1} A_2 C_\delta . \qquad (4)$$

M_2 is the "measurement" vector of the cross sections derived from the nuclear model, C_2 is the corresponding covariance matrix, and A_2 is the coefficient matrix for the additional data. C_δ is the covariance matrix of the "first-step" evaluated parameters and follows from Eq. (2). C_δ is non-singular but C_2 is in general singular; however, in the one example of interest here, it has been shown that $A_2 C_\delta A_2^T + C_2$ can be inverted. This "second-step" approach of adding more complex data information (as angular distributions, polarization etc.) is currently being considered as an option for the evaluation proposed for ENDF/B-VI. Another option of combining theoretical nuclear model results with evaluated pointwise data has been discussed elsewhere.[1] It is interesting that the same results were obtained with either approach. In either case, it proved necessary in the example discussed here to use some cross section data in the nuclear model fit which could have been used in the first step of the evaluation.[1]

IV. THE UTILIZATION OF NUCLEAR MODELS

Though some data obtained from a nuclear model can be utilized in a "second-step" procedure as shown in Section III, the desire to use a multi-model fit of the pre-evaluated cross sections remains. The main advantage of a separate "second-step" addition of data derived from a nuclear model is that a final step requires less complicated nuclear model modules, i.e. modules which only calculate the cross sections which are the objects of the evaluation, and thus require less computer time and space. The total parameter space is somewhat reduced as only the cross sections described by the nuclear models can be included in the fit, i.e. thermal parameters and energy interval integrals are excluded.

For this third step of the evaluation in which the pre-evaluated cross sections are fit with a multi-nuclear model code, the (cross section) parameters evaluated in the prior steps become measureable quantities, m_i, which can be derived from nuclear models, and the nuclear model parameters become the new parameters. Assuming an a priori nuclear model parameter vector $\hat{p}$, the adjusted quantity (evaluated cross section) is again based upon a Taylor series expansion

$$f_i(\vec{p}) = f_i(\hat{p}) + \sum_j \frac{\partial f_i(\vec{p})}{\partial p_j} (p_j - \hat{p}_j) = m_i , \qquad (5)$$

$$= f_i(\hat{p}) \, (1 + \sum_j S_{ij} \delta_j), \qquad \delta_j = \frac{p_j - \hat{p}_j}{\hat{p}_j}$$

where $f_i(\hat{p})$ is the derived quantity obtained from the nuclear model based upon the a priori parameter vector $\hat{p}$. The

$$S_{ij} = \frac{\hat{p}_j}{f_{i(\hat{p})}} \frac{\partial f_i}{\partial p_j}$$

are the coefficients of the "sensitivity" matrix which replaces the coefficient matrix A in Eqs. (1) and (2). The derivatives, $\partial fi/\partial pj$ are obtained from the nuclear model either in analytical form (R-matrix) or from finite differences. The adjustment vector δ for the nuclear model parameters and its covariance can be obtained with analogous use of Eqs. (1) and (2). However, $\hat{p}$ needs to be close to the final solution $\vec{p}$ in order for the linearity assumption (Eq. (5)) to hold. This can be achieved by prior non-linear fitting of the cross sections of individual nuclei by simple χ^2 minimization. At this stage, other cross sections can be included in order to further constrain some parameters. Alternatively, if a nuclear model parameter set and its covariance are available based upon data which are uncorrelated with the m_i's, δ and its covariance can be obtained from Eqs. (3) and (4). In this case, the uncertainties of the a priori nuclear model parameters restrain the adjustment called for by the additional data. The covariance matrix of the evaluated quantities, $fi(\vec{p})$, follows from error propagation from the covariance matrix of the parameters[7-9]

$$C_f = D C_p D^T ,$$

where D is the matrix of the derivatives, $\partial fi/\partial pj$, and C_p is from Eq. (2) or (4). Formally, the covariance of the evaluated cross sections, C_f, is derived from the covariance of the measured data, C_M, by propagation through the covariance of the nuclear model parameters, C_p. Additional uncertainties which are due to the approximations of the nuclear models are ignored at this point.

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COVARIANCES FOR MEASURED ACTIVATION AND FISSION RATIOS DATA

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ABSTRACT

Methods which are routinely used in the determination of covariance matrices for both integral and differential activation and fission-ratios data acquired at the Argonne National Laboratory Fast-Neutron Generator Facility (FNG) are discussed. Special consideration is given to problems associated with the estimation of correlations between various identified sources of experimental error. Approximation methods which are commonly used to reduce the labor involved in this analysis to manageable levels are described. Results from some experiments which have been recently carried out in this laboratory are presented to illustrate these procedures.

INTRODUCTION

The number of applications for nuclear data covariance matrices is growing. Many contemporary neutron spectrum unfolding codes require this information [1]. Modern nuclear data evaluation procedures demand covariance information for the conduct of unbiased evaluations [2]. Covariances are routinely included in analyses of integral reactor experiments (i.e., sensitivity analyses) [3]. The list could go on. Because of these applications, contemporary evaluated neutron data files generally include covariance information for a variety of interaction processes (e.g., File 33 for the ENDF/B-V System [4]).

Considerable attention is being given within the nuclear data community to the mechanics associated with routine utilization of covariance information in applications (e.g., the present conference). Ultimately, the worth of all this activity rests upon the quality of the covariance information available. Computations involving covariances are often quite sensitive to the detailed structure of these matrices. However, much of the covariance information available in the evaluated files is of marginal quality. The reasons for this are many, but the most important one is probably that knowledge of covariances for the underlying experimental data base is fragmentary. Most of the older data sets do not provide sufficient information to permit generation of reliable covariance matrices. Unfortunately, most

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contemporary experiments don't either. Until more experimentalists make the effort to compile and report the necessary detailed information about their experiments, this problem is very likely to persist and may very well undermine the successful implimentation of covariance methodology in nuclear data applications. Why is this such a problem? First, many experimentalists are not convinced of the need to provide this information for their experiments. Furthermore, most do not know how to do the job properly, or do not wish to make the effort. It is our experience that generation of reliable covariance information not only involves probing deeper into the details of an experiment than most experimentalists care to do, but it also requires a rather sophisticated understanding of statistical methods. In short, it is tedious, time consuming and nontrivial work. An important challenge for the covariance community is to encourage and to educate their associates -- particularly those who do experiments -- concerning the importance of this issue.

In this laboratory we have been exploring this matter since about 1980, in the context of our fission ratio and activation cross section measurement program [5,6]. Our detailed procedures have undergone considerable evolution during this period since we have refined our experimental methods and have learned more about the underlying statistical concepts associated with data error analysis. The objective of this paper is to summarize our experiences, and to illustrate our approach with some examples from recent work in this laboratory.

GENERAL FORMALISM

In principle, an experiment can be completely described by a set of random variables x_k (k=1,K). They represent fundamental physical quantities which can be measured in the laboratory, e.g., count rates, lengths, masses, voltages, pressures, etc. Collectively, these variables form a random vector $\bar{x}$. This representation is, of course, not unique. A single measurement under defined conditions corresponds to sampling the space of these vectors and selecting, in an unbiased fashion, a particular vector $\bar{x}$. In a well designed experiment, the possible values will tend to cluster around the population mean $\langle\bar{x}\rangle$ with relatively small dispersion. The experiment is then said to be "precise". Since most experiments are performed only once, or are repeated a few times at most, it is important that they be designed to be relatively "precise" so that any value $\bar{x}$ obtained will approximate the mean value $\langle\bar{x}\rangle$ rather closely. The probability distribution which governs $\bar{x}$ is seldom known. However, of greater interest is the associated covariance matrix $\bar{V}_x$. The random variables x_k can be viewed as parameterizing the "raw data" of an experiment. From them we compute a set P_i (i=1,n) of derived results which are the quantities actually sought from the experiment (e.g., cross sections or cross section ratios). Collectively, these form the vector $\bar{P}$. The components of $\bar{P}$ are uncertain (exhibit dispersion) because the corresponding measured raw data (in the present context, the $\bar{x}$) are uncertain. The covariance matrix $\bar{V}_P$ for $\bar{P}$ is of special interest. It can be derived from $\bar{V}_x$ using the law of error propagation, i.e., $\bar{V}_P = \bar{T}^+ \bar{V}_x \bar{T}$, where $\bar{T}$ is the matrix of partial derivatives, $\partial P_i/\partial x_k$, and $\bar{T}^+$ is its transpose.

In reality, the individual components of $\bar{x}$ are rarely defined and traced in explicit detail, although attempts are being made to do this at some laboratories, e.g., in certain experiments at ORELA [7] Usually, various independent attributes which are considered by the experimenter to be adequately descriptive of an experiment (e.g., detector counts, normalizations, standards, geometry factors, etc.) are identified. These are followed in detail throughout the experiment. This amounts to re-arranging the components and then partitioning $\bar{x}$ so that $\bar{x} = (\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_l, \ldots \bar{x}_L)$. The various subvectors $\bar{x}_l$ are then treated as mutually independent, but the components x_k within a particular subvector need not be independent. Under these conditions, the covariance matrix $\bar{V}_P$ assumes the form $\bar{V}_P = \sum_{l=1}^{L} \bar{T}_l^+ \bar{V}_{xl} \bar{T}_l$. The portions of $\bar{T}$ and $\bar{V}_x$ corresponding to attribute l are labelled accordingly. The components $\bar{V}_P$ are usually expressed in the equivalent form, $(\bar{V}_P)_{ij} = \sum_{l=1}^{L} S_{ijl} e_{il} e_{jl}$ [5,8]. Here, e_{il} is the partial error of P_i due to attribute l, and S_{ijl} is a "micro correlation" coefficient which measures the correlation between the partial errors e_{il} and e_{jl}. All these correlations satisfy the relationship $-1 \le S_{ijl} \le 1$, with $S_{iil} = 1$. Negative correlation coefficients indicate anticorrelation, i.e., the corresponding partial errors affect the values involved in an opposing manner. For each l, these coefficients form a micro correlation matrix $\bar{S}_l$ with dimension n x n.

In practice, the preceding equation for $(\bar{V}_P)_{ij}$ is an appropriate starting point for determination of the covariance matrix for a set of experimental data. The experimenter defines the attributes of the experiment to be considered and prepares a table of partial error components, as discussed in Ref. 5. This is generally

the easiest part of the job. The micro correlation coefficients are typically more difficult to provide. It is here where the analytical skills and intuition of the experimenter are tested. If the attributes to be considered are wisely chosen, then many of the micro correlation matrices $\bar{S}_l$ will be relatively simple, e.g., consisting mainly of the values 0 and 1. In more complex situations, it is sometimes possible to determine the matrix $\bar{S}_l$ from rigorous analysis. For example, if a functional curve is fitted to calibration data using covariance methodology, as demonstrated in examples from Ref. 6, the needed micro correlation parameters will be readily available as a byproduct of the fitting process. Otherwise, the micro correlation coefficients will have to be estimated subjectively. It was recently demonstrated that the consequences of subjectivity need not be as serious as might be expected *a priori* [8]. So long as the number of independent attributes L considered in the experiment is sizeable (typically in excess of 10), the uncertainty in determining the covariance matrix $\bar{V}_P$, and thus the matrix $\bar{C}_P$ $\{ (\bar{C}_P)_{ij} = (\bar{V}_P)_{ij}/[(\bar{V}_P)_{ii}(\bar{V}_P)_{jj}]^{1/2}$ for i,j=1,n $\}$ of corresponding "macro correlations" between the various P_i, tends to be substantially less than that of estimating the various micro correlation coefficients involved in the analysis. This result is really a consequence of the Central Limit Theorem from statistics [8]. On the basis of this, we have often found it convenient to confine our choice of possible values for micro correlation coefficients to 0, ±0.25, ±0.5, ±0.75 or ±1 in cases where they have to be estimated from very subjective considerations.

PROCEDURE FOR THE COMPOSITION OF COVARIANCE MATRICES

If the numbers n of values P_i and L of error attributes are substantial, then the task of composing $\bar{V}_P$ can be a formidable one. We have learned that it is usually impractical to do this by hand and have therefore developed a computer procedure which is quite convenient. A table of partial errors errors e_{il} (i=1,n and l=1,L) is entered into the computer initially. Attention is then turned to the micro correlation matrices $\bar{S}_l$. These are addressed in ascending order of l. Quite often, most of the elements of $\bar{S}_l$ assume a single value (commonly 0 or 1). This majority value is therefore entered first into all positions of the matrix array. Then, different values S_{ijl} are introduced as needed to "over-ride" the majority selection. They can be entered as single values, or as uniform rectangular or triangular arrays within $\bar{S}_l$, as required. This procedure is greatly simplified by judiciously choosing the attributes to be considered and by organizing the indices for the set of experimental values $\bar{P}$ so that those with the greatest number of common attributes are situated adjacent to each other. Usually there is a trade off between the labor involved because the number of attributes L selected is large, and the effort required due to the complexity of individual micro correlation matrices $\bar{S}_l$ (i.e., it is generally the case that the larger L is, the simpler the individual micro correlation matrices become). For the uninitiated, this procedure can be frustrating, but we have found that skill comes with experience, and the task has proved to be quite manageable in our experimental program. Finally, we have learned that it always pays to conduct the exercise of error analysis as soon after completion of the measurements as possible in order to avoid forgetting potentially important experimental details.

ERROR SOURCES AND THEIR CORRELATIONS

The list of attributes to be employed in the analysis of errors by necessity varies considerably from one experiment to another. However, the major sources of uncertainty which arise in the activation and fission ratios experiments considered in this paper can be categorized under a few headings. There are many similarities between these experiments. This should be apparent from their rather similar geometric configurations, as indicated schematically in Fig. 1. All of the experiments discussed here incorporate similarly designed low-mass fission chambers. For the activation measurements, thin disk samples are attached to the exterior of the chamber. What is measured is the cross section ratio for induced activation in the sample relative to fission for the standard deposit in the chamber. In this geometry (Fig. 1.A), the sensitivity of the measured ratios to geometric effects is rather modest. For the fission ratio experiments, the geometry is considerably more symmetric (Fig. 1.B), and consequently the sensitivity to geometry is further reduced. The error sources (and their correlations) associated with these experiments are discussed below. It is misleading to designate certain types of error as "random" and others as "systematic". It depends entirely upon the context in which an error is encountered. A particular error is considered to be random if it affects only one data point, P_i. It is systematic, however, if it affects two or more data points in a correlated manner. This distinction is made evident in the discussion below.

The sources of error described here are summarized in Table 1. Event statistics (E_1) includes all errors which are traced to statistical errors of measured counts (e.g., fission events from the chamber, activity decay counts from a samples, alpha counts of a fission foil, etc.). These are generally uncorrelated, but under certain circumstances they can be correlated. For example, if two activation cross sections are deduced from a single irradiation, then the statistical error in the measured fission events during that irradiation affects both of the activation measurements and is thus fully correlated. Background (E_2) corrections generally induce

uncorrelated errors, unless the same background factor is applied to several data points. An example of the latter would be the application of a correction for background 511-keV annihilition radiation (measured once during the course of an experiment) in the process of determining annihilation radiation activity for a set of samples activated by neutron irradiation. This error is fully correlated. Event determination procedures (E_3) labels a broad category which includes consideration of methods used in the determination of corrected fission and activation events from raw data. Examples included procedures for measuring sample activity, extrapolation and thickness corrections to measured fission detector events, etc. For convenience these experimental features are grouped together here, but in practice distinctions would be made and the various factors would be treated separately. These types of errors are generally correlated to some extent, though certain items may well be random. As an example, consider fissions extrapolation. This is a correction for spectrum fission events which are unavoidably lost in the low pulse height alpha particle and noise distribution. If this correction is determined separately for each measured spectrum, then random error will be present. However, a fully correlated error to account for method-induced bias must also be included if the same method is used to extrapolate all the fission spectra obtained from the experiment. Event determination calibration standards (E_4) are those which are used to calibrate detectors. Included are activity standards, energy scale standards, etc. The errors in this category are usually fully correlated. Sample assay (E_5) covers mass determinations for activation samples and fission foils. The associated errors are fully correlated. However, when we say "correlated", we do not exclude anti correlation. As an example, suppose that a data set includes two ratios. (A/B) and (B/C). An error involving the assay of B is, in fact, anti correlated for these two points since the same error effects the ratios in an opposite manner. Activity half life (E_6) refers to all types of error which come about due to imprecise knowledge of relevant half lives. Examples include sample activities, alpha activities which are utilized in fission foil mass determinations, etc. These are generally fully correlated errors. Activity decay factors (E_7) are those which take into account details of the decay process (other than half life), e.g., decay branching. These are generally fully correlated so long as the process involved affects more than one data point. Uncertainties due to imperfect knowlege of isotopic abundances (E_8) can influence experiments in various ways. They can affect mass determinations (e.g., sample masses, fission masses deduced through the measurement of the alpha activity for a specific isotope, etc.). They can also affect the correction of fission yields for indistinguishable contributions from minor isotopes present in the the fission foils. These errors are fully correlated so long as the same material is involved in more than one data point. The term geometry (E_9) covers a number of complex experimental issues. Errors due to geometric uncertainty can be both random and systematic in nature (and thus partially correlated in general). Random error is usually associated with reproducibility in the positioning of apparatus while systematic error arises from errors in measurement of fixed geometric factors (e.g., detector dimensions, deposit dimensions, etc.). The random errors tend to dominate in this category. The magnitudes of these errors, and their correlations, can be determined quite readily by computer modeling for the simple geometries of the present experiment. We do this on occasion, but not for every experiment. Errors due to uncertain specification of neutron source parameters (E_{10}) tend to be systematic, but correlations smaller than unity are often assumed. Details of the neutron source impact significantly upon the determination of cross sections or ratios whenever the source exhibits energy dependence (i.e., multiple discrete groups or a continuum) or is strongly anisotropic. For ratio measurements, absolute neutron fluence (E_{11}) is irrelevant. However, if cross sections are sought (as is the case for activation measurements), then the neutron fluence must be determined from the yield of a standard reaction. The main source of error is then due to the standard cross section itself. This error is systematic if all the data points in the set are based upon the same standard reaction. If energy dependence is involved, then the correlation depends upon the correlation introduced by the differential cross section covariance matrix for the standard reaction. This information can usually be obtained from evaluated data files (e.g., Ref. 4). Uncertainties due to neutron absorption (E_{12}) tend to be small for these experiments. These corrections are usually calculated, and any uncertainties can be traced to total cross section and geometry factors which are usually well known. Correlations arise if the data points share common features (same sample, same fission foil backing, same fission chamber, etc.). Neutron scattering (E_{13}) corrections for these experiments are sometimes measured, but most often are calculated. For measured corrections, the errors range from random to fully correlated, depending on the details of experimental procedure. Errors in calculated scattering corrections are almost always systematic, but are seldom fully correlated. Since these corrections are computed by the Monte Carlo method in our laboratory, this introduces a degree of randomness into the correction process. However, the various data points in a set generally involve a number of common features (e.g., common cross section sets, similar geometries, etc.) which introduce correlations. These correlations are always estimated and are not well known. Finally, whenever a particular quantity is measured more than once, and discrepancies are observed which cannot be explained otherwise, an additional error should be included to account for non reproducibility (E_{14}). This error is always treated as random in our error analyses.

EXAMPLES FROM RECENT EXPERIMENTS IN THIS LABORATORY

Material from four recent experiments conducted in this laboratory are presented in this section for illustrative purposes. Two of these experiments involve activation and two fission ratios. Use was made of two very distinct neutron sources in this work. Two of the experiments involved a 14.7-MeV neutron field from the D-T reaction. The other two were performed using the Be(d,n) thick target

reaction at 7 MeV deuteron energy as a "clean integral benchmark field". Attention is restricted in this paper to consideration of the error analyses for these experiments. Since most of the data sets are fairly large (20 or more points), we have decided to show only selected portions of the total error matrices for the examples presented below.

