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EVALUATION AND PROCESSING OF COVARIANCE DATA

Oak Ridge National Laboratory, USA, 7th - 9th October 1992

COMPTE RENDU D'UNE RÉUNION DE SPÉCIALISTES

ÉVALUATION ET TRAITEMENT DES DONNÉES DE COVARIANCE

Oak Ridge National Laboratory, USA, 7 - 9 Octobre 1992

Edited by

M. Wagner

Institut für Radiumforschung und Kernphysik, Vienna, Austria

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Scientific program committee:

F.H. FRÖHNER
Kernforschungszentrum Karlsruhe
Institut für Neutronenphysik und Reaktortechnik
Postfach 3640
W-7500 Karlsruhe 1
GERMANY
Telephone: 07247/82-2336
FAX: 07247/82-4874
Telex: 724716-KFK

Douglas W. MUIR
Nuclear Data Section
Division of Physical and Chemical Sciences
International Atomic Energy Agency
P. O. Box 100
A-1400 Vienna, AUSTRIA
Telephone: 43-1-2360
FAX: 43-1-234564
E-Mail: "RNDS@IAEA1"

Harm GRUPPELAAR
Netherlands Energy Research Foundation
Postbus 1
NL-1755 Petten
THE NETHERLANDS
Telephone: 31-2246-4083
FAX: 31-2246-3490
E-Mail: ESU0123@HPEENR51

M. SALVATORES
Head Reactor Physics & Fuel Cycle Service
Building 230
CE/CADARACHE
13108 Saint Paul Lez Durance
Cedex, FRANCE
Telephone: (33) 42-25-33-65
FAX: (33) 42-25-48-49
Telex: CEACA 440678F

Yukinori KANDA
Department of Energy Conversion
Engineering
Kyushu University
Kasuga Fukuoka 816
JAPAN
Telephone: 81-92-573-9611 EX. 390
FAX: 81-92-575-1352
E-Mail:

Donald L. SMITH
Energy Physics Division
Building 314
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439-4841
U.S.A.
Telephone: (708) 252-6021
FAX: (708) 252-6022
E-Mail: B18245@ANLOS.BITNET

Robert W. PEELLE
Building 6010, MS-6356
P. O. Box 2008
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831-6356, U.S.A.
Telephone: (615) 574-6113
TS 624-6113
FAX: (615) 576-8746
E-Mail: "PEELLER@CESARVAX
OREP01::PEELLER

Herbert VONACH
Institut für Radiumforschung
und Kernphysik
der Universität Wien
Boltzmanngasse 3
A-1090 Wien
AUSTRIA
Telephone: 43-1-34-72-05
FAX: 43-1-31-91-458 - 482

Local organizing committee:

D.C. Larson, Chairman
C.Y. Fu
D.M. Hetrick
R.W. Roussin
A.M. McCoy

Conference Participants and Addresses

Claude Bastian
CEC-IRC
Central Bureau for Nuclear