Activation: 14-MeV Data

Activation cross sections have been measured at 14.7 MeV for the following reactions: $^{7}Li(n,n't)^{4}He$, $^{27}Al(n,p)^{27}Mg$, $^{27}Al(n,\alpha)^{24}Na$, $Si(n,X)^{28}Al$, $Ti(n,X)^{46}Sc$, $Ti(n,X)^{47}Sc$, $Ti(n,X)^{48}Sc$, $^{51}V(n,p)^{51}Ti$, $^{51}V(n,\alpha)^{48}Sc$, $Cr(n,X)^{52}V$, $^{55}Mn(n,2n)^{54}Mn$, $^{54}Fe(n,\alpha)^{51}Cr$, $Fe(n,X)^{56}Mn$, $^{59}Co(n,p)^{59}Fe$, $^{59}Co(n,2n)^{58}Co$, $^{59}Co(n,\alpha)^{56}Mn$, $^{58}Ni(n,2n)^{57}Ni$, $^{65}Cu(n,p)^{65}Ni$, $^{65}Cu(n,2n)^{64}Cu$, $Zn(n,X)^{64}Cu$ and $^{64}Zn(n,2n)^{63}Zn$ [9,10]. In this experiment, the irradiations were performed using a fission foil which was enriched in ^{238}U, however, a precise $^{238}U/^{235}U$ fission ratio measurement was performed under the same experimental conditions so that the final results could be expressed in terms of the better known ^{235}U fission cross section standard [4]. The apparatus used is indicated in Fig. 1. The sample/fission detector arrangement is as indicated in Fig. 1.A, while the 14.7 MeV neutron source assembly is as shown in Fig. 1.B. The dominant error sources for this experiment were activity measurement statistics (uncorrelated), the ^{235}U fission cross section (fully correlated), calibration of the fission monitor (fully correlated) and calibration of activity measurement processes (uncorrelated for the tritium activity but partially to fully correlated for all the other activities, which were measured by gamma ray detection). The magnitudes of the errors considered are summarized in Table 1. Total errors and the corresponding correlation matrix for the final cross sections of the first eight reactions from the list above are shown in Table 2.

Activation: Be(d,n) Integral Data

Integral cross section ratios were measured for the activation reactions $^{7}Li(n,n't)^{4}He$, $^{27}Al(n,p)^{27}Mg$, $^{27}Al(n,\alpha)^{24}Na$, $^{58}Ni(n,p)^{58}Co$ and $^{60}Ni(n,p)^{60}Co$ relative to ^{238}U fission in the continuum benchmark field produced by the Be(d,n) thick target reaction at 7 MeV deuteron energy [11]. The apparatus used is shown in Fig. 1.A. The dominant error sources for this experiment were activity measurement statistics (uncorrelated), determination of corrected fission events (partially correlated), neutron source anisotropy effects (partially correlated) and calibration of activity measurement processes (uncorrelated for the tritium activity but partially correlated for all the other activities, which were measured by gamma ray detection). The magnitudes of the errors considered are summarized in Table 1. Total errors and the corresponding correlation matrix for the final measured ratios are shown in Table 3.

Fission Ratios: 14-MeV Data

In this experiment, fission cross section ratios of ^{230}Th, ^{232}Th, ^{233}U, ^{234}U, ^{236}U, ^{238}U, ^{237}Np, ^{239}Pu and ^{242}Pu were measured at 14.7 MeV relative to ^{235}U [12]. The apparatus used is as shown in Fig. 1.B. In order to improve the precision of this experiment, the measurements were repeated several times under somewhat varying conditions, and a variety of calibrated fission foils were employed. Consequently, the error analysis, while straightforward, was quite tedious to carry out. The dominant sources of error in this experiment were statistical errors in the fission counts (uncorrelated), extrapolation and thickness corrections to these counts (partially to fully correlated depending on context) and various foil calibration errors, including those related to alpha counting and isotopic content effects (partially to fully correlated depending on context). The magnitudes of the errors considered are summarized in Table 1. Total errors and the corresponding correlation matrix for eight of the individually measured ratios from this experiment are shown in Table 4.

Fission Ratios: Be(d,n) Integral Data

The following integral fission cross section ratios have been measured in the continuum benchmark field produced by the Be(d,n) thick target reaction at 7 MeV deuteron energy [13]: $^{232}Th/^{235}U$, $^{237}Np/^{235}U$, $^{238}U/^{235}U$, $^{237}Np/^{238}U$, $^{232}Th/^{237}Np$, $^{236}U/^{235}U$, $^{239}Pu/^{235}U$, $^{233}U/^{235}U$, $^{234}U/^{235}U$, $^{234}U/^{238}U$ and $^{236}U/^{238}U$. The apparatus used is indicated in Fig. 1. The detector arrangement is as shown in Fig. 1.B. while the neutron source assembly used to produce the benchmark spectrum is as shown in Fig. 1.A. The dominant sources of error in this experiment were statistical errors in the fission counts (uncorrelated), extrapolation and thickness corrections to these counts (partially to fully correlated depending on context), various foil calibration errors, including those related to alpha counting and isotopic content effects (partially to fully correlated depending on context), and an error assigned to cover differences between ratios measured with the fission foils in two different orientations. Total errors and the corresponding correlation matrix for eight of the individually measured ratios from this experiment are shown in Table 5.

SUMMARY

We have developed a procedure for providing reliable covariance matrices for the results of our activation cross section and fission ratio measurement program at the Argonne National Laboratory FNG Facility. Our approach is founded on the basic principles of statistics and error propagation, while at the same time it employs valid approximation methods which reduce the required labor to manageable levels. This effort requires careful attention to the experimental details, a task which is made relatively tractable by the inherently simple design of these experiments.

ACKNOWLEDGEMENTS

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Table 1: Error sources for the experiments discussed in this paper

		Error Magnitudes (%)[a]			
		Activation		Fission Ratios	
	Source of Error	14 MeV	Be(d,n)	14 MeV	Be(d,n)
E_1	Event statistics	0.1-4.6	0.3-3.0	0.6-0.8	0.3-0.6
E_2	Background	N[b]-0.1	< 0.5	NA[c]	NA
E_3	Event determination procedures	1.7-2.0	0.5-2.5	0.6-2.5	0.5-1.7
E_4	Event determination calibration standards	0.6-2.1	0.6-2.0	NA	NA
E_5	Sample assay	1.4-1.7	2.0-2.2	NA	0.3
E_6	Activity half life	N-0.5	N-0.4	0.1-0.4	0.1-0.5
E_7	Activity decay factors	< 1.0	N-1.0	N	N
E_8	Isotopic abundance	< 0.5	N	N-0.4	N-0.4
E_9	Geometry	0.3-1.0	0.3-1.7	N	N
E_{10}	Neutron source	N-0.2	0.1-4.7	N	N-0.6
E_{11}	Neutron fluence	4.0	NA	NA	NA
E_{12}	Neutron absorption	0.1-0.5	0.5	< 0.2	0.1-0.2
E_{13}	Neutron scattering	0.1-1.5	0.6	0.2-0.7	0.1-0.4
E_{14}	Reproducibility	NA	NA	< 0.3	0.3-2.5

[a] Range of errors encountered in these particular experiments.

[b] N = Negligible (< 0.1%).

[c] NA = Not applicable to this experiment.

Table 2: Errors and correlations: 14 MeV activation data

	Reaction[a]	Error (%)[b]	Correlation Matrix 1	2	3	4	5	6	7	8
1	$^{7}Li(n,n't)^{4}He$	4.6	1							
2	$^{27}Al(n,p)^{27}Mg$	5.3	.76	1						
3	$^{27}Al(n,\alpha)^{24}Na$	5.5	.74	.64	1					
4	$Si(n,X)^{28}Al$	4.8	.85	.74	.71	1				
5	$Ti(n,X)^{46}Sc$	5.0	.83	.72	.70	.81	1			
6	$Ti(n,X)^{47}Sc$	6.2	.65	.56	.54	.63	.61	1		
7	$Ti(n,X)^{48}Sc$	5.8	.70	.60	.59	.67	.66	.51	1	
8	$^{51}V(n,p)^{51}Ti$	5.1	.79	.68	.67	.77	.75	.58	.63	1

[a]Cross section normalized to ^{235}U neutron fission.
[b]Total error.

Table 3: Errors and correlations: Be(d,n) activation data

	Reaction[a]	Error (%)[b]	Correlation Matrix 1	2	3	4	5
1	$^{7}Li(n,n't)^{4}He$	4.0	1				
2	$^{27}Al(n,p)^{27}Mg$	3.9	.34	1			
3	$^{27}Al(n,\alpha)^{24}Na$	5.9	.28	.55	1		
4	$^{58}Ni(n,p)^{58}Co$	4.1	.30	.63	.43	1	
5	$^{60}Ni(n,p)^{60}Co$	3.7	.41	.62	.52	.46	1

[a]Cross section ratio relative to ^{238}U neutron fission.
[b]Total error.

Table 4: Errors and correlations: 14 MeV fission ratio data

	Ratio[a]	Error (%)[b]	Correlation Matrix 1	2	3	4	5	6	7	8
1	$^{230}Th/^{235}U(\#1)$	2.2	1							
2	$^{230}Th/^{235}U(\#2)$	2.2	.46	1						
3	$^{230}Th/^{235}U(\#3)$	2.2	.72	.49	1					
4	$^{232}Th/^{235}U(\#1)$	2.3	.49	.34	.34	1				
5	$^{232}Th/^{235}U(\#2)$	2.9	.26	.29	.40	.27	1			
6	$^{232}Th/^{235}U(\#3)$	2.2	.50	.34	.34	.51	.28	1		
7	$^{233}U/^{235}U(\#1)$	1.3	.23	.46	.29	.19	.19	.19	1	
8	$^{233}U/^{235}U(\#2)$	1.2	.25	.24	.25	.20	.16	.20	.14	1

[a]Multiple measurements of the same ratio are so indicated.
[b]Total error.

Table 5: Errors and correlations: Be(d.n) fission ratio data

	Ratio[a]	Error (%)[b]	Correlation Matrix 1	2	3	4	5	6	7	8
1	$^{232}Th/^{235}U(d_1)$	2.5	1							
2	$^{232}Th/^{235}U(d_2)$	2.5	.87	1						
3	$^{237}Np/^{235}U(d_1)$	2.1	.35	.40	1					
4	$^{237}Np/^{235}U(d_2)$	2.6	.32	.40	.70	1				
5	$^{238}U/^{235}U(d_1)$	2.6	.39	.41	.49	.49	1			
6	$^{238}U/^{235}U(d_2)$	2.8	.34	.41	.49	.50	.68	1		
7	$^{237}Np/^{238}U(d_1)$	2.6	.21	.24	.58	.54	.20	.20	1	
8	$^{237}Np/^{238}U(d_2)$	2.7	.18	.25	.58	.55	.18	.20	.79	1

[a]Ratio labels (d_1 and d_2) refer to two different detector distances.
[b]Total error.

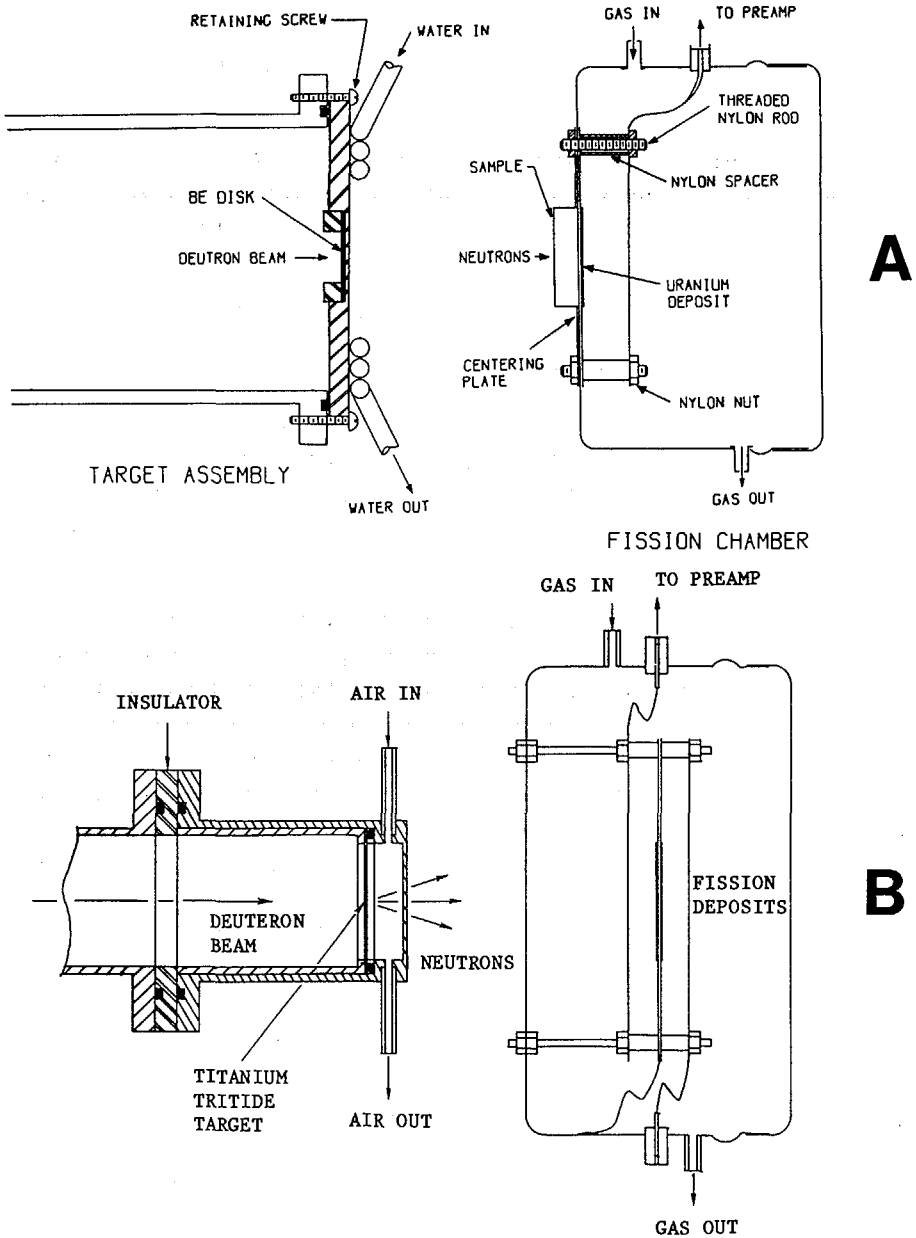

Figure 1: Schematic diagrams of the apparatus used in activation (A) and fission ratio (B) measurements at the Argonne FNG. Both of the neutron source assemblies used in this work are shown.

A Method to Evaluate Covariances for Correlated Nuclear Data

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Abstract

A method to evaluate covariances for nuclear data has been developed by applying Bayesian method with B-spline functions and logarithms of experimental data. A point of the method is adoption of the B-spline function. Applicability of the method to nuclear data evaluation is presented with few simple exsamples.

1. Introduction

It had been becoming evident in spite of endeavors of many experimenters that cross sections newly measured with currently-developed techniques did not always converge to a definite range within an expected uncertainty. Therefore, it is reasonable that the evaluated cross sections are associated by uncertainties estimated from the errors of available measurements. The covariance between energy segments can explicitly describe correlation of the cross sections at specific energies. The author (YK) had tried to calculate confidence bands along the evaluated cross sections of a few nuclear reaction in the early works [1,2]. In the study, the author did not introduce the covariances of cross sections between energy segments as a present-day manner but used the ones among coefficients in a quadratic function fitted to the experimental data in a limited energy range. Physical meaning of these covariances is obscure; they implicitly relate to the uncertainties of the evaluated cross sections. They were estimated by applying a least squares method. Although polynomial functions of higher order may be fitted to a cross section curve, they correlate so strong between even far-separated energy segments: for example, the polynomial function fitted to many experimental points in the one energy region hardly is suitable in the other energy region where

experimental data are scarce. To solve this difficulty, B-spline functions are applied in our work.

2. Basic formulae

In a Bayesian method, basic formulae for the parameter vector θ to be estimated and its covariance matrix M are given by

$$\theta = \theta_0 + (\Phi^t V^{-1} \Phi + M_0^{-1})^{-1} \Phi^t V^{-1} (y - \Phi \theta_0) \quad (1)$$

and

$$M = (\Phi^t V^{-1} \Phi + M_0^{-1})^{-1}, \quad (2)$$

respectively. The super-scripts t and -1 denote the transpose and inverse, respectively. The experimental data vector y can be approximately expressed as $y = \Phi \theta$, where Φ is a design matrix. The matrix V is a covariance matrix for the experimental data. The vector θ_0 and matrix M_0 are a priori parameter vector and its covariance matrix, respectively. In the case of unknown a priori covariance M_0^{-1} is null and θ_0 disappears in eq.(1). It is a generalized least squares method.

3. Smoothing of Experimental Data

In our work, B-spline functions are applied to smooth scattered experimental data. The r-th order B-splines are defined by the recurrent formula:

$$M_{rj}(x) = \{(x - \xi_{jr-1}) M_{r-1\,j-1}(x) + (\xi_j - x) M_{r-1\,j-1}(x)\} / (\xi_j - \xi_{j-r-1}) \quad (3)$$

$$M_{0j}(x) = \begin{cases} (\xi_j - \xi_{j-1}) & \xi_j > x \geq \xi_{j-1} \\ 0 & \text{otherwise} \end{cases} \quad (4)$$

where the points ξ_j (j=1,2,...) are called "knots" and characterize the finite intervals. The B-spline functions represent any functions with the linear combination of B-splines such as

$$f(x) = \Sigma\, M_{rj}(x) s_j, \quad (5)$$

where the s_j is the j-th parameter for B-spline functions.

In our work, the first or second order B-spline function is applied to smooth experimental data. An example of the second order function is shown in Fig.1, where 38 data are smoothed with given 13 knots. This makes it possible to choose arbitrary knots on energy axes of every reaction cross section included in a simultaneous evaluation. The spline functions fitted to the data can be used also to interpolate at those energies common to every reaction. They can appropriately smooth and interpolate the data.

Except for practical convenience described above, spline functions are very useful to represent correlation of measured data between different energies. The r-th order spline functions are determined by the data being in r+1 intervals and r+1 functions are obtained in a interval. The correlation of the data in the neighbouring intervals are naturally introduced.

The 0-th B-spline function $M_{0j}(x)$ is constant in the interval and does not correlate with the neighbouring intervals. This is the case that experimental values are averaged in a interval. The use of $M_{0j}(x)$ is resulted in not only discontinuity at the boundaries of the intervals but also inconvenience that common knots must be set for the every reaction in the simultaneous evaluation to make the evaluating energies match.

4. Representation of Experimental Data

Although our method can be applied to the evaluation of one reaction cross section, it prove its real worth when it is just applied to the simultaneous evaluation. In the early works, the validity and usefulness is shown practically [3,4,5]. Experiments of cross sections are summarized into four categories are following,

(1) Absolute measurement,
(2) Shape measurement of a cross section curve,
(3) Ratio measurement to a reference cross section,
(4) Shape measurement of cross section ratio curve.

When the least-squares method or the Bayesian method is applied to each case, the design matrix in eq.(1) must be formulated to be suitable for it. When the ratios of cross sections are treated in the simultaneous evaluation, logarithms of the cross sections are used.

There are two reaction cross sections $\sigma_1(E)$ and $\sigma_2(e)$. The absolute measurements $y(E_1)$ and $y(E_2)$ can be expressed by eq.(6) referring Fig.2. The data for $\sigma_2(e)$ are shown by eq.(7).

$$\begin{pmatrix} y(E_1) \\ y(E_2) \end{pmatrix} = \begin{pmatrix} B_1^-(E_1) & B_2^+(E_1) & 0 \\ 0 & B_2^-(E_2) & B_3^+(E_2) \end{pmatrix} \begin{pmatrix} \Theta_1 \\ \Theta_2 \\ \Theta_3 \end{pmatrix} \quad (6)$$

$$\begin{pmatrix} z(e_1) \\ z(e_2) \end{pmatrix} = \begin{pmatrix} b_1^-(e_1) & b_2^+(e_1) & 0 \\ 0 & b_2^-(e_2) & b_3^+(e_2) \end{pmatrix} \begin{pmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \end{pmatrix} \quad (7)$$

The ratio measurement of σ_1 to σ_2 at e_1 and e_2, which are represented as $R(e_1)$ and $R(e_2)$, respectively, are presented as

$$\begin{pmatrix} R(e_1) \\ R(e_2) \end{pmatrix} = \begin{pmatrix} B_1^-(e_1) & B_2^+(e_1) & 0 & -b_1^-(e_1) & -b_2^+(e_1) & 0 \\ 0 & B_2^-(e_2) & B^+(e_2) & 0 & -b_2^-(e_2) & -b_3^+(e_2) \end{pmatrix} \begin{pmatrix} \Theta 1 \\ \Theta 2 \\ \Theta 3 \\ \theta 1 \\ \theta 2 \\ \theta 3 \end{pmatrix} \quad (8)$$

The covariances are computed by applying eq.(2).

5. Conclusion

The Bayesian method presented in this report have been successfully applied to evaluate simultaneously the cross sections [3,4,5] and the parameters in the nuclear reaction model [6,7] by adopting the B-spline function to represent experimental data. Estimation of the covariances for the experimental data used in the evaluation is an essential work in these application.

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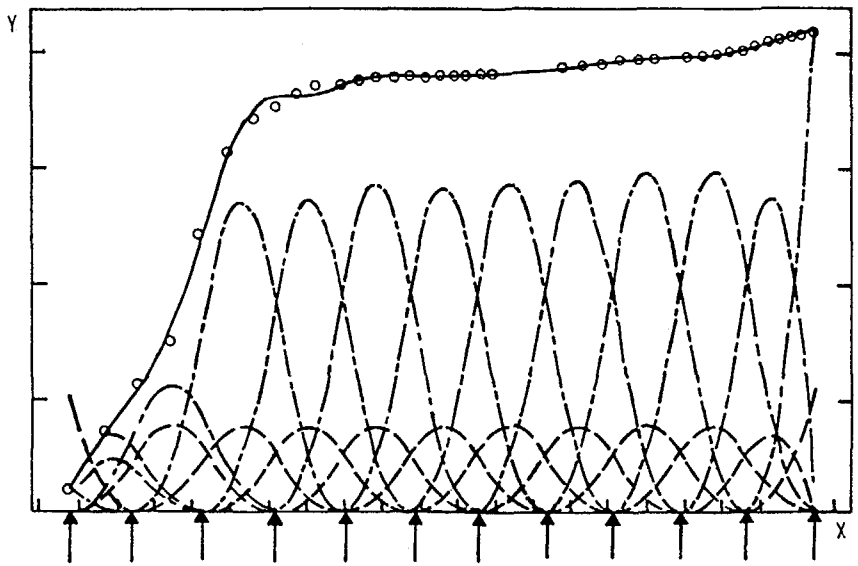

Fig.1 An example of smoothing of experimental data by second order B-spline functions. The open circles are the experimental data. The arrows point the knots on the X-axis, the dashed-lines and dot-dashed lines are the elementary and normalized B-spline functions, respectively. The solid line is the resulted smoothing curve.

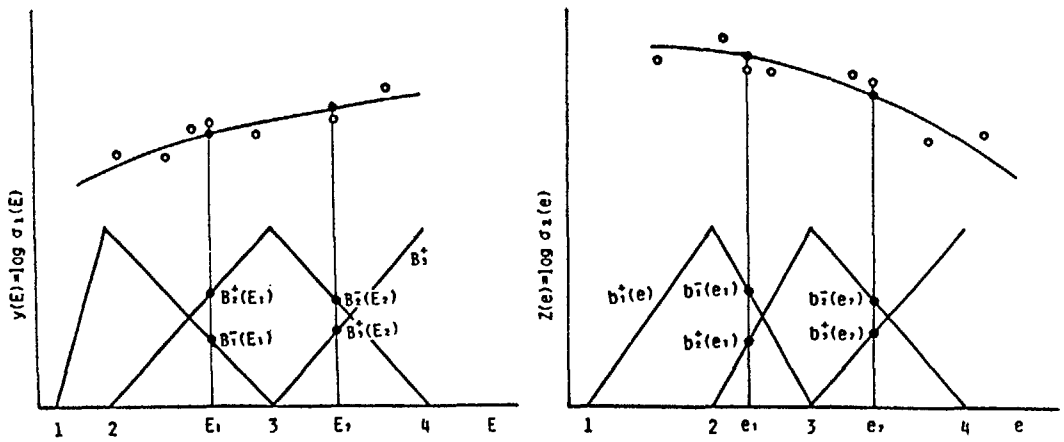

Fig.2 The logarithms y(E) and z(e) of the cross sections $\sigma_1(E)$ and $\sigma_2(e)$, respectively, are represented by the 1st order B-spline function B(E) and b(e). The super-scripts + and - denote the 1st order polymomials having positive and negative gradients, respectively. The numbers 1,2,··· are knots. The sub-scripts of B(E) and e(e) denote the lowest knot of the interval where they are defined. The E_1 and E_2, and e_1 and e_2 are the experimental points for σ_1 and σ_2, respectively. The solid lines along the experimental data are the smoothing curves represented by the spline functions. The closed circle on the y(E) curve at E_1, for instance, shows the sum of $B_1^-(E_1)$ and $B_2^+(E_1)$ and approximately represents the open circle over it.

Covariances Obtained in Simultaneous Evaluation of Fission and Capture Cross Sections for Heavy Nuclides

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Abstract

Simultaneous evaluation of the fission cross sections for five nuclides and capture cross sections for two nuclides have been performed by using fourteen experiments including absolute and ratio measurements. A generalized least squares method is applied with the B-spline functions and logarithms of the data. The obtained covariances are presented and discussed.

1. Introduction

Fission and capture cross sections of uranium and plutonium isotopes evaluated with high accuracy have been demanded in fast breeding reactor development in order to calculate reactor parameters. Most of their measurements scatter in the region insufficient to evaluate them with an expected certainty. Many experiments have been hard performed to solve the problem. It seems to be achieved it partly but it is not sufficient to answer the whole needs of users.

These measurements have correlation in experimental conditions. In early evaluations, a kind of cross section was singly treated not to consider entirely experimental correlation. The simultaneous evaluation has been studied to take account of it and developed effectively by introducing experimental covariances into a generalized least-squares method.

The results shown in this report are obtained by the simultaneous evaluation method presented separately in this meeting. The covariances between evaluated cross sections obtained in this study are given and discussed. The results shown in this report are an extension of the previous work presented at Santa Fe [1]. Several data are added; some of them are new and others are old.

2 Simultaneous Evaluation

The cross sections evaluated in this study are the capture cross sections of ^{197}Au and ^{238}U and the fission cross sections of ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu and ^{241}Pu in the energy range from 50 keV to 20 MeV. The experimental data used in the simultaneous evaluation are the absolute measurements of these cross sections and seven kinds of relative measurement of their combinations. The formulae used for the simultaneous evaluation are found in the paper presented else at this meeting [2] and Ref.[3]. The design matrix [2] is given to relate the cross sections to be evaluated with the experimental data. We present the simple example in which the $^{235}U(n,f)$ and $^{238}U(n,f)$ cross sections are evaluatied from their absolute measurements and ratio data for both the cross sections. The experiment vector $(y_{25}, y_{28}, y_{8/5})$ can be expressed as,

$$\begin{pmatrix} y_{25} \\ y_{28} \\ y_{8/5} \end{pmatrix} = \begin{pmatrix} \Phi_{25} & 0 \\ 0 & \Phi_{28} \\ -\Phi_{25} & \Phi_{28} \end{pmatrix} \begin{pmatrix} \theta_{25} \\ \theta_{28} \end{pmatrix} \qquad (1)$$

The matrix in the right member is the design matrix whose elements are sub-design-matrices which is expressed with B-spline functions described in Ref. [2]. The elements of the experiment vector are logarithms of experimental values. The vector in the right member of eq.(1) is the parameter vector to be estimated and expresses the amplitude of the B-spline functions.

The experiments used in this study is 126 sets. Their experimental covariances are evaluated from standardized correlalion factors for partial errors and information available in the report. If the experimental covariances can not be estimated because of insufficient information on the partial errors in the report, they were assumed to be 30 %. From our experience in covariance studies, the value of 30 % is to be judged a boundary of significant correlation.

3 Results and Discussion

The result for the ^{235}U fission cross section is shown in Fig.1. Although the figures for the other cross sections are not shown in this report, the result is affected from the cross sections including in the simultaneous evaluation. It is a principle that the total error given by the experimenter is adopted as the variance of the experimental covariance matrix. In an early step of the evaluation, the result shown in Fig.2 is obtained. To show clearly the difference of both the results, a lower energy region is presented in Fig.3 with two curves. It seems to be unreasonably lower than the bulk of the experimental data. The evaluated curves for the other cross sections show similar tendency. The cause of disagreement between the evaluation and experiment is that one experiment gives much smaller errors than the others. It is Lindner et al.'s measurements for the capture cross sections of ^{197}Au and ^{238}U relative to the fission cross section of ^{235}U [4]. They gave the standard deviations less than 1 %. If they are reasonable the results shown in Fig.2 and the dashed curve in Fig.3 should be accepted. There are no reasons that their experiment is extremely accurate comparing with the others. Therefore, it is assumed that the partial error not taken into account by the experiments are 5 %. The number for the partial error is arbitrary but it may be valid by comparing with the other experiments. It means that their experiment is comparable with the others.

Since the dimension of the whole covariance matrix obtained in the simultaneous evaluation is very large, a part of it is presented in Fig.4. They are not diagonal except for the self-correlation matrices because the numbers of knots on the energy axes are different for every reaction. It can be seen in Fig.4 that the values next to the diagonal elements of the self-correlation sub-matrices are systematically smaller than the neighbour elements for every reaction. It is a proper difficulty in our method applying spline functions. Amplitudes at neighbouring knots have negative correlation in order to make a spline-function fitting to the experimental points between the knots. The obtained covariances are affected by the proper difficulty. Since this effect is limited for the nearest neighbours, they can be corrected by interpolation from both side values. Application of the spline function to the nuclear data evaluation, however, is useful beyond this difficulty.

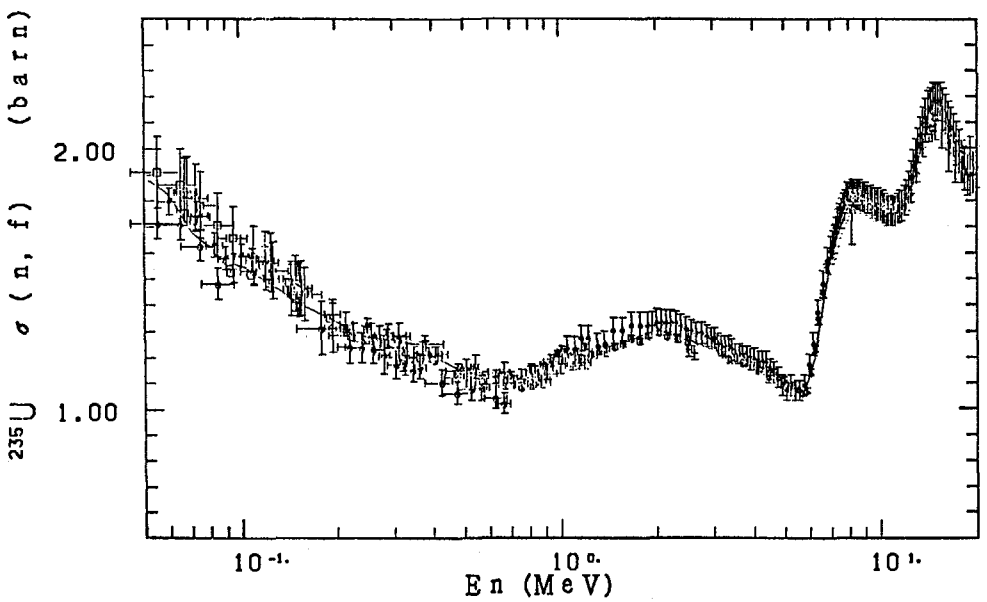

Fig.1 Simultaneously evaluated $^{235}U(n,f)$ cross sections. This result was obtained by revising the erros of Lindner's data.

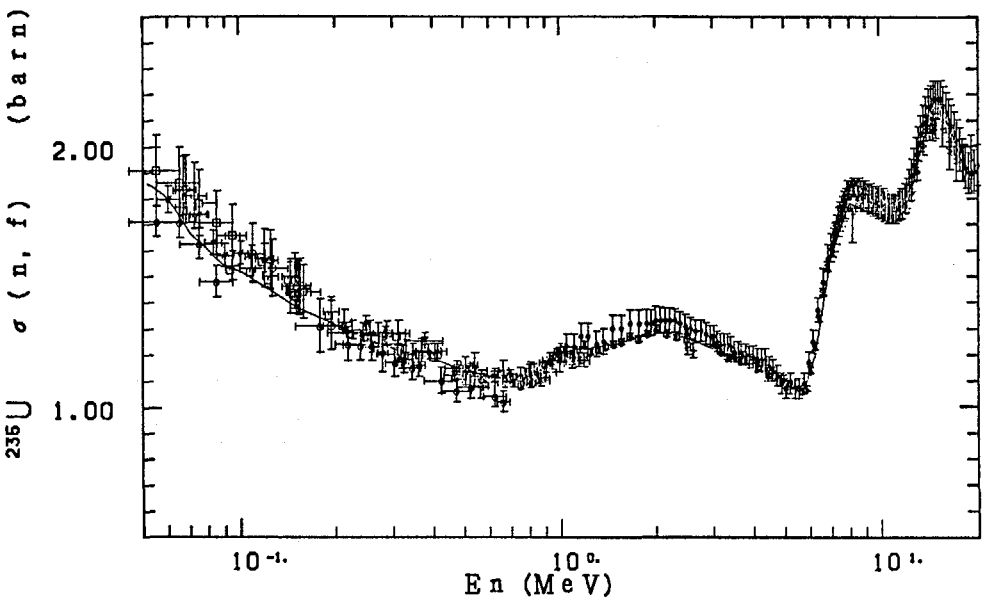

Fig.2 Simultaneously evaluated $^{235}U(n,f)$ cross sections. This result was obtained by using the original errors of Lindner's data.

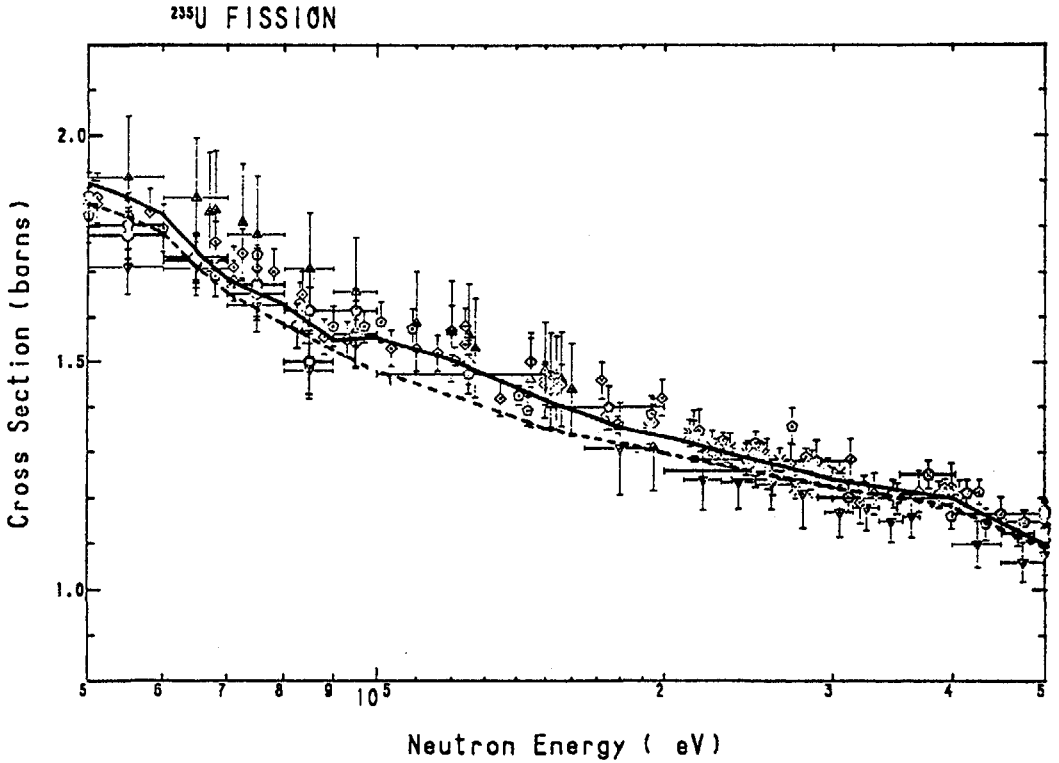

Fig.3 The lower energy region in Figs.1 and 2. The solid line is the result for the revised errors of Lindner's data and the dashed line is for the original ones.

$^{235}U(n,f)$

1# 2.20E+01(MEV) #	100									
2# 2.00E+01(MEV) #	-33	100								
3# 1.90E+01(MEV) #	22	4	100							
4# 1.80E+01(MEV) #	9	27	5	100						
5# 1.70E+01(MEV) #	12	22	26	6	100					
6# 1.60E+01(MEV) #	10	18	17	23	0	100				
7# 1.50E+01(MEV) #	1	2	3	2	6	-8	100			
8# 1.40E+01(MEV) #	1	3	3	4	3	9	-19	99		
9# 1.30E+01(MEV) #	3	6	6	6	7	9	14	-16	100	
10# 1.20E+01(MEV) #	3	7	8	8	8	13	8	13	0	99

$^{238}U(n,f)$

41# 2.20E+01(MEV) #	73	-23	16	7	9	7	0	1	1	2
42# 2.00E+01(MEV) #	-21	64	2	17	14	11	1	2	3	5
43# 1.90E+01(MEV) #	13	2	61	3	16	10	1	1	3	5
44# 1.80E+01(MEV) #	6	17	4	62	4	14	1	2	3	5
45# 1.70E+01(MEV) #	8	14	17	4	64	0	4	1	4	5
46# 1.60E+01(MEV) #	6	11	10	14	0	61	-7	5	5	7
47# 1.55E+01(MEV) #	2	3	3	4	0	17	15	-2	2	3
48# 1.50E+01(MEV) #	0	1	1	1	2	-2	39	-8	9	3
49# 1.40E+01(MEV) #	0	1	1	1	0	3	-9	47	-18	6
50# 1.30E+01(MEV) #	1	4	4	4	4	6	9	-15	63	0
51# 1.20E+01(MEV) #	2	4	5	5	5	8	4	7	1	56

41# 2.20E+01(MEV) #	100									
42# 2.00E+01(MEV) #	-39	100								
43# 1.90E+01(MEV) #	17	-12	100							
44# 1.80E+01(MEV) #	2	17	-18	100						
45# 1.70E+01(MEV) #	7	8	18	-14	100					
46# 1.60E+01(MEV) #	5	8	4	15	-16	100				
47# 1.55E+01(MEV) #	2	3	4	1	11	-20	100			
48# 1.50E+01(MEV) #	0	1	1	2	0	9	-23	100		
49# 1.40E+01(MEV) #	0	1	1	1	2	-1	11	-33	100	
50# 1.30E+01(MEV) #	1	3	3	4	4	6	0	16	-34	100
51# 1.20E+01(MEV) #	2	4	4	4	5	6	5	1	10	-9	100

$^{235}U(n,f)$

Fig.4 An example of correlation matrices for evaluated cross sections.

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EVAL: AN INTERACTIVE FACILITY FOR MULTIPARAMETRIC COVARIANT EVALUATION

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Abstract:

EVAL is designed for the evaluation of a set of nuclear parameters out of an overdetermined set of measurements of their combinations. Written in the interpreted language APL, it allows the full-screen interactive input and edition of the evaluation data base. Sorting of the measurements in independant groups, least-squares fitting and display of the fitted parameter values are performed by further interactive commands. As a cross-check, an inference procedure may situate the measured data with respect to the evaluated parameters on common diagrams.

1. Evaluation as a least squares minimization problem

1.1 Formulation

Consider a set of n measurements $M_1, M_2, .. M_n$

(together as vector **M**)

of quantities otherwise expressed as functions $F_1, F_2, .. F_n$

(together as vector **F**)

of p physical parameters $x_1, x_2, .. x_p$ to be evaluated

(together as vector **x**)

M_i is thus a measurement of $F_i(x_1, x_2, .. x_p)$

The parameter set is assumed overdetermined by the measurement set, i.e. $n > p$.

Assume that the measurement uncertainties are given by the n times n matrix **Z** such that $Z_{ij} = \langle dM_i . dM_j \rangle$

The purpose of the evaluation is to find the value of **x** which minimizes the expression:

(i) $(\mathbf{M} - \mathbf{F}(\mathbf{x}))^t . \mathbf{Z}^{-1} . (\mathbf{M} - \mathbf{F}(\mathbf{x})) = \text{Chisquare}$

If the covariance estimate is correct, the evaluation should provide a value of Chisquare of the order of n.

Fig 1 illustrates a simple case of evaluation ($n = 5$, $p = 2$)

1.2. Linearisation

A practical solution to (i) may be found using a linear expansion of **F** in the vicinity of an initial guess value x_0 of **x**.

We thus introduce:

$\mathbf{X} = \mathbf{x} - \mathbf{x_0}$ Parameter variation

$\mathbf{Y} = \mathbf{M} - \mathbf{F}(\mathbf{x_0})$ Observation vector

$\mathbf{F}(\mathbf{x}) = \mathbf{F}(\mathbf{x_0}) + \mathbf{A} \cdot \mathbf{X}$,whereby

$A_{ik} = dF_i/dx_k$ Design or Gradient matrix

Equation (i) then becomes in linear approximation:

(ii) $(\mathbf{Y}-\mathbf{A}.\mathbf{X})^t.\mathbf{Z}^{-1}.(\mathbf{Y}-\mathbf{A}.\mathbf{X})$ = Chisquare ▮ minimum

A special matrix inversion-factorisation technique was developed to solve equation (ii) . The mathematical procedure is given in Appendix I of this paper.

1.3 Specific requirements of multiparametric. evaluation

Curve fitting methods as used e.g. in neutron resonance shape analysis mostly rely on a least-squares approach leading to a matrix equation formally identical to eq. (ii).

However, all quantities measured for a curve fit (e.g. cross-section values) are expressed by the same analytical function of the parameters to be fitted, plus a running parameter (e.g. neutron energy), so that:

M_i is a measurement of $F(E_i, X_1, X_2, .. X_3)$

The specific coding task in the case of a curve fit thus reduces to the design of one function or subroutine, which will be used for the computation of all components of the observation vector **Y** and of the gradient matrix **A** .

Differently in multiparametric evaluation, every measurement may relate to a different quantity. There may be a priori as many different functions as there are measurements. Although the amount of data involved in an evaluation is sometimes orders of magnitude less than in curve fitting, the coding of all these functions (and their logical links to the data) promises to be a (human) time-swallowing task with a compiled programming language like FORTRAN.

A similar remark applies to the covariance data. Whereas in curve fitting a smooth evolution of the covariance terms may be implied -thus leading to approximations with relatively small covariance input- point multiparametric evaluation requires every non-zero term of the covariance matrix to be exactly given -and possibly corrected - by the evaluator himself.

These requirements comforted us in the choice of the interactive language APL for the design of our facility. The advantages of APL vs FORTRAN for this type of application are summarised in Appendix II of this paper. Essentially, our APL workspace EVAL is a relational data base system with full-screen input and output, plus interactive fitting and graphic display possibilities.

2 Building and editing the evaluation data base

2.1 Individual edition of the measurements

The input of the evaluation is handled by EVAL as a database of which every measurement is a record. By "measurement" we understand here all the data related with it, i.e.

a literature reference (12 char.),

an executable expression representing the corresponding function measured (22 char.- see subsection 2.2)

the measured value (1 number)

the uncorrelated error in % (1 number)

a string of codes for the correlated errors (12 or more char.- see subsection 2.3)

The function EDIT displays these data in full-screen mode, allowing to append or delete records or to correct them directly. Every measurement is represented by one line on the screen panel (See Fig 2), thus 20 different measurements may be displayed at a time.

EDIT is the basic function of EVAL. The bottom line of its panel display the options which may be started by Programmed Function Keys of the keyboard. The simplest are the screen hardcopy, the Quit and the Scroll options by which the whole input may be accessed.

2.2 Executable expressions, parameters and base functions

In the interpreted language APL used by EVAL, a string of characters may be treated as a literal variable, or passed as such to the interpreter for execution. Column 2 of the EDIT panel consists of such executable expressions. More precisely, every of them is executed as a function of the vector x_0 of Section 1.2 (vector of the guess values of the parameters).

This of course implies that x_0 was introduced before the execution, using a dedicated full-screen panel as shown in Fig 4. Note that a variation value must be given for each parameter, in order to compute the partial derivatives composing the gradient matrix **A**.

Executable APL expressions may involve user programmed APL functions. It is therefore advisable to design a set of base functions addressing the position of the guess values in x_0 with names appealing to the evaluator's mind, like those listed in column 2 of Fig 4.

2.3 Edition of common sources of uncertainty

Correlated uncertainties are coded in the last column of the EDIT panel. Their details may be accessed for every measurement on an individual panel showing what are the sources of uncertainty and to how much they amount in percent, as to be seen on Fig 3. This representation is simpler to understand and update than a series of covariance terms. EVAL uses data in this form to build the covariance matrix actually used in the least-squares fit operation.

3 Fitting and using the evaluated parameters

3.1 Reordering the measurements in independant groups

In practice, an individual measurement does not involve all the parameters considered in the evaluation. Accordingly, the corresponding row in the gradient matrix **A** contains only few non-zero partial derivative terms. Also, not all the common sources of uncertainty are relevant for a measurement, so that the covariance matrix **Z** is usually sparse.

It may thus occur in an evaluation data base that a group of measurements involves only parameters and sources of uncertainty which are irrelevant to other groups of measurements. In that case, the groups may be evaluated separately, leading to several uncoupled groups of evaluated parameters.

This situation may be checked in EVAL with the Reorder option. Reorder will then associate the measurements and parameters which belong together and mark them with a running index (column 1 of the EDIT panel) in order to split the evaluation in independent groups.

3.2 Fit and iteration operations

When the edition of the evaluation data base is completed, the least-square fit of the parameters may be started with one keystroke. EVAL then builds the observation vector, the covariance and the gradient matrices. In fact these quantities are computed in EVAL as normalised or relative deviations. In the present paper the theoretical development was done with absolute expressions for the sake of clarity.

The fit operation uses the technique detailed in Appendix I. On our IBM4381 mainframe, data sets of up to 200 measurements involving up to 50 parameters can be fitted in the order of a minute of central processor unit time.

The result of the fit consists of a list of parameters and their covariance matrix. Both may be displayed/scrolled on the screen, as shown on Fig 5.

In general, the guess values used to start an evaluation are already close to the result, and convergence problems will not be so frequent as in curve fitting. Nevertheless evaluators are interested in the quality of the convergence process. This can be checked using the Recycle option of EVAL, which simply sets the guess values to the values produced by the last fit. EVAL is then ready for a new fitting step, and the iteration process may be repeated to the will of the evaluator.

3.3 Filing the evaluation data base and the fitted results

The whole information about an evaluation case is held in the EVAL workspace in a set of literal and numeric vectors and matrices. It represents an important investment of human an machine time. As such, it should better be filed before a new case is treated. For this purpose we used the APL component file system developed at CBNM [1]. It allows to file or retrieve a whole evaluation data base under a single name. Directory display and merging options are also available there like in conventional data base systems.

3.4 Cross checking the evaluation base by inference

The fit procedure illustrated by Fig 1 can be grossly described by saying that the fitted point in the x_p space has to be nearest to the hypersurfaces representing the measurements in that space. Conversely, one may infer that the point on an hypersurface which is nearest to the fitted point gives the combination of parameters which is most likely to represent the corresponding measurement.

The nearest point on the hypersurface is obtained by drawing the normal to the hypersurface from the fitted point. The direction of the normal is given by the gradient of the corresponding function. This is just given by the corresponding row of the gradient matrix **A** which was used for the fit.

Gathering our good old differential geometry, we find that the displacement from the fitted point x_0 to the hypersurface $F_i(x) = M_i$ is given by:

$$(M_i - F_i(x_0)) \times \mathbf{grad}\, F_i \div (\mathbf{grad}\, F_i)^2$$

The global uncertainty on a measurement is also deducible from the data base. It leads to two hypersurfaces represented by

$$F_i(x) = M_i + dM_i \qquad \text{and} \qquad F_i(x) = M_i - dM_i.$$

Fig 6 shows how they may be used to infer the error bar on each measurement, as a vector in the x_p space.

The inference method was applied on the evaluation data base put up by E.J.Axton for the evaluation of thermal constants of actinides during his recent stay at Geel [2].

It is a pleasure to acknowledge Mr Axton's kind permission to use his data for our demonstration purposes.

Fig 7 is a biparametric inference diagram of measurements related with the fission and/or nubar of ^{233}U. The literature references are ordered by increasing distance to the fitted point (axes are labelled in %). The dashed ellipse around the

central fitted point is deduced from the covariance matrix resulting from the evaluation. Its tilted orientation indicates a coupling between the fitted values of fission and nubar, as otherwise suggested by the presence of measured points- typically measurements of eta - on the upwards diagonal.

Fig 8 is a monoparametric inference diagram- i.e. a projection of the inferred points on the axis of x_p corresponding to the fission of ^{233}U. There, the references are ordered by increasing overall uncertainty, and the error bars have been inferred by the method illustrated on Fig 6. The two dashed vertical lines give the standard deviation as deduced from the covariance matrix of the fitted parameters.

Mr Axton's data base involves 167 measurements and 38 evaluated parameters. It is our belief that a thorough and competent cross-checking of data bases of this complexity by systematic inference would reveal trends and relations hitherto unnoticed.

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Appendix I: Inversion-factorisation of a covariance matrix

The Least Squares solution of an evaluation problem involving n observations and p parameters (n > p) is a vector X of p parameter values which minimizes:

(1) Chisquare = $(Y-A.X)^t.Z^{-1}.(Y-A.X)$

whereby

- **Y** is the n-valued observation vector, i.e. the deviation between the values measured and those computed from the initial (guess) parameters
- **A** is the (n × p) design matrix - we call it here the gradient matrix, as it consists of a rectangular table of partial derivatives of all observations with respect to all parameters. The observation set is assumed overdetermined, so that A must have more lines (n) than columns (p).
- **Z** is the (n × n) covariance matrix of the observations.

when Z is a unit matrix, the "normal equation" minimization of expression (1) is given by :

(2) $A^t.Y - A^t.A.X = 0$

leading to:

(3) $X = (A^t.A)^{-1}.A^t.Y$

Alternatively, the Householder transform provides a pseudo- inverse matrix A_P such that:

(4) $A_P.A = 1$ (unit matrix)

which leads to:

(5) $X = A_P.Y$

The pseudoinverse approach leads theoretically to the same result as the normal equation approach. However it involves less computing steps. It is implemented in APL as a standard primitive operation of the language.

When Z is not a unit matrix, the normal equation minimization of (1) is:

(3') $X = (A^t.Z^{-1}.A)^{-1}.A^t.Z^{-1}.Y$

the covariance of X is thereby:

(3") $V = (A^t.Z^{-1}.A)^{-1}$

Let us show that even for a non-unit covariance matrix, expression (1) may still be brought to a form which is solved by a matrix division in APL, or a Householder-like method in another language.

Defining **R** such that

(7) $\mathbf{R}^t.\mathbf{R} = \mathbf{Z}^{-1}$,

equation (1) becomes :

Chisquare = $(\mathbf{Y}-\mathbf{A}.\mathbf{X})^t.\mathbf{R}^t.\mathbf{R}.(\mathbf{Y}-\mathbf{A}.\mathbf{X})$

Now, transforming

$\mathbf{Y1} = \mathbf{R}.\mathbf{Y}$

$\mathbf{A1} = \mathbf{R}.\mathbf{A}$

we obtain:

Chisquare = $(\mathbf{Y1} - \mathbf{A1}.\mathbf{X})^t.(\mathbf{Y1} - \mathbf{A1}.\mathbf{X})$

solved in the pseudo-inverse approach by:

$\mathbf{X} = \mathbf{A1}^p.\mathbf{Y1}$

with the associated covariance:

$\mathbf{V} = (\mathbf{A1}^t.\mathbf{A1})^{-1}$

Obviously there, we need a procedure to deduce from **Z** a matrix **R** fulfilling eq (7), or equivalently:

(7') $\mathbf{Z}.\mathbf{R}^t.\mathbf{R} = \mathbf{1}$

Recurrence procedure on a triangular matrix **R** and a covariance matrix **Z**.

Z is a symmetric covariance matrix. It may be thus factorized using the Cholesky method to the product of a lower triangular matrix **U** by its transpose. (7') may be thus replaced by:

(8) $\mathbf{Z} = \mathbf{U}.\mathbf{U}^t$

(9) $\mathbf{U}.\mathbf{U}^t.\mathbf{R}^t\mathbf{R} = 1$

eq (9) is satisfied if

(10) $\mathbf{U}.\mathbf{R} = \mathbf{R}.\mathbf{U} = 1$

Assuming that the solution for $(n \times n)$ **Z**,**R**, and **U** matrices is known, let us extend it to matrices of dimension $(n+1) \times (n+1)$.

Eq. (8) becomes:

$$\begin{vmatrix} \mathbf{Z} & \mathbf{f}^t \\ \mathbf{f} & \mathbf{z} \end{vmatrix} = \begin{vmatrix} \mathbf{U} & \mathbf{0} \\ \mathbf{g} & \mathbf{u} \end{vmatrix} \times \begin{vmatrix} \mathbf{U}^t & \mathbf{g}^t \\ \mathbf{0} & \mathbf{u} \end{vmatrix}$$

or, in detail:

(11) $\mathbf{Z} = \mathbf{U}.\mathbf{U}^t$ (by assumption)

(12) $\mathbf{f}^t = \mathbf{U}.\mathbf{g}^t$

(13) $\mathbf{f} = \mathbf{g}.\mathbf{U}^t$

(14) $\mathbf{z} = \mathbf{g}.\mathbf{g}^t + \mathbf{u}^2$

We assume now that **R** is a lower triangular matrix and write the extension of equation (10):

$$\begin{vmatrix} \mathbf{U} & \mathbf{0} \\ \mathbf{g} & \mathbf{u} \end{vmatrix} \times \begin{vmatrix} \mathbf{R} & \mathbf{0} \\ \mathbf{h} & \mathbf{r} \end{vmatrix} = \begin{vmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{vmatrix}$$

or,in detail:

(15) $\mathbf{U}.\mathbf{R} = \mathbf{1}$ (by assumption)

(16) $\mathbf{0} = \mathbf{0}$ .. obvious

(17) $\mathbf{g}.\mathbf{R} + \mathbf{u}.\mathbf{h} = \mathbf{0}$

(18) $u.r = 1$

combining (13) and (15):

(19) $\mathbf{f}.\mathbf{R}^t = \mathbf{g}$

then, with (14):

(20) $u = (z - \mathbf{f}.\mathbf{R}^t.\mathbf{R}.\mathbf{f}^t)^{1/2}$

(17) and (19) give:

(21) $\mathbf{f}.\mathbf{R}^t.\mathbf{R} + \mathbf{u}.\mathbf{h} = \mathbf{0}$

The recurrence relations giving the terms r and h extending matrix **R** with one more line and one more column may now be combined from (18), (20) and (21), as follows:

$$(22)\quad r = (z - \mathbf{f}.\mathbf{R}^t.\mathbf{R}.\mathbf{f}^t)^{-1/2}$$

$$(23)\quad h = -r.\mathbf{f}.\mathbf{R}^t.\mathbf{R}$$

To start the recurrence procedure, we observe that if **Z** is a 1×1 matrix of one value, **U** and **R** satisfying (8) and (10) are easy to obtain as 1×1 matrices containing the square root and the inverse of the square root of this value, respectively. We may thus extend the solution using (22) and (23) recurrently to covariance matrices of any dimension.

The method was implemented in APL as function RCHOL, It minimizes the number of matrix inversions in the case of a non-unit covariance matrix, thus reducing the memory occupation and the computing time, typically by 30%.

Appendix II: Salient features of APL

(A Programming Language - K.Iverson)

Constants and variables

Type: Numeric, Literal or Boolean
Shape: Scalar, Vector, Matrix or Array of any rank

Type and Shape of a variable may be modified any time by an assignment statement.
(No declaration, high fexibility)

Functions

Powerful and strongly structured **set of primitive functions** (e.g. Matrix division in the L.S. sense implemented in standard)

User-written **functions** using primitives **executed directly** (Interpreted language- no Compile & Link)

Functions work on **scalar and array variables as well** (e.g. sum of vector and matrices without DO-loops)

The **execute** primitive may pass literal strings to the APL interpreter for execution (no External Function Declaration)

Interactive access to peripheral devices (VSAPL- IBM)

Programmable **fullscreen** Input/Output

Graphic display and plot (Tektronix)

Disk **file access**

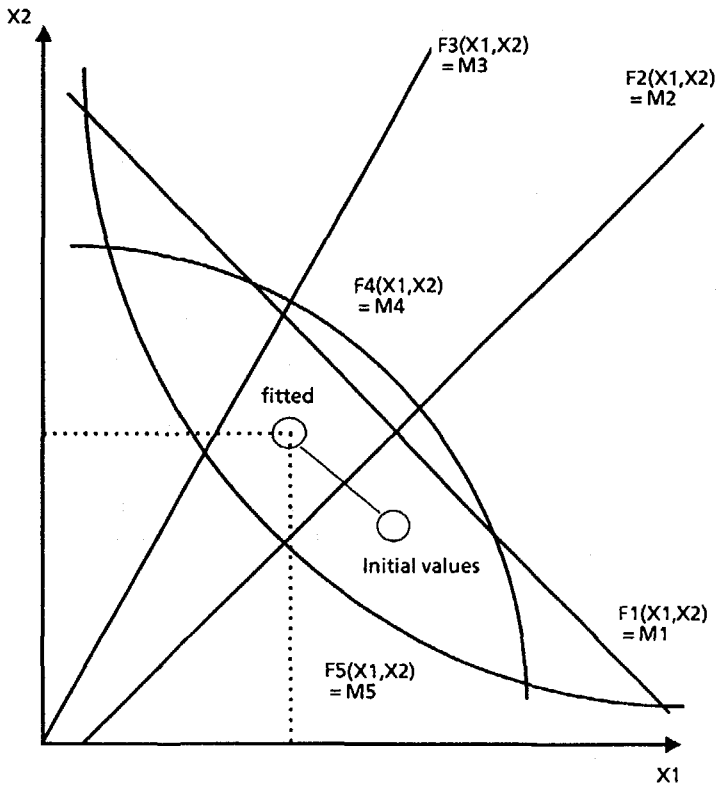

Fig 1. Evaluation of 2 parameters with 5 measurements

```
 **** EDIT ****   : individual data input
┌─Nr──┐ ┌Reference┐ ┌──────Quantity──────┐ ┌─Measured──┐ ┌─ΔU %─┐ ┌─ΔC Codes─┐
  1.101 BERCEANO   77 34 FH1 35                1.44303E03      .722 C⊃
  1.102 RAFFLE     59 33 FH1 33                8.34259E02     3.300 C
  1.103 RAFFLE     59 FIS 35                   5.81971E02     3.092
  1.104 RAFFLE     59 39 FH1 39                1.71480E03     2.840 n
  1.105 RAFFLE     56 (FIS 41)÷FIS 39          1.33190E00     6.000
  1.106 MASLIN     65 FIS 35                   5.83707E02     1.049 E
  1.107 SAPLAKOGLU59 FIS 35                    5.93171E02      .991 E
  1.108 WATANABE   64 FIS 41                   9.85451E02     4.569
  1.109 FRAYSSE    65 (39 FH1 39)÷34 FH1 35    1.24252E00     1.547 n⊃
  1.110 BORCEA     70 (39 FH1 39)÷34 FH1 35    1.25781E00     1.615 n⊃
  1.111 BOLDEMAN   77 NUB 52                   3.75491E00      .408 LYZC
  1.112 BOLDEMAN   80 (NUB 33)÷NUB 52         6.60490E-01      .172 HLMNUYZΔC
  1.113 BOLDEMAN   80 (NUB 35)÷NUB 52         6.43183E-01      .117 ILMNVYZΔC
  1.114 BOLDEMAN   80 (NUB 39)÷NUB 52         7.66143E-01      .159 JLMNWYZΔC
  1.115 BOLDEMAN   80 (NUB 41)÷NUB 52         7.80276E-01      .120 KLMNXYZΔC
  1.116 SPENCER    82 NUB 52                   3.78311E00      .185 LMOYZ
  1.117 GWIN       84 (NUB 33)÷NUB 52         6.59956E-01      .266 UYZA
  1.118 GWIN       84 (NUB 35)÷NUB 52         6.47006E-01      .208 VYZA
  1.119 GWIN       84 (NUB 39)÷NUB 52         7.65301E-01      .173 WYZA
  1.120 GWIN       84 (NUB 41)÷NUB 52         7.84231E-01      .222 XYZA
PF1=Hcpy 3=Reor 4=Resid 5=Recy 6=Fit 7=Err 8=ParIn 9=ParOut 10=Quit 11=↑ 12=↓
Global edit: nA,nD,or nR in Nr field   Indiv.edit: Cursor in ΔC field, ENTER
```

Fig. 2. Global edition of measurements

```
(NUB 33)÷NUB 52          1.112 BOLDEMAN  80
          ↓    ┌-------Cause of correlated error--------┐   ┌Rel.err.%-┐
          H    Energy Uncertainty of U233 Neutrons                  .074
          L    Energy Uncertainty of CF252 Neutrons                -.056
          M    Detector slope (Different Authors)                  -.033
          N    Boldeman Detector Slope                             -.104
          U    U233 Delayed Neutrons                                .009
          Y    CF252 Delayed Neutrons                              -.106
          Z    Delayed  Gamma-rays                                  .040
          Δ    Boldemans Foil Thickness corrections                 .024
          C    Boldeman Common Uncertainty                          .041

PF1=Hcpy  10=Quit  11=↑  12=↓
Input corr. uncert. by its code char. in  err. survey- Delete with /
in col 1
```

Fig. 3 Individual edition of measurements

```
PARIN: parameter input
     ┌-Param.-┐    ┌-Meaning--┐      ┌Guess value┐   ┌Variat.-┐
       GP[ 1]     ABS 33             5.76217E02      1.00E-04
       GP[ 2]     SCA 33             1.21865E01      1.00E-04
       GP[ 3]     FIS 33             5.30695E02      1.00E-04
       GP[ 4]     NUB 33             2.49497E00      1.00E-04
       GP[ 5]     ABS 35             6.81830E02      1.00E-04
       GP[ 6]     SCA 35             1.59833E01      1.00E-04
       GP[ 7]     FIS 35             5.82784E02      1.00E-04
       GP[ 8]     NUB 35             2.43336E00      1.00E-04
       GP[ 9]     ABS 39             1.01897E03      1.00E-04
       GP[10]     SCA 39             7.89726E00      1.00E-04
       GP[11]     FIS 39             7.47627E02      1.00E-04
       GP[12]     NUB 39             2.88217E00      1.00E-04
       GP[13]     ABS 41             1.37321E03      1.00E-04
       GP[14]     SCA 41             1.21877E01      1.00E-04
       GP[15]     FIS 41             1.01188E03      1.00E-04
       GP[16]     NUB 41             2.94627E00      1.00E-04
       GP[17]     HLF 33             1.59200E00      0.00E00
       GP[18]     WGA 33             9.99461E-01     1.00E-04
       GP[19]     WGF 33             9.95536E-01     1.00E-04
       GP[20]     SCR 33             1.09181E01      1.00E-04
PF1=Hcpy  3=Check  10=Quit  11=↑  12=↓
Editor commands in GP field :nA, nD or nR  -Confirm changes with ENTER
```

Fig. 4. Guess Parameter input

```
 GROUT 1: fitted par. in grp 1                          Error correlations %
 Param. ┌-Meaning--┐  Fitted value   Error %      1   2   3   4   5   6   7   8
 GP[ 1] ABS 33          5.76217E02      .226   1 100 -27  86 -16  27 -12  28  -7
 GP[ 2] SCA 33          1.21861E01     5.483   2 -27 100 -23   4  -7   3  -7   2
 GP[ 3] FIS 33          5.30695E02      .253   3  86 -23 100 -27  25 -11  28 -10
 GP[ 4] NUB 33          2.49497E00      .161   4 -16   4 -27 100  -7   3 -10  57
 GP[ 5] ABS 35          6.81830E02      .192   5  27  -7  25  -7 100 -46  82 -11
 GP[ 6] SCA 35          1.59828E01     6.914   6 -12   3 -11   3 -46 100 -38   5
 GP[ 7] FIS 35          5.82784E02      .196   7  28  -7  28 -10  82 -38 100 -22
 GP[ 8] NUB 35          2.43336E00      .147   8  -7   2 -10  57 -11   5 -22 100
 GP[ 9] ABS 39          1.01897E03      .282   9  14  -4  11  -1  29 -12  28  -2
 GP[10] SCA 39          7.89659E00    12.333  10  -1   0  -1   0  -3   2  -3   0
 GP[11] FIS 39          7.47624E02      .269  11  16  -4  18  -6  31 -13  36  -8
 GP[12] NUB 39          2.88217E00      .177  12  -6   2 -10  51  -6   3 -10  56
 GP[13] ABS 41          1.37320E03      .662  13   6  -2   4   0  10  -4   9   0
 GP[14] SCA 41          1.21878E01    21.470  14   0   0   0   0  -1   0  -1   0
 GP[15] FIS 41          1.01187E03      .652  15   6  -2   7  -3  10  -5  12  -4
 GP[16] NUB 41          2.94627E00      .196  16  -6   2 -10  47  -6   3 -10  51
 GP[18] WGA 33          9.99461E-01     .107  18 -21   6  -5  -9   5  -2   7  -4
 GP[19] WGF 33          9.95535E-01     .142  19 -20   5 -49   9   5  -2   2   4
 GP[20] SCR 33          1.09169E01     8.050  20 -36  72 -31   6 -10   4 -10   2
 GP[22] WGA 35          9.78926E-01     .084  22   5  -1   6  -4 -19   9  11  -1
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Position cursor on wanted group or corr origin, press ENTER to page/scroll
```

Fig. 5. Fitted Parameters output

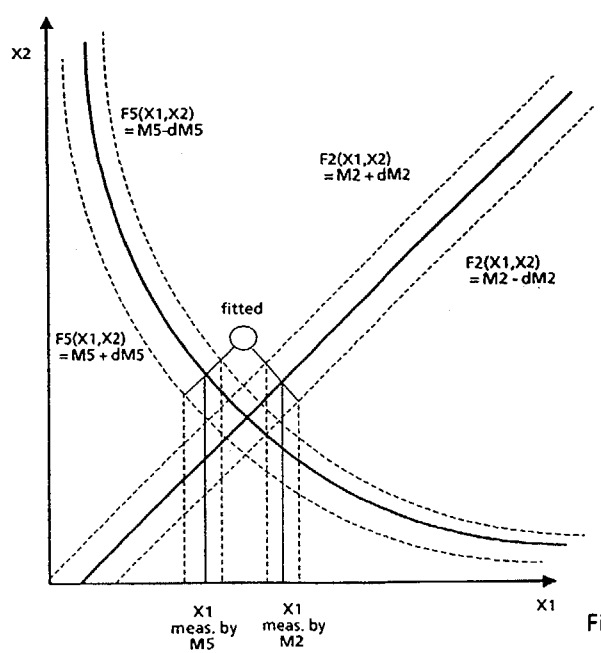

Fig 6. Inference method

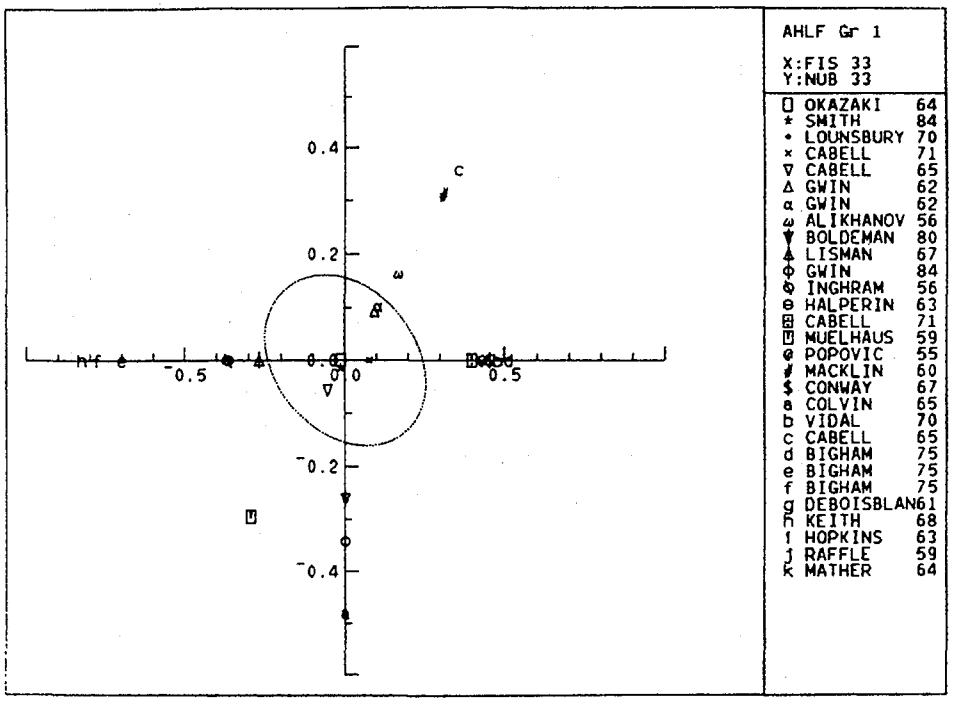

Fig. 7. Bi-parametric inference diagram

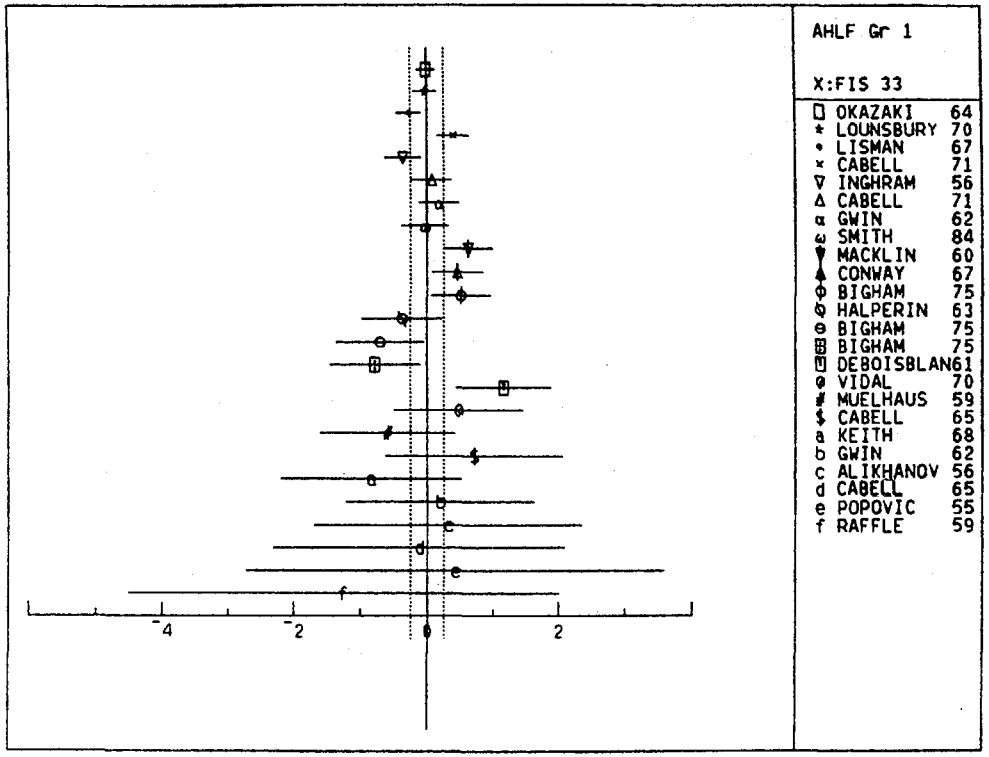

Fig. 8. Mono-parametric inference diagram

Covariances of Nuclear Model Parameters generated from Experimental Information

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Abstract

Bayesian method have been applied to estimate level density parameters and optical model parameters from experimental data of cross sections and emitted-particle spectra. The level density parameters for 17 nuclides and optical model parameters for n, p and α and their covariances have been obtained from 13 kinds of experimental data. The results of the estimated cross sections, parameters and covariances are presented.

1. Introduction

Nuclear-reaction model calculation in nuclear data evaluation has become more important in the high neutron energy region for which the nuclear data are required in fusion reactor development and application of spallation neutron sources, because the available experimental data in these energy region are scarce and their measurements sufficient to evaluate the required data are not expected in near future. Accordingly, the model calculation must be applied in the nuclear data evaluation. The reaction models which have been developed in nuclear physics are presently valid to certain extent if parameters in the model formulae are appropriately estimated.

Multi-step Hauser-Feshbach model is widely applied to calculate neutron reaction cross sections. In the model formulae, many parameters are included. They must be empirically determined so as to reproduce experimental data. The nuclear data evaluation by the model calculation is equivalent to the determination of the parameters in the formulae. It is very troublesome to estimate the appropriate parameters for the nuclides taking into account of calculation, since the numbers of the nuclides and parameters including in the calculation are large and these parameters are strongly correlated each other.

The authors have applied the Bayesian method to obtain the level density parameters for the residual nuclides in Ni(n,x) and Co(n,x) reactions. In this report, the covariances resulted from the parameter estimation [1,2,3] are presented.

2. Estimation of the Parameters

The formulae used in the present study are represented as,

$$p = p_0 + (F_0{}^t V^{-1} F_0 + X_0^{-1})^{-1} F_0{}^t V^{-1} (y - f(p_0)),$$

$$M = (F_0{}^t V^{-1} F_0 + X_0^{-1})^{-1},$$

$$F_0 = (Vf(p))^t{}_{p=p_0},$$

where p is the parameter vector to be estimated, y the experimental data vector, V the covariance matrix for the experimental data, f(p) the calculated value vector by a nuclear reaction model with the a priori parameter p_0, X_0 the covariance matrix of the a priori parameter p_0, and F_0 the sensitivity matrix of cross sections to the parameter p_0.

The nuclear reaction model used in this study is a multi-step Hauser-Feshbach model. The GNASH [4] was used to calculate the cross sections. The level density for the nuclides included in the multi-step reactions was represented by the Gilbert-Cameron's formula [5]. The initial values of the level density parameters were taken from are Gilbert-Cameron's work. The covariances for the experimental data were assumed that diagonal elements were equal to the errors given by the experimenters and off-diagonal elements were neglected. The diagonal elements of the covariances for a priori level density parameters were given to be 30% because their values shown in Gilbert-Cameron's report distributed within about 30% region. Their off-diagonal elements were assumed to be null because the data of level density in the report seemed to scatter like at random. Transmission coefficients were calculated by ELIESE-3 [6].

Three cases have been performed. The parameters to be estimated are,

(1) Level density parameters,

(2) Level density parameters and pairing energies,

(3) Level density parameters and optical parameters.

The experimental data were used in the estimation for every case.

The estimated parameters are listed as following.

Case 1 Level Density Parameters of 17 Nuclides,
$^{54,55}M$, $^{54-59}Fe$, $^{57-60}Co$ and $^{57-61}Ni$.

Case 2 Level Density Parameters of 17 Nuclides,
Pairing Energies of 17 Nuclides.
The nuclides are same as Case 1.

Case 3 Level Density Parameters of 17 Nuclides,
Optical Model Parameters for n,p and α.
The nuclides are same as Case 1.
n; r_0, V_0, r_s, W_{s1} (Surface potential)
p; r_0, V_0, r_s, W_{s1} (Surface potential)
α; r_0, V_0, r_s, W_{v1} (Volume potential)

The results of the case 3 are mainly discussed in this report.

A priori parameters of the optical model for n,p and α are taken from Becchetti-Greenlees [7], Menet et al. [8] and Huizenga-Igo [9], respectively.

The target nucleus and experiments used in the estimation are presented as following.

Target Nucleus	Experimental Data
^{60}Ni	σ(total)
^{58}Ni	σ(n,p), Spectra of p and α (En= 14.8 MeV)
^{59}Co	σ(total), σ(n,p), σ(n,α), σ(n,2n)

The sensitivities of the cross sections to the parameters were computed with changing them by 5%. The examples are shown in Figs.1, 2, and 3.

3. Results and discussion

The level density parameters of a priori and a posteriori values are shown in Fig.1 for Case 3.

The covariance matrices obtained for the case 1 and 3 are presented in Figs. 1 and 3, respectively. For the case 3, only a part of the level density is shown. The results depend naturally on the kind of number of the estimated parameters and the experiments used in the estimation. Generally speaking, however, common tendency in both the results. It is reasonable that correlation between the target and residual nuclide used in the estimation is large. There are large covariances else for target-residual-nuclides pairs far from the reactions whose experimental data were used in the estimation. It represents that the experiments for those reactions are very effective to determine the level density parameters relating nuclides. They are difficult reactions to measure their cross sections because target nuclides are unstable and/or reactions are multi-particle emission processes. In the present work, the reactions for Fe are not considered. Therefore, information for Fe is uncertain.

If the study is extend to neighboring nuclides, the knowledge on the level density parameters and optical model parameters to calculate the reaction cross sections and emitted-particle spectra is made certain and accurate results are expected. The covariances obtained in these procedures are suitable for representing correlation between calculations and experiments in evaluated nuclear data.

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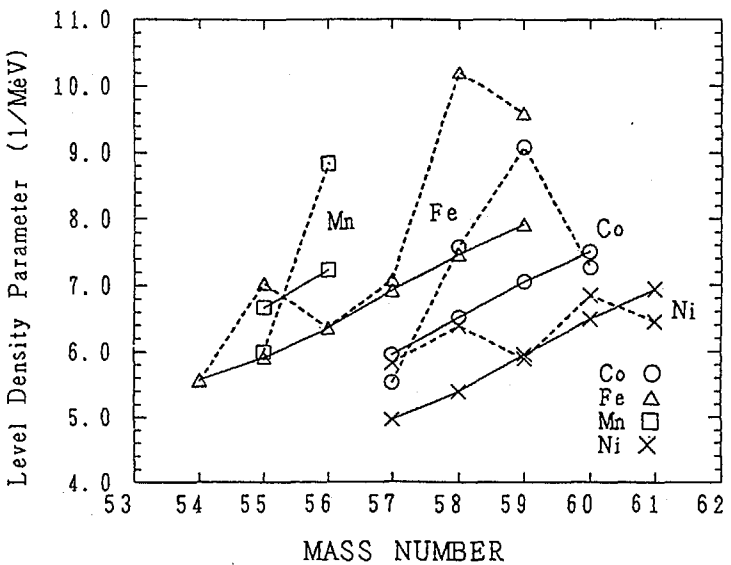

The level densities estimated in case 3. The solid lines are a priori data and the dotted lines a posteriori data.

Fig.1

Level Density Parameters

		^{55}Mn 1	^{56}Mn 2	^{54}Fe 3	^{55}Fe 4	^{56}Fe 5	^{57}Fe 6	^{58}Fe 7	^{59}Fe 8	^{57}Co 9	^{58}Co 10	^{59}Co 11	^{60}Co 12	^{57}Ni 13	^{58}Ni 14	^{59}Ni 15	^{60}Ni 16	^{61}Ni 17
^{55}Mn	1	1000																
^{56}Mn	2	1	1000															
^{54}Fe	3	0	0	1000														
^{55}Fe	4	0	28	0	1000													
^{56}Fe	5	0	0	0	0	1000												
^{57}Fe	6	0	-4	0	4	0	1000											
^{58}Fe	7	-50	-239	0	236	0	-7	1000										
^{59}Fe	8	1	835	0	44	0	-6	-347	1000									
^{57}Co	9	0	-5	-1	-77	0	-10	-43	-8	1000								
^{58}Co	10	0	29	0	976	0	4	241	46	-181	1000							
^{59}Co	11	0	930	0	25	0	-8	-222	865	-4	26	1000						
^{60}Co	12	0	-6	0	4	0	791	-10	-8	-9	4	-11	1000					
^{57}Ni	13	0	-3	13	-42	0	-8	-29	-5	914	-123	-3	-7	1000				
^{58}Ni	14	0	24	0	904	0	0	206	39	246	855	22	0	206	1000			
^{59}Ni	15	0	0	0	58	0	59	9	1	-168	41	0	45	-134	-29	1000		
^{60}Ni	16	0	-6	0	4	0	774	-9	-8	-7	3	-10	941	-6	0	45	1000	
^{61}Ni	17	0	0	0	0	0	-71	0	0	2	0	0	-47	2	0	-15	-194	1000

The covariances for the level density parameters evaluated in case 1.

Fig.2

Level Density Parameters and Optical Model Parameters

		^{55}Mn 1	^{56}Mn 2	^{54}Fe 3	^{55}Fe 4	^{56}Fe 5	^{57}Fe 6	^{58}Fe 7	^{59}Fe 8	^{57}Co 9	^{58}Co 10	^{59}Co 11	^{60}Co 12	^{57}Ni 13	^{58}Ni 14	^{59}Ni 15	^{60}Ni 16	^{61}Ni 17	ron 18	rsn 19	Von 20	Wsn 21	rop 22	rsp 23	Vop 24	Wsp 25	roα 26	rsα 27	Voα 28	Wsα 29
^{55}Mn	1	1000																											
^{56}Mn	2	10	1000																										
^{54}Fe	3	0	0	1000																									
^{55}Fe	4	-57	-203	0	1000																								
^{56}Fe	5	0	0	0	0	1000																							
^{57}Fe	6	-5	67	0	-179	0	1000																						
^{58}Fe	7	-109	-344	0	514	0	-88	1000																					
^{59}Fe	8	5	847	0	-143	0	218	-306	1000																				
^{57}Co	9	0	-18	1	-12	0	-153	56	21	1000																			
^{58}Co	10	0	-93	-80	949	0	-258	486	10	30	1000																		
^{59}Co	11	9	974	0	-231	0	87	-335	882	-25	-90	1000																	
^{60}Co	12	-4	271	0	-177	0	785	-90	571	-76	-135	343	1000																
^{57}Ni	13	0	7	31	-113	0	-63	-18	13	921	-80	-35	-35	1000															
^{58}Ni	14	1	-78	0	934	0	-153	454	1	-1	970	-66	-79	-87	1000														
^{59}Ni	15	2	30	-1	-57	0	128	-25	74	9	116	58	180	72	206	1000													
^{60}Ni	16	-4	267	0	-245	0	856	-155	463	-152	-255	335	930	-63	-140	173	1000												
^{61}Ni	17	0	24	0	60	0	-235	47	121	60	102	37	126	19	69	60	40	1000											
ron	18	-4	61	1	-71	0	-22	-7	-124	-34	-180	4	-211	36	-239	-355	-106	-165	1000										
rsn	19	4	-56	-1	69	0	19	12	125	39	177	0	205	-33	238	348	105	163	-997	1000									
Von	20	4	-66	-1	73	0	24	1	122	29	184	-10	216	-38	239	362	105	167	-995	989	1000								
Wsn	21	-4	100	1	-79	0	-41	47	-96	16	-192	54	233	54	-215	-375	-95	-164	859	-837	-886	1000							
rop	22	-1	48	0	-170	0	48	-103	-50	-114	-273	32	-123	-34	-231	-222	0	-237	418	-410	-426	436	1000						
rsp	23	0	40	0	-89	0	242	-61	-54	-97	-83	42	158	-40	-30	241	260	43	126	-127	-123	93	-636	1000					
Vop	24	2	-14	0	80	0	329	-92	-58	-30	-18	18	211	9	103	-109	362	-27	-281	278	238	-271	-320	392	1000				
Wsp	25	0	0	0	-3	0	-7	0	4	-9	-3	0	2	-2	8	32	-4	17	-9	9	10	-11	-48	-191	11	1000			
roα	26	3	421	0	-139	0	-133	-149	425	-26	-7	533	65	0	0	-35	89	-19	161	-158	-164	164	120	-1	-27	-3	1000		
rsα	27	1	12	0	-67	0	159	-64	-104	11	-165	-120	15	17	-171	28	13	6	-8	8	8	-9	-51	66	-18	4	-650	1000	
Voα	28	0	-16	0	-1	0	-17	5	0	-3	11	1	-1	-2	12	0	0	-1	5	-5	-5	4	3	0	2	0	-477	-4	1000	
Wsα	29	0	1	0	-5	0	12	-5	-7	0	-12	-9	1	1	-13	2	1	0	0	0	0	0	-4	5	-1	0	-42	-63	0	1000

Fig.3 The covariances for the parameters estimated in case 3.

USE OF COVARIANCE INFORMATIONS FOR INTEGRAL EXPERIMENT PLANNING

by

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INTRODUCTION

The present note describes briefly the application of basic data covariance matrix informations to the optimization of integral experiments, in order to reduce design parameter uncertainties.

In planning an integral experiment, the main guideline is to set-up an experiment that will be useful to reduce the uncertainty in the calculation of a specific design parameter (e.g. the reactivity worth of the control-rods).

The first step is then to assess the a-priori uncertainty of the chosen design parameter. Standard sensitivity profile calculations and use of data covariance matrices allow to obtain that information.

Since most integral experiments cannot simulate exactly the reference system under study, there is the need to verify that the planned integral experiment is "representative" of the reference situation.

Intuitively, a sensitivity analysis will be the most suited tool. In fact, even the qualitative inspection of the relevant sensitivity profiles, will help to understand if unknown error in the nuclear data will have the same effects in the integral experiment and in the reference system. In that case, using the same calculation tools both in the experiment analysis and in design, one can apply as "bias factor" to the design calculation, i.e. the Calculation-Experiment value obtained from the experiment and one can apply as residual uncertainty, the experimental uncertainty on the integral quantity measurement.

This is obviously an idealized situation. Sensitivity profiles may differ for some cross-section type and it is generally difficult to established quantitative rules to define bias factors and uncertainties only on a qualitative basis. L.N. USACHEV has developed a simple algorithm [1], that we have already applied in a general study on experiment planning [2], which allows to define a "representativeness" parameter "r" defined as :

$$r = \frac{S_R^+ D S_E}{[(S_R^+ D S_R)\,(S_E^+ D S_E)]^{1/2}} \qquad (1)$$

where S_R and S_E are the sensitivity vectors related both to the reference system and to the experiment.
D is the basic data dispersion matrix.

In Reference [1], it is shown that the dispersion ΔR_1^2 on the parameter R is reduced after having performed the experiment in the following way :

$$\Delta R_1^2 = \Delta R_0^2 (1 - r^2) \qquad (2)$$

where ΔR_0^2 is the dispersion before running the experiment (and then due to the a-priori basic data uncertainty estimation).

It is clear that the best result is obtained when $r \to 1$, which means that the two vectors S_R and S_E should be as close as possible.

COVARIANCE DATA INFLUENCE ON EXPERIMENT REPRESENTATIVENESS

We have applied the method previously presented to a practical situation.

We considered as reference system a SUPER-PHENIX 1 type reactor with two control-rod rings, and as experiment the RACINE-1E configuration [3], also with two rod rings.

The integral parameters considered were the control-rod reactivity worths of :

- inner ring completely inserted, ρ_1 ;
- outer ring completely inserted, ρ_2 ;
- both rings completely inserted $\rho_1 + \rho_2$.

We considered a six-group energy structure and the cross-section data uncertainties given in Table 1. The first hypothesis was to use these data without any correlation (i.e. a diagonal D matrix).

The results of the uncertainty analysis, namely the standard deviations for the integral parameters R defined as :

$$\Delta R = (S^{+} D S)^{1/2} \qquad (3)$$

are shown in Tables II-VII.

The second hypothesis was to introduce cross-sections correlations both in energy, and among cross-sections of the same isotope. The values of the off-diagonal elements of D are given in Table VIII.

In Table IX, we give the results, both with and without correlations for the following quantities :

- total uncertainty on R (standard deviation) both for the reference system and the experiment ;
- the values of the "r" parameter (called "correlation between system and experiment"), equation (1) ;
- the reduced uncertainty in the prediction of the integral parameter R, according to equation (2).

DISCUSSION AND CONCLUSIONS

The impact of the introduction of the correlations is not negligeable, even if we have considered only a limited number of them. It is then evident that appropriate estimates of the dispersion matrices should be used to properly assess the interest of a specific series of experiments. A substantial reduction of uncertainty can justify an experiment, only if reliable uncertainty data are used. It is also evident that for this type of study, only simple, broad group averaged data, easy to handle, are useful.

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TABLE 1

THE FOLLOWING UNCERTAINTIES WILL BE USED

COMPONENT : U-235

GROUP	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.
1	1.00000E-01	4.00000E-02	5.00000E-03	5.00000E-02	1.00000E-01	1.50000E-01
2	1.00000E-01	4.00000E-02	5.00000E-03	5.00000E-02	1.00000E-01	1.50000E-01
3	1.00000E-01	4.00000E-02	5.00000E-03	5.00000E-02	1.00000E-01	1.50000E-01
4	1.00000E-01	4.00000E-02	5.00000E-03	5.00000E-02	1.00000E-01	1.50000E-01
5	1.00000E-01	4.00000E-02	5.00000E-03	5.00000E-02	1.00000E-01	1.50000E-01
6	1.00000E-01	4.00000E-02	5.00000E-03	5.00000E-02	1.00000E-01	1.50000E-01

COMPONENT : U-238

GROUP	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.
1	5.00000E-02	8.00000E-02	1.00000E-02	5.00000E-02	1.00000E-01	1.00000E-01
2	5.00000E-02	8.00000E-02	1.00000E-02	5.00000E-02	1.00000E-01	1.00000E-01
3	5.00000E-02	8.00000E-02	1.00000E-02	5.00000E-02	1.00000E-01	1.00000E-01
4	5.00000E-02	8.00000E-02	1.00000E-02	5.00000E-02	1.00000E-01	1.00000E-01
5	1.00000E-01	8.00000E-02	1.00000E-02	5.00000E-02	1.00000E-01	1.00000E-01
6	1.00000E-01	8.00000E-02	1.00000E-02	5.00000E-02	1.00000E-01	1.00000E-01

COMPONENT : PU-239

GROUP	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.
1	1.00000E-01	5.00000E-02	1.00000E-02	5.00000E-02	1.00000E-01	2.00000E-01
2	1.00000E-01	5.00000E-02	1.00000E-02	5.00000E-02	1.00000E-01	2.00000E-01
3	1.00000E-01	5.00000E-02	1.00000E-02	5.00000E-02	1.00000E-01	2.00000E-01
4	1.00000E-01	5.00000E-02	1.00000E-02	5.00000E-02	1.00000E-01	2.00000E-01
5	1.00000E-01	5.00000E-02	1.00000E-02	5.00000E-02	1.00000E-01	2.00000E-01
6	1.00000E-01	5.00000E-02	1.00000E-02	5.00000E-02	1.00000E-01	2.00000E-01

COMPONENT : PU-240

GROUP	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.
1	2.00000E-01	1.50000E-01	4.00000E-02	1.00000E-01	1.00000E-01	5.00000E-01
2	2.00000E-01	1.50000E-01	4.00000E-02	1.00000E-01	1.00000E-01	5.00000E-01
3	2.00000E-01	1.50000E-01	4.00000E-02	1.00000E-01	1.00000E-01	5.00000E-01
4	2.00000E-01	1.50000E-01	4.00000E-02	1.00000E-01	1.00000E-01	5.00000E-01
5	2.00000E-01	1.50000E-01	4.00000E-02	1.00000E-01	1.00000E-01	5.00000E-01
6	2.00000E-01	1.50000E-01	4.00000E-02	1.00000E-01	1.00000E-01	5.00000E-01

COMPONENT : PU-241

GROUP	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.
1	2.00000E-01	2.00000E-01	4.00000E-02	1.00000E-01	1.00000E-01	5.00000E-01
2	2.00000E-01	2.00000E-01	4.00000E-02	1.00000E-01	1.00000E-01	5.00000E-01
3	2.00000E-01	2.00000E-01	4.00000E-02	1.00000E-01	1.00000E-01	5.00000E-01
4	2.00000E-01	2.00000E-01	4.00000E-02	1.00000E-01	1.00000E-01	5.00000E-01
5	2.00000E-01	2.00000E-01	4.00000E-02	1.00000E-01	1.00000E-01	5.00000E-01
6	2.00000E-01	2.00000E-01	4.00000E-02	1.00000E-01	1.00000E-01	5.00000E-01

TABLE 1 (follows)

COMPONENT : FE

GROUP	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.
1	2.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	1.50000E-01
2	2.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	1.50000E-01
3	2.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	1.50000E-01
4	2.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	1.50000E-01
5	2.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	1.50000E-01
6	2.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	1.50000E-01

COMPONENT : CR

GROUP	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.
1	3.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	3.00000E-01
2	3.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	3.00000E-01
3	3.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	3.00000E-01
4	3.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	3.00000E-01
5	3.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	3.00000E-01
6	3.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	3.00000E-01

COMPONENT : NI

GROUP	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.
1	3.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	3.00000E-01
2	3.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	3.00000E-01
3	3.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	3.00000E-01
4	3.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	3.00000E-01
5	3.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	3.00000E-01
6	3.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	3.00000E-01

COMPONENT : OX

GROUP	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.
1	2.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	2.00000E-01
2	2.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	2.00000E-01
3	2.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	2.00000E-01
4	2.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	2.00000E-01
5	2.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	2.00000E-01
6	2.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	2.00000E-01

COMPONENT : NA

GROUP	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.
1	2.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	2.00000E-01
2	2.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	2.00000E-01
3	2.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	2.00000E-01
4	2.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	2.00000E-01
5	2.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	2.00000E-01
6	2.00000E-01	0.0	0.0	1.00000E-01	1.00000E-01	2.00000E-01

TABLE II

UNCERTAINTY ANALYSIS FOR A REFERENCE SYSTEM (SUPER-PHENIX 1 TYPE)
CASE OF THE INNER ROD RING WORTH

SUMMARY BY COMPONENT FOR UNCERTAINTY ON SYSTEM

COMPON.	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.	TOTAL
U-235	2.91 E-4*	3.28 E-4	1.46 E-4	6.20 E-5	5.02 E-6	2.19 E-5	4.67 E-4
U-238	2.15 E-2	8.66 E-4	2.66 E-4	1.19 E-2	1.04 E-3	2.17 E-3	2.47 E-2
Pu-239	3.82 E-3	5.92 E-3	4.98 E-3	3.14 E-3	1.29 E-4	1.41 E-3	9.29 E-3
Pu-240	1.69 E-3	2.51 E-3	2.08 E-3	1.62 E-3	4.06 E-5	7.32 E-4	4.08 E-3
Pu-241	2.09 E-4	9.46 E-4	1.04 E-3	2.18 E-4	4.38 E-6	1.16 E-4	1.44 E-3
FE	2.41 E-3	0.0	0.0	1.95 E-2	3.86 E-3	1.96 E-3	2.01 E-2
CR	1.47 E-3	0.0	0.0	6.39 E-3	5.93 E-4	5.22 E-4	6.60 E-3
NI	1.65 E-3	0.0	0.0	7.85 E-3	1.28 E-3	2.81 E-4	8.13 E-3
OX	2.99 E-4	0.0	0.0	2.51 E-2	1.15 E-2	9.91 E-6	2.77 E-2
NA	6.15 E-4	0.0	0.0	1.32 E-2	4.58 E-3	1.54 E-3	1.41 E-2
TOTAL	2.22 E-2	6.56 E-3	5.51 E-3	3.80 E-2	1.31 E-2	3.72 E-3	4.69 E-2

* E-4 = 10^{-4}

COMPONENT : U-238 SUMMARY BY GROUP FOR UNCERTAINTY ON SYSTEM

GROUP	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC.	INELAS.	TOTAL
1	5.33 E-5*	8.65 E-4	2.66 E-4	3.62 E-3	1.94 E-5	1.31 E-3	3.96 E-3
2	4.06 E-4	3.98 E-5	1.00 E-5	4.26 E-3	1.41 E-4	1.45 E-3	4.52 E-3
3	5.83 E-3	0.0	0.0	1.01 E-2	1.03 E-3	9.44 E-4	1.17 E-2
4	6.31 E-3	0.0	0.0	2.69 E-3	7.60 E-5	0.0	6.86 E-3
5	1.96 E-2	0.0	0.0	8.76 E-4	2.60 E-5	0.0	1.96 E-2
6	2.37 E-3	0.0	0.0	2.54 E-4	0.0	0.0	2.39 E-3
TOTAL	2.15 E-2	8.66 E-4	2.66 E-4	1.19 E-2	1.04 E-3	2.17 E-3	2.47 E-2

* E-5 = 10^{-5}

COMPONENT : Pu-239 SUMMARY BY GROUP FOR UNCERTAINTY ON SYSTEM

GROUP	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC.	INELAS.	TOTAL
1	1.93 E-5*	3.37 E-3	1.99 E-3	1.44 E-3	1.03 E-5	1.36 E-3	4.39 E-3
2	3.27 E-4	3.19 E-3	2.10 E-3	1.26 E-3	1.27 E-5	1.93 E-4	4.04 E-3
3	7.46 E-4	2.65 E-3	1.21 E-3	2.44 E-3	1.23 E-4	2.56 E-4	3.89 E-3
4	2.77 E-4	2.12 E-4	1.22 E-3	4.02 E-4	3.56 E-5	1.38 E-4	1.34 E-3
5	3.41 E-3	2.34 E-3	3.59 E-3	1.10 E-4	7.19 E-6	0.0	5.48 E-3
6	1.50 E-3	9.31 E-4	7.68 E-4	1.67 E-5	0.0	0.0	1.92 E-3
TOTAL	3.82 E-3	5.92 E-3	4.98 E-3	3.14 E-3	1.29 E-4	1.41 E-3	9.29 E-3

* E-5 = 10^{-5}

TABLE III

UNCERTAINTY ANALYSIS FOR AN INTEGRAL EXPERIMENT (RACINE TYPE)
CASE OF THE INNER ROD RING WORTH

SUMMARY BY COMPONENT FOR UNCERTAINTY ON EXPERIMENT

COMPON.	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.	TOTAL
U-235	5.96 E-3*	8.39 E-3	2.93 E-3	1.42 E-3	3.67 E-5	1.50 E-3	1.10 E-2
U-238	2.37 E-2	3.03 E-3	9.14 E-4	5.65 E-3	2.01 E-4	7.41 E-3	2.57 E-2
Pu-239	9.28 E-3	8.35 E-3	5.66 E-3	1.00 E-3	4.41 E-5	4.02 E-4	1.37 E-2
Pu-240	3.93 E-3	3.53 E-4	2.93 E-4	4.63 E-4	1.24 E-5	1.93 E-4	3.99 E-3
Pu-241	6.77 E-4	2.32 E-3	1.62 E-3	8.17 E-5	1.72 E-6	3.69 E-5	2.91 E-3
FE	1.85 E-3	0.0	0.0	7.27 E-3	9.52 E-4	4.77 E-3	8.94 E-3
CR	1.04 E-3	0.0	0.0	2.39 E-3	2.04 E-4	2.14 E-3	3.38 E-3
NI	1.04 E-3	0.0	0.0	2.07 E-3	2.50 E-4	1.00 E-3	2.54 E-3
OX	6.04 E-5	0.0	0.0	1.20 E-2	6.34 E-3	1.13 E-5	1.36 E-2
NA	9.78 E-4	0.0	0.0	8.94 E-3	3.00 E-3	1.54 E-3	9.61 E-3
TOTAL	2.66 E-2	1.25 E-2	6.65 E-3	1.79 E-2	7.09 E-3	9.39 E-3	3.70 E-2

* E-3 = 10^{-3}

COMPONENT : U-238 SUMMARY BY GROUP FOR UNCERTAINTY ON EXPERIMENT

GROUP	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.	TOTAL
1	2.17 E-4*	3.03 E-3	9.13 E-4	2.15 E-3	7.46 E-5	7.40 E-3	8.33 E-3
2	8.68 E-4	1.02 E-4	4.96 E-5	2.87 E-3	3.29 E-5	2.44 E-4	3.01 E-3
3	1.24 E-3	0.0	0.0	4.36 E-3	1.76 E-4	2.59 E-4	4.54 E-3
4	6.02 E-3	0.0	0.0	1.67 E-4	3.67 E-5	0.0	6.02 E-3
5	2.22 E-2	0.0	0.0	3.38 E-5	3.77 E-5	0.0	2.22 E-2
6	5.56 E-3	0.0	0.0	7.38 E-5	0.0	0.0	5.56 E-3
TOTAL	2.37 E-2	3.03 E-3	9.14 E-4	5.65 E-3	2.01 E-4	7.41 E-3	2.57 E-2

* E-4 = 10^{-4}

COMPONENT : Pu-239 SUMMARY BY GROUP FOR UNCERTAINTY ON EXPERIMENT

GROUP	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.	TOTAL
1	1.26 E-8*	2.73 E-6	4.33 E-5	7.97 E-4	2.79 E-6	3.90 E-4	8.88 E-4
2	4.13 E-5	3.94 E-4	1.60 E-4	2.22 E-4	6.73 E-7	7.63 E-6	4.82 E-4
3	1.66 E-3	4.93 E-3	3.07 E-3	1.15 E-4	4.32 E-5	9.75 E-5	6.05 E-3
4	3.23 E-3	3.04 E-3	2.28 E-3	3.85 E-4	4.93 E-6	1.95 E-5	5.00 E-3
5	7.90 E-3	5.63 E-3	3.99 E-3	2.81 E-4	6.81 E-6	0.0	1.04 E-2
6	3.23 E-3	2.06 E-3	1.19 E-3	2.91 E-4	0.0	0.0	4.02 E-3
TOTAL	9.28 E-3	8.35 E-3	5.66 E-3	1.00 E-3	4.41 E-5	4.02 E-4	1.37 E-2

* E-8 = 10^{-8}

TABLE IV

UNCERTAINTY ANALYSIS FOR A RERFERENCE SYSTEM (SUPER-PHENIX 1 TYPE)
CASE OF THE OUTER ROD RING WORTH

SUMMARY BY COMPONENT FOR UNCERTAINTY ON SYSTEM

COMPON.	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.	TOTAL
U-235	1.56 E-4*	1.79 E-4	5.91 E-5	2.83 E-5	1.06 E-6	4.52 E-5	2.51 E-4
U-238	1.20 E-2	4.40 E-3	1.31 E-3	6.85 E-3	3.70 E-4	7.80 E-3	1.65 E-2
Pu-239	1.87 E-3	2.98 E-3	1.36 E-3	5.13 E-4	3.77 E-5	5.60 E-4	3.85 E-3
Pu-240	8.54 E-4	4.66 E-4	3.22 E-4	2.65 E-4	1.16 E-5	2.73 E-4	1.09 E-3
Pu-241	1.05 E-4	5.47 E-4	2.45 E-4	3.69 E-5	1.25 E-6	4.12 E-5	6.11 E-4
FE	1.30 E-3	0.0	0.0	7.15 E-3	1.09 E-3	7.13 E-3	1.02 E-2
CR	7.90 E-4	0.0	0.0	2.32 E-3	4.35 E-4	3.39 E-3	4.20 E-3
NI	1.56 E-3	0.0	0.0	3.57 E-3	3.21 E-4	1.98 E-3	4.38 E-3
OX	4.34 E-4	0.0	0.0	1.06 E-2	4.50 E-3	2.57 E-5	1.16 E-2
NA	3.33 E-4	0.0	0.0	4.71 E-3	1.26 E-3	2.19 E-3	5.36 E-3
TOTAL	1.24 E-2	5.37 E-3	1.93 E-3	1.59 E-2	4.85 E-3	1.15 E-2	2.44 E-2

* E-4 = 10^{-4}

COMPONENT : U-238 SUMMARY BY GROUP FOR UNCERTAINTY ON SYSTEM

GROUP	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.	TOTAL
1	3.13 E-4*	4.40 E-3	1.31 E-3	2.49 E-3	7.39 E-5	7.79 E-3	9.39 E-3
2	9.91 E-4	1.11 E-4	4.60 E-5	2.22 E-3	3.91 E-5	3.70 E-4	2.46 E-3
3	2.92 E-3	0.0	0.0	5.70 E-3	2.51 E-4	2.25 E-4	6.41 E-3
4	3.43 E-3	0.0	0.0	1.71 E-3	2.57 E-4	0.0	3.84 E-3
5	1.10 E-2	0.0	0.0	6.35 E-4	2.29 E-5	0.0	1.10 E-2
6	1.36 E-3	0.0	0.0	5.63 E-5	0.0	0.0	1.37 E-3
TOTAL	1.20 E-2	4.40 E-3	1.31 E-3	6.85 E-3	3.70 E-4	7.80 E-3	1.65 E-2

* E-4 = 10^{-4}

COMPONENT : Pu-239 SUMMARY BY GROUP FOR UNCERTAINTY ON SYSTEM

GROUP	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.	TOTAL
1	1.60 E-6*	2.96 E-4	2.56 E-4	1.81 E-4	4.25 E-6	5.51 E-4	7.00 E-4
2	7.34 E-5	7.70 E-4	3.08 E-4	7.34 E-5	8.86 E-7	4.45 E-6	8.36 E-4
3	7.97 E-4	2.61 E-3	1.20 E-3	3.55 E-4	3.34 E-5	8.31 E-5	3.01 E-3
4	1.61 E-4	1.73 E-4	2.16 E-4	2.70 E-4	1.55 E-5	5.49 E-5	4.23 E-4
5	1.50 E-3	1.05 E-3	3.72 E-4	1.45 E-4	7.07 E-6	0.0	1.88 E-3
6	7.56 E-4	4.82 E-4	2.10 E-4	6.51 E-5	0.0	0.0	9.24 E-4
TOTAL	1.87 E-3	2.98 E-3	1.36 E-3	5.13 E-4	3.77 E-5	5.60 E-4	3.85 E-3

* E-6 = 10^{-6}

TABLE V

UNCERTAINTY ANALYSIS FOR AN INTEGRAL EXPERIMENT (RACINE TYPE)
CASE OF THE OUTER ROD RING WORTH

SUMMARY BY COMPONENT FOR UNCERTAINTY ON EXPERIMENT

COMPON.	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.	TOTAL
U-235	2.60 E-3*	3.84 E-3	1.35 E-3	9.58 E-4	2.99 E-5	1.01 E-3	5.03 E-3
U-238	1.02 E-2	4.25 E-3	1.22 E-3	1.20 E-3	2.90 E-4	1.21 E-2	1.65 E-2
Pu-239	6.29 E-3	6.62 E-3	3.16 E-3	6.30 E-4	3.50 E-5	1.53 E-3	9.81 E-3
Pu-240	2.71 E-3	3.32 E-4	1.76 E-4	2.95 E-4	9.58 E-6	5.95 E-4	2.81 E-3
Pu-241	4.55 E-4	1.75 E-3	8.78 E-4	5.15 E-5	1.36 E-6	1.64 E-4	2.02 E-3
FE	8.53 E-4	0.0	0.0	2.50 E-3	5.83 E-4	6.60 E-3	7.14 E-3
CR	5.20 E-4	0.0	0.0	8.09 E-4	2.25 E-4	3.27 E-3	3.42 E-3
NI	8.37 E-4	0.0	0.0	7.41 E-4	1.51 E-4	1.41 E-3	1.80 E-3
OX	2.77 E-4	0.0	0.0	2.59 E-3	4.34 E-3	3.10 E-5	5.07 E-3
NA	4.75 E-4	0.0	0.0	2.57 E-3	1.76 E-3	3.74 E-3	4.89 E-3
TOTAL	1.27 E-2	8.93 E-3	3.75 E-3	4.86 E-3	4.74 E-3	1.48 E-2	2.28 E-2

* E-3 = 10^{-3}

COMPONENT : U-238 SUMMARY BY GROUP FOR UNCERTAINTY ON EXPERIMENT

GROUP	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.	TOTAL
1	3.05 E-4*	4.24 E-3	1.22 E-3	8.16 E-4	1.07 E-4	1.20 E-2	1.28 E-2
2	9.32 E-4	1.00 E-4	5.14 E-5	6.55 E-4	1.69 E-4	1.61 E-3	1.98 E-3
3	2.68 E-4	0.0	0.0	5.47 E-4	2.05 E-4	1.42 E-4	6.58 E-4
4	2.80 E-3	0.0	0.0	2.13 E-4	4.12 E-5	0.0	2.81 E-3
5	9.66 E-3	0.0	0.0	2.81 E-5	8.30 E-6	0.0	9.66 E-3
6	1.83 E-3	0.0	0.0	1.09 E-5	0.0	0.0	1.83 E-3
TOTAL	1.02 E-2	4.25 E-3	1.22 E-3	1.20 E-3	2.90 E-4	1.21 E-2	1.65 E-2

* E-4 = 10^{-4}

COMPONENT : Pu-239 SUMMARY BY GROUP FOR UNCERTAINTY ON EXPERIMENT

GROUP	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.	TOTAL
1	1.57 E-6*	2.79 E-4	3.98 E-5	1.84 E-4	7.25 E-6	1.47 E-3	1.51 E-3
2	2.37 E-5	2.27 E-4	4.50 E-5	1.51 E-4	2.37 E-5	4.02 E-4	4.89 E-4
3	1.58 E-3	4.72 E-3	2.06 E-3	5.75 E-4	2.35 E-5	5.29 E-5	5.43 E-3
4	2.65 E-3	2.50 E-3	1.19 E-3	4.86 E-5	6.37 E-6	2.52 E-5	3.83 E-3
5	5.24 E-3	3.75 E-3	2.00 E-3	3.95 E-5	3.88 E-6	0.0	6.75 E-3
6	1.58 E-3	1.01 E-3	5.37 E-4	7.75 E-5	0.0	0.0	1.95 E-3
TOTAL	6.29 E-3	6.62 E-3	3.16 E-3	6.30 E-4	3.50 E-5	1.53 E-3	9.81 E-3

* E-6 = 10^{-6}

TABLE VI

UNCERTAINTY ANALYSIS FOR A REFERENCE SYSTEM (SUPER-PHENIX TYPE)
CASE OF BOTH ROD RINGS WORTH

SUMMARY BY COMPONENT FOR UNCERTAINTY ON SYSTEM

COMPON.	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.	TOTAL
U-235	5.24 E-5*	6.26 E-5	3.00 E-5	4.99 E-5	1.67 E-6	4.67 E-5	1.10 E-4
U-238	4.37 E-3	3.86 E-3	1.09 E-3	1.03 E-2	4.10 E-4	8.82 E-3	1.48 E-2
Pu-239	2.19 E-3	2.56 E-3	2.05 E-3	1.69 E-3	5.75 E-5	1.56 E-3	4.57 E-3
Pu-240	1.03 E-3	8.98 E-4	7.43 E-4	8.74 E-4	1.78 E-5	7.03 E-4	1.92 E-3
Pu-241	1.30 E-4	5.11 E-4	4.72 E-4	1.20 E-4	1.92 E-6	1.14 E-4	7.27 E-4
FE	5.35 E-4	0.0	0.0	1.40 E-2	1.50 E-3	7.89 E-3	1.61 E-2
CR	3.52 E-4	0.0	0.0	4.53 E-3	4.57 E-4	3.80 E-3	5.94 E-3
NI	1.32 E-3	0.0	0.0	6.86 E-3	4.78 E-4	2.23 E-3	7.35 E-3
OX	4.79 E-4	0.0	0.0	1.90 E-2	5.54 E-3	3.17 E-5	1.98 E-2
NA	1.43 E-4	0.0	0.0	9.23 E-3	1.80 E-3	2.47 E-3	9.73 E-3
TOTAL	5.24 E-3	4.74 E-3	2.49 E-3	2.86 E-2	6.07 E-3	1.29 E-2	3.29 E-2

* E-5 = 10^{-5}

COMPONENT : U-238 SUMMARY BY GROUP FOR UNCERTAINTY ON SYSTEM

GROUP	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.	TOTAL
1	2.70 E-4*	3.86 E-3	1.09 E-3	2.15 E-3	8.03 E-5	8.78 E-3	9.89 E-3
2	6.32 E-4	7.31 E-5	3.47 E-5	2.60 E-3	8.26 E-5	7.92 E-4	2.80 E-3
3	5.18 E-4	0.0	0.0	9.10 E-3	3.38 E-4	3.20 E-4	9.13 E-3
4	1.36 E-3	0.0	0.0	3.36 E-3	2.00 E-4	0.0	3.63 E-3
5	3.99 E-3	0.0	0.0	1.33 E-3	3.64 E-6	0.0	4.21 E-3
6	7.91 E-4	0.0	0.0	4.15 E-4	0.0	0.0	8.93 E-4
TOTAL	4.37 E-3	3.86 E-3	1.09 E-3	1.03 E-2	4.10 E-4	8.82 E-3	1.48 E-2

* E-4 = 10^{-4}

COMPONENT : Pu-239 SUMMARY BY GROUP FOR UNCERTAINTY ON SYSTEM

GROUP	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.	TOTAL
1	7.81 E-6*	1.35 E-3	6.93 E-4	4.08 E-4	9.99 E-6	1.55 E-3	2.21 E-3
2	9.91 E-5	9.25 E-4	8.08 E-4	4.24 E-4	9.59 E-6	1.59 E-4	1.31 E-3
3	3.94 E-4	1.16 E-3	6.02 E-5	1.46 E-3	4.91 E-5	1.10 E-4	1.91 E-3
4	8.96 E-4	8.36 E-4	7.52 E-4	5.27 E-4	2.64 E-5	9.91 E-5	1.53 E-3
5	1.85 E-3	1.28 E-3	1.55 E-3	2.48 E-4	1.23 E-6	0.0	2.75 E-3
6	6.55 E-4	3.99 E-4	3.29 E-4	1.44 E-4	0.0	0.0	8.47 E-4
TOTAL	2.19 E-3	2.56 E-3	2.05 E-3	1.69 E-3	5.75 E-5	1.96 E-3	4.57 E-3

* E-6 = 10^{-6}

TABLE VII

UNCERTAINTY ANALYSIS FOR AN INTEGRAL EPERIMENT (RACINE TYPE)
CASE OF BOTH ROD RINGS WORTH

SUMMARY BY COMPONENT FOR UNCERTAINTY ON EXPERIMENT

COMPON.	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.	TOTAL
U-235	3.79 E-3*	5.53 E-3	1.91 E-3	1.21 E-3	3.58 E-5	1.25 E-3	7.19 E-3
U-238	1.34 E-2	3.94 E-3	1.14 E-3	2.10 E-3	1.88 E-4	1.08 E-2	1.78 E-2
Pu-239	7.09 E-3	7.26 E-3	3.99 E-3	6.72 E-4	2.11 E-5	1.11 E-3	1.09 E-2
Pu-240	3.04 E-3	3.57 E-4	2.36 E-4	3.13 E-4	5.56 E-6	4.33 E-4	3.11 E-3
Pu-241	5.14 E-4	1.94 E-3	1.11 E-3	5.41 E-5	8.05 E-7	1.16 E-4	2.29 E-3
FE	1.08 E-3	0.0	0.0	4.07 E-3	4.85 E-4	6.12 E-3	7.45 E-3
CR	6.35 E-4	0.0	0.0	1.33 E-3	1.89 E-4	2.95 E-3	3.30 E-3
NI	9.03 E-4	0.0	0.0	1.18 E-3	1.49 E-4	1.30 E-3	1.99 E-3
OX	1.86 E-4	0.0	0.0	5.02 E-3	3.18 E-3	2.40 E-5	5.94 E-3
NA	5.98 E-4	0.0	0.0	4.41 E-3	1.36 E-3	2.85 E-3	5.47 E-3
TOTAL	1.60 E-2	1.01 E-2	4.71 E-3	8.42 E-3	3.51 E-3	1.32 E-2	2.53 E-2

* E-3 = 10^{-3}

COMPONENT : U-238 SUMMARY BY GROUP FOR UNCERTAINTY ON EXPERIMENT

GROUP	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.	TOTAL
1	2.84 E-4*	3.94 E-3	1.14 E-3	7.86 E-5	1.00 E-4	1.07 E-2	1.15 E-2
2	9.51 E-4	1.03 E-4	5.24 E-5	1.36 E-3	1.19 E-4	1.12 E-3	2.01 E-3
3	2.70 E-4	0.0	0.0	1.59 E-3	1.02 E-4	2.93 E-5	1.61 E-3
4	3.41 E-3	0.0	0.0	1.70 E-4	1.77 E-5	0.0	3.41 E-3
5	1.26 E-2	0.0	0.0	9.42 E-5	1.71 E-5	0.0	1.26 E-2
6	2.70 E-3	0.0	0.0	3.39 E-5	0.0	0.0	2.70 E-3
TOTAL	1.34 E-2	3.94 E-3	1.14 E-3	2.10 E-3	1.88 E-4	1.08 E-2	1.78 E-2

* E-4 = 10^{-4}

COMPONENT : Pu-239 SUMMARY BY GROUP FOR UNCERTAINTY ON EXPERIMENT

GROUP	CAPTURE	FISSION	PRODUC.	TRANSP.	ELASTIC	INELAS.	TOTAL
1	2.55 E-7*	4.60 E-5	7.77 E-5	4.03 E-4	5.41 E-6	1.08 E-3	1.15 E-3
2	4.60 E-5	4.40 E-4	1.30 E-4	1.89 E-4	1.67 E-5	2.81 E-4	5.73 E-4
3	1.70 E-3	5.06 E-3	2.59 E-3	4.73 E-4	6.41 E-6	1.45 E-5	5.96 E-3
4	2.85 E-3	2.69 E-3	1.54 E-3	5.92 E-5	8.62 E-6	3.42 E-5	4.21 E-3
5	5.95 E-3	4.25 E-3	2.52 E-3	9.63 E-5	4.81 E-6	0.0	7.73 E-3
6	1.94 E-3	1.24 E-3	6.76 E-4	1.26 E-4	0.0	0.0	2.40 E-3
TOTAL	7.09 E-3	7.26 E-3	3.99 E-3	6.72 E-4	2.11 E-5	1.11 E-3	1.09 E-2

* E-7 = 10^{-7}

Covariances for Adjusted Derived Quantities

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ABSTRACT

A procedure is reviewed for the adjustment of derived quantities and the derivation of their covariance based upon a set of parameters and additional data with their covariances.

I. INTRODUCTION

The utilization of additional experimental data for the adjustment of a set of evaluated data has received considerable attention in recent years, mainly in the context of group cross section adjustments with integral experimental values (see for example Ref. 1). A major distinction is being made between the evaluation of the basic parameters and the adjustment procedures, though both can use the same or similar formalisms. The evaluation of the basic parameters involves predominantly differential cross section data and is based upon direct measurements of the cross sections or simple combinations thereof, e.g. cross section ratios. Such evaluations lead to evaluated nuclear data files like ENDF, KEDAK etc. An example of the evaluation procedures involved which provide a sensible covariance matrix of the evaluated differential data, including cross material covariances, is given elsewhere.[2] The evaluated differential data files are occasionally updated and provide references for a period of time. In contrast, the adjustments of group cross sections with experimental integral data lead to adjusted group cross section sets which are locally used for reactor design calculations and are less well defined references.

The major difference between the differential experimental data and the experimental integral data is that the former depend in analytical form on one or a few parameters whereas the latter depend on many parameters and their calculation involves a model, as well as calculational approximations which introduce further uncertainties and biases. Thus, it has been argued[3] that the adjustments of differential data with integral quantities not only reflect differential data deficiencies but represent compensations for model shortcomings and calculational approximations as well.

An adjustment code, GMADJ,[4] has been recently developed in which the derived quantities are adjusted based upon implicitly adjusted parameters. The use and extraction of explicitly adjusted group cross sections is avoided and the evaluated nuclear data file remains the well defined reference. The parameters include the group cross sections but are not restricted to such quantities. Corrections required for the models and the calculational approximations may be defined as parameters based upon characterizations of the reactor with features like heterogeneity, core size etc.

II. THE ADJUSTMENT PROCEDURE

A Taylor series expansion around a priori parameters $\hat{p} = \{\hat{p}_1, \hat{p}_2 \ldots \hat{p}_n\}$ and terminated with its linear term yields for the integral quantity

$$f_i(\vec{p}) = f_i(\hat{p}) + \sum_j \left.\frac{\partial f_i(\vec{p})}{\partial p_j}\right|_{\hat{p}} (P_j - \hat{P}_j) = m_i + \varepsilon_i \qquad (1)$$

where m_i is the measured quantity and ε_i is the error. A positive-definite and non-singular covariance matrix is assumed to be available for the a priori parameters. In most cases, the integral experimental data are uncorrelated with the differential data or such correlations are very small and can be neglected, i.e. the combined covariance has the form

$$C = \begin{pmatrix} C_D & 0 \\ 0 & C_I \end{pmatrix}$$

where C_D is the covariance of the differential data and C_I is the covariance of the integral data. In this case, one can derive for the adjustments of the parameters[4,5]

$$\delta = C_D A_I (A_I C_D A_I^T + C_I)^{-1} M_I \qquad (2)$$

with covariance

$$C_\delta = C_D - C_D A_I^T (A_I C_D A_I^T + C_I)^{-1} A_I C_D \,. \qquad (3)$$

The coefficients of the design matrix A follow from the Taylor series expansion of Eq. (1)

$$A_{ij} = S_{ij} \frac{f_i(\hat{p})}{\Delta m_i}, \qquad S_{ij} = \left.\frac{\delta f_i(\vec{p})}{\delta p_j}\right|_{\hat{p}} \frac{\hat{p}_j}{f_{i(\hat{p})}}$$

where S_{ij} are the sensitivities which are defined as the percent change of the quantity per percent change of the parameter and are obtained from perturbation theory. The components of the measurement vector are given by

$$M_i = \frac{m_i - f_i(\hat{p})}{\Delta m_i}$$

and the Δm_i are the uncertainties of the measured quantities.

III. THE COVARIANCES OF THE GROUP CROSS SECTIONS AND OF THE INTEGRAL DATA

The covariances of the group cross sections have been generated with the NJOY module ERROR[6] based on ENDF/B-V.2[7] data files.[8] The generation of these covariances requires a reactor spectrum but, fortunately, proves to be rather insensitive to it.[8] Some improvements of these covariances are required, e.g. the uncertainties for the $^{10}B(n,\alpha)$ cross section are less than 2% at all energies and zero above 1.35 MeV, but more realistic values would be 5-15% above 0.2 MeV. Additions have to be considered as well where no cross covariances are available. For example, no covariance information is given between $^{235}U(n,\gamma)$ and $^{235}U(n,f)$ but the capture is derived from alpha measurements, thus strongly correlated with fission. The same applies for the fission cross sections of the higher actinides which, with very few exceptions, are all derived from ratio measurements relative to $^{235}U(n,f)$.

A file of the experimental integral data has been created which contains updated experimental values, uncertainty components and correlation information in a similar format as used on a file created for differential data evaluations.[9] This is a renewed effort to construct an integral data file with all required uncertainty information for use in adjustment procedures and is similar to prior work in this area.[13] The covariance of the integral data is being constructed based upon the uncertainty and correlation information on this file.

IV. ADJUSTMENTS OF DERIVED QUANTITIES

The adjustment of the parameters has been discussed in Section II. However, an explicit adjustment of the parameters is not required if the main interest is in derived quantities. Adjusted derived quantities for which no measurements exist are obtained from the same Taylor series expansion of Eq. (1). Reformulated it yields

$$f_i(\vec{p}) = f_i(\hat{p})\ (1 + \sum_j S_{ij}\delta_j), \qquad (4)$$

thus the adjusted quantity is obtained without explicit adjustments of the parameters. For this equation to be valid requires that the higher order terms neglected in Eq. (1) are small. This has been shown to be the case by comparison of adjusted reactor parameters with calculations based upon adjusted group cross sections.[10]

The covariance of the adjusted derived quantities is obtained from the covariance matrix of the adjusted parameters

$$C_f = D \cdot C_p \cdot D^T \qquad (5)$$

with

$$D = \begin{pmatrix} \frac{\delta f_1}{\delta p_1} & \frac{\delta f_1}{\delta p_2} & \cdots & \frac{\delta f_1}{\delta p_n} \\ \frac{\delta f_m}{\delta p_1} & \frac{\delta f_m}{\delta p_2} & \cdots & \frac{\delta f_m}{\delta p_n} \end{pmatrix}$$

This is the generalization of the derivations given by Usachev[11] for one quantity and by Peelle[12] for two quantities. After appropriate transformation of Eq. (5), one obtains the relative covariance of the adjusted derived quantities"

$$C_{f(rel)} = S.C_\delta.S^T$$

where S is the sentivitity matrix and C_δ is from Eq. (3).

The same formalism can be used for the evaluation of the differential data involving a nuclear model which has been discussed elsewhere.[2]

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THE EVALUATION AND APPLICATION OF REDUNDANT-CROSS-SECTION COVARIANCES

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ABSTRACT

Certain multigroup covariance libraries, notably COVFILS-2, omit all redundant (or summed) reactions on the grounds that the information content of a well-measured total cross section, for example, is implicitly contained in the covariances of the component, or partial, reactions that add up to the total. We analyze this strategy and show that, while redundant reactions can play an important role in cross-section and covariance evaluation, their omission from libraries intended for applications is justifiable.

We consider the problem of estimating the uncertainty in some function $f(\sigma)$, induced by the uncertainties in the cross-section set σ. Normally, some of the reactions affecting f are "redundant," having cross sections that are, by definition, obtainable by simply summing the cross sections for particular non-redundant (NR) reactions. Examples of typical redundant reactions are the total, nonelastic, and total-inelastic reactions. Certain multigroup covariance libraries, notably COVFILS-2,[1] omit all redundant reactions on the grounds that the information content of a well-measured total cross section, for example, is implicitly contained in the covariances of the component, or partial, reactions that add up to the total. In this paper, we analyze this strategy in some detail. While redundant reactions can play an important role in cross-section evaluation, we conclude that their omission from libraries intended for sensitivity and uncertainty analysis can be justified, provided the cross-section and covariance data have been evaluated consistently.

Suppose that the function $f(\sigma)$ is at least approximately linear in the neighborhood of some reference point $\{\sigma_{i,ref}\}$, where it takes on the value

$$f_{ref} = f[\sigma_{i,ref}] \tag{1}$$

In the neighborhood of the reference point, we can, to a good approximation, write

$$f = f_{ref} + \sum_k c_k \, [\sigma_k - \sigma_{k,ref}] \quad , \tag{2}$$

where the index k runs over all reaction types and over all energies. We can simplify Eq. (2) by collecting all of the constant terms together,

$$f_0 = f_{ref} - \sum_k c_k \sigma_{k,ref} \quad , \tag{3}$$

so that

$$f - f_0 = \sum_k c_k \sigma_k \quad . \tag{4}$$

We next rewrite Eq. (4) with a slight notational change, in order to emphasize the separate contributions of the two types of data,

$$f - f_0 = \sum_i a_i s_i + \sum_j b_j t_j \quad , \tag{5}$$

where i ranges over all non-redundant reaction types (with cross sections s_i) and over all energies, and j ranges over all redundant reaction types (with cross sections t_j) and over all energies.

We next introduce row vectors A and B, containing the a_i and b_j, respectively, and column vectors S and T, containing the s_i and t_j. Then Eq. (5) becomes

$$f - f_0 = A\,S + B\,T \quad . \tag{6}$$

The fixed relationship of the two types of data can be written as

$$T = H\,S, \tag{7}$$

where H is a rectangular matrix of constant coefficients, normally having magnitude zero or unity. Combining Eqs. (6) and (7) gives us an alternate form for f,

$$f - f_0 = K\,S \quad , \tag{8}$$

where we have introduced a new row vector,

$$K = A + B\,H \quad . \tag{9}$$

We now turn to the subject of covariances. It is useful, at least conceptually, to break the evaluation process into two parts. We suppose that the vector S is initially determined by use of direct measurements, and these measurements have a covariance, or dispersion, matrix D(S). We assume that T is initially determined strictly by "theory," T = H S. At this point then, all covariances are determined entirely by the measurement uncertainties of S.

In the second step, one incorporates direct measurements M of the redundant cross sections into the covariance assessment. The M play a role exactly analogous to the integral measurements in a conventional, neutronics-oriented statistical "adjustment" exercise, while the S play the role of the differential data. Because of this clear equivalence, we shall use the term "adjusted" to refer to the data evaluator's final combined evaluation of the redundant and NR cross sections. The final, or adjusted, values will be identified in our discussions by the use of the prime symbol (').

The new information provided by the measurements M is most compactly expressed in terms of the "discrepancy" vector P,

$$P = M - T = M - H\,S \quad . \tag{10}$$

In the Appendix (see also Ref. 2), it is shown under very general conditions that, given P and its pre-adjustment covariances D(P), the "best" (minimum-variance) estimate for an arbitrary vector Z is given by

$$Z' = Z - \mathrm{cov}(Z,P)\,G\,P \quad , \tag{11}$$

with covariances

$$D(Z') = D(Z) - \mathrm{cov}(Z,P)\,G\,\mathrm{cov}(Z,P)^{\dagger} \quad , \tag{12}$$

where

$$G = [D(P)]^{-1} \quad . \tag{13}$$

In these relations, the elements of the vector Z can be any quantity that "covaries" with P: integral or differential data, functions of the data (even nonlinear functions), or a mixture of data and functions. The notation cov(Z,P)

denotes a rectangular matrix whose ij-th element is the pre-adjustment covariance $\mathrm{cov}(z_i, p_j)$, and the symbol (†) denotes the matrix transpose.

Equations (11)-(13) can be applied immediately to the problem of combining the redundant and NR measurements. First, we identify the arbitrary matrix Z with the redundant cross sections T. The adjusted values are then given by

$$T' = T - \mathrm{cov}(T,P)\ G\ P \quad . \tag{14}$$

The adjusted NR values are similarly obtained by identifying Z with S,

$$S' = S - \mathrm{cov}(S,P)\ G\ P \quad . \tag{15}$$

Covariances, such as D(T') and D(S'), are immediately obtainable from Eq. (12) with these same identifications.

Equations (14) and (15) provide the optimum evaluated results for all cross sections, taking full account of all available measurements. Of course, stating that this approach is optimum does not mean that all evaluations in a file such as ENDF/B were performed in this way. Even so, this indicates the desired direction that evaluations should take, in order to extract the maximum possible information content from available experimental data.

In fact, a large number of current evaluations do follow this path, at least to the extent of using well-measured total cross sections as a constraint in determining the less well-known reactions, such as elastic scattering. In the covariance files, the frequently occurring statement that reaction-type 2 (MT2) is "derived" in some energy range, from the relation MT1 - MT102, for example, directs the multigroup processing program to reconstruct[3] all covariances involving MT2 in that energy range. In the usual use of this format (an "NC-type" sub-subsection with LTY = 0), the evaluator is, in effect, making the approximation that the covariances of the direct measurements of MT2 are essentially infinite. The experimental data and the associated covariances for MT1 and MT102 would be completely unchanged by an adjustment, Eqs. (11)-(15), in this case (because G approaches 0), so they can go directly into the data file as "measured." The "derived" covariances calculated for MT2 by the processing program are identical to what the evaluator would have obtained, using Eqs. (11)-(15) with very large input covariances for MT2.

It is still mathematically correct to use the LTY = 0 format when the covariances for MT1 and MT102 (to continue with our example) have been substantially adjusted, and this is sometimes done, even though this was not the intent of the original proposers of this format. In such cases, the adjusted covariances for MT1 and MT102 are placed in the file, and adjusted covariances for MT2, although known to the evaluator, are again left to be reconstructed by the processing program. In this case, the use of the LTY = 0 format is not a transparent statement about the method of evaluation, but merely a mechanical convenience to shorten the data files. (The number of reaction pairs is reduced from six down to three in our example.) The use of LTY = 0 is still possible here because the mathematical connection between the final covariances for the three reactions is the same, whatever magnitude is assumed for the covariances of the direct measurements of MT2.

Evaluations that do not follow the approach, described in the preceding several paragraphs, of enforced consistency between the data and covariances for various reactions (incorporating, for example, only direct-measurement covariances for MT1, MT2, and MT102 and ignoring their logical connection) are seriously flawed and are thus clear candidates for re-evaluation. On this basis, we assume that the evaluations of the more important materials either are already "consistent," in the above sense, or soon will be. This is important, because, when creating processed covariance libraries from consistent evaluations, one can dispense with redundant reactions entirely. To show this, we calculate the uncertainty in the post-adjustment value of f.

$$\begin{aligned} \mathrm{var}(f') &= \mathrm{var}(f' - f_0) = \mathrm{var}(A\ S' + B\ T') \\ &= \mathrm{cov}(A\ S' + B\ T',\ A\ S' + B\ T') \\ &= A\ D(S')\ A^{\dagger} + A\ \mathrm{cov}(S',T')\ B^{\dagger} + B\ \mathrm{cov}(T',S')\ A^{\dagger} + B\ D(T')\ B^{\dagger} \quad . \end{aligned} \tag{16}$$

ENDF/B-V provides, in general, covariance information for both redundant and NR data. Covariance processing programs, such as the ERRORR module[3] of NJOY, can easily retrieve all of the covariances and put them out in the multigroup structure specified by the code user. The question at hand is whether all, or just a portion, of these output covariances actually need to be incor-

porated into multigroup covariance libraries in order to permit the computation of uncertainties such as var(f'). Superficially, it would seem that all are required, because three of the four terms in Eq. (16) involve the uncertainties of T'. This first impression turns out to be untrue. To show why, we first multiply Eq. (15) from the left by H, yielding

$$H\,S' = H\,S - H\,\mathrm{cov}(S,P)\,G\,P = T - \mathrm{cov}(T,P)\,G\,P \quad , \tag{17}$$

where the last result follows from Eq. (7). Comparing Eqs. (17) with Eq. (14), we see that

$$T' = H\,S' \quad . \tag{18}$$

Thus, at least when one is considering linear functions, the best estimates of the functions are equal to the functions of the best estimates of the data. Because of the existence of this simple linear connection (even after taking into account direct measurements of both types of reaction and correlations between the two), the uncertainty in the redundant data can still be propagated from the uncertainty of NR data. We can use this fact to simplify Eq. (16),

$$\begin{aligned}\mathrm{var}(f') &= A\,D(S')\,A^{\dagger} + A\,\mathrm{cov}(S',H\,S')\,B^{\dagger} + B\,\mathrm{cov}(H\,S',S')\,A^{\dagger} + B\,\mathrm{cov}(H\,S',H\,S')\,B^{\dagger} \\ &= A\,D(S')\,(A^{\dagger} + H^{\dagger}\,B^{\dagger}) + B\,H\,D(S')\,(A^{\dagger} + H^{\dagger}\,B^{\dagger}) \\ &= (A + B\,H)\,D(S')\,(A + B\,H)^{\dagger} \quad .\end{aligned}$$

Recalling Eq. (9), we have simply

$$\mathrm{var}(f') = K\,D(S')\,K^{\dagger} \quad . \tag{19}$$

Equation (19) summarizes our main conclusion, namely, that sensitivity and uncertainty analysis does <u>not</u> require covariances of the redundant cross sections.

In addition to saving space in a covariance library such as COVFILS-2, there is an additional reason for restricting the library to the subset of non-redundant reactions. Sensitivity-analysis programs are specifically coded to calculate the effect on f, for example, of changing a single NR cross section while holding all other NR reactions fixed. In this process, redundant cross sections are allowed to change in response to changes in their NR components. This is exactly the point of view adopted in deriving Eq. (8). The calculated sensitivities can thus be immediately identified with the elements k_i of the vector K. With the k_i in hand, one is immediately ready to calculate the uncertainty in f using Eq. (19). The vectors A and B, on the other hand, are fundamentally ambiguous.

To illustrate this point, consider a case in which there is a single redundant reaction, namely the total, so that $t = \sigma_{tot}$ for some specified energy group. One can simply <u>define</u> the coefficient b to be, for example, the rate of change of f with respect to a correlated change in all partial reactions in that group, holding all partial-to-partial ratios constant. Other definitions are also possible. Since there is only one redundant reaction, the matrix H is just a row vector, and it contains all ones. The matrix product B H is also a row vector, with an entry of b in each position. Once b is specified, the elements of A are then determined by Eq. (9),

$$a_i = k_i - b \quad . \tag{20}$$

Thus, one can, indeed, include redundant reactions explicitly in a sensitivity and uncertainty analysis, but only if one simultaneously reduces the NR-reaction sensitivities so as to cancel the net effect of this inclusion. There seems to be little point to performing the analysis in this way.

REFERENCES

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APPENDIX

A NON-RESTRICTIVE DERIVATION OF THE GENERALIZED METHOD OF LEAST SQUARES

In the general field of data evaluation, one frequently needs to combine data from two or more different sources. A powerful and general technique for performing this task is the generalized method of least squares. (The term "Bayes' Method" is sometimes used as a synonym for the generalized method of least squares, but for reasons given below, this usage is not really appropriate.)

Most derivations of the generalized method of least squares begin by assuming a linear relationship between the fundamental parameters of interest (differential data) and various important functions of the parameters (integral data). Unfortunately, in some applications it may be difficult or impossible to determine the needed linear "sensitivity coefficients" relating the functions to the parameters. For example, in multigroup neutronics studies, coefficients relating detector responses to multigroup cross sections are usually obtained by applying first-order perturbation theory to the relevant forward and adjoint fluxes, calculated with one- or two-dimensional discrete ordinates. In some applications, this may be impractical--the geometry may be intrinisically three-dimensional, so that Monte Carlo analysis is required, or the number of integral measurements may be so numerous that the required number of adjoint calculations is impractically large. In the evaluation of nuclear-model parameters, two main difficulties arise. First, the calculational procedure may involve the application of a whole series of complex computer programs, so that it may be difficult to develop theoretical expressions for the sensitivities. Secondly, the calculated cross sections can be significantly nonlinear functions of the parameters.

Since we wish to apply least square techniques in some of these areas, we have examined[2] the question of whether or not the generalized method of least squares could be developed outside the usual linear framework. At the same time, it was also hoped that the use of other restrictive assumptions could be held to a minimum. In the following development, then, we do not make any of the following assumptions:

(a) that the integral quantities of interest are linear functions of the parameters;

(b) that the measurements of the functions and of the parameters are uncorrelated;

(c) that the results of the measurements are drawn from normal distributions.

We begin by stating the generic problem: one has an initial data base of parameters λ_i that one wishes to improve by taking into account new measurements of certain relevant physical quantities. We denote by the column-vector Λ the initial data set and by M the results of the new measurements. Corresponding to M are the values $C(\lambda)$ of the same physical quantities, as obtained by calculation from the Λ. The information content of the new measurements is most compactly represented in terms of the discrepancy vector,

$$P = M - C \ . \tag{A-1}$$

In analyzing the question of how to use the new information P in an optimum way, we adopt a minimum-variance point of view. The reason we do so is that the alternative maximum-likelihood, or "Bayesian," approach to the development of the least squares equations requires the assumption of normal probability distributions, whereas the minimum-variance approach does not.

Without sacrificing generality, we can assume that the ultimate object here is to provide increased accuracy in a set of "target" functions Z, which may depend on the parameters Λ, the measurements M, or both. The nature of the target functions is totally arbitrary at this point.

Improved estimates Z' are formed as the sum of the initial values, Z, plus an "adjustment," which is taken to be a general linear combination of the discrepancies,

$$Z' = Z + F P \ . \tag{A-2}$$

From the form of Eq. (A-2), it is clear that, even in nonlinear applications, Z' will provide an unbiased estimate as long as the expectation value E(P) is zero, i.e., as long as E(M) = E(C).

The matrix of arbitrary constants F is determined from the requirement that Z' be a "best" estimate. By this we mean that $\mathrm{var}(z'_k)$ is minimized, with respect to changes in F, for every target function z_k.

It is convenient to introduce a second arbitrary matrix Q, related to F by

$$F = Q - \mathrm{cov}(Z,P)\ G, \tag{A-3}$$

where

$$G = [D(P)]^{-1} \quad . \tag{A-4}$$

The covariance matrices cov(Z,P) and D(P) are defined in the main text of this paper.

For any particular choice of Q, the dispersion matrix of Z' can be written as follows:

$$\begin{aligned} D(Z') &= \mathrm{cov}(Z',Z') \\ &= \mathrm{cov}[Z + Q\,P - \mathrm{cov}(Z,P)\ G\ P,\ Z + Q\,P - \mathrm{cov}(Z,P)\ G\ P] \\ &= D(Z) + \mathrm{cov}(Z,P)\ Q^{\dagger} - \mathrm{cov}(Z,P)\ G\ \mathrm{cov}(Z,P)^{\dagger} + Q\ \mathrm{cov}(Z,P)^{\dagger} \\ &\quad + D(Q\,P) - Q\ D(P)\ G\ \mathrm{cov}(Z,P)^{\dagger} - \mathrm{cov}(Z,P)\ G\ \mathrm{cov}(Z,P)^{\dagger} \\ &\quad - \mathrm{cov}(Z,P)\ G\ D(P)\ Q^{\dagger} + \mathrm{cov}(Z,P)\ G\ D(P)\ G\ \mathrm{cov}(Z,P)^{\dagger} \quad . \end{aligned} \tag{A-5}$$

After applying Eq. (A-4) here, many terms cancel, leaving only

$$D(Z') = D(Z) - \mathrm{cov}(Z,P)\ G\ \mathrm{cov}(Z,P)^{\dagger} + D(Q\,P) \ . \tag{A-6}$$

The diagonal elements of the dispersion matrix D(Q P) in Eq. (A-6) are variances and, hence, cannot be made negative by any choice of Q. Thus, the diagonal elements of D(Z') are minimized by choosing the arbitrary matrix Q to be null, Q = 0. Thus, the minimum-variance solution for the z'_k (the solution having the smallest "error bars"), is obtained by substituting Q = 0 in Eqs. (A-3) and (A-6); hence,

$$Z' = Z - \mathrm{cov}(Z,P)\ G\ P \quad , \tag{A-7}$$

and

$$D(Z') = D(Z) - \mathrm{cov}(Z,P)\ G\ \mathrm{cov}(Z,P)^{\dagger} \quad . \tag{A-8}$$

These very general results can be applied in many ways. For example, in Ref. 2 it is pointed out that the covariances in Eqs. (A-7) and (A-8) can be evaluated directly, via a Monte Carlo technique, without ever explicitly calculating linear sensitivity coefficients.

Equation (A-7) can be applied to adjust either the measurements or the corresponding calculations,

$$M' = M - \mathrm{cov}(M,P)\ G\ P \quad ,$$

$$C' = C - \mathrm{cov}(C,P)\ G\ P \quad .$$

In fact, from these results we see that M' is <u>equal</u> to C'. Recalling Eq. (A-1),

$$M' - C' = P - \mathrm{cov}(P,P)\ G\ P = 0 \quad .$$

This should have been expected, since M' and C' are best estimates of the very same physical quantities.

For the purposes of the present paper, where the redundant cross sections (C) are rigorously linear functions of the non-redundant cross sections (Λ), as shown in Eq. (7) of the main text, it is useful to rewrite the results in a more conventional form. To do this, we specialize Eq. (A-7) to the case where Z is identical to Λ and where $C(\lambda)$ is explicitly linear, $C = H\,\Lambda$.

$$\Lambda' - \Lambda = [D(\Lambda)\ H^{\dagger} - \mathrm{cov}(\Lambda,M)]\ G\ P \quad . \tag{A-9}$$

Similarly, if we identify Z with M,

$$M' - M = [\mathrm{cov}(M,\Lambda)\ H^{\dagger} - D(M)]\ G\ P. \tag{A-10}$$

These linearized relations are identical to those published relatively recently by Barhen et al.[A1]

An important feature of the least squares equations, whether written in the general or the linearized form, is that, even when correlations exist between the integral and differential measurements, it is still possible to reduce the matrix-inversion requirements to the fairly simple task of inverting D(P). Integral-differential correlations can be expected to be important in the simultaneous evaluation of different cross-section types, because the redundant cross sections and their components may well be measured with similar experimental techniques.

APPENDIX REFERENCES:

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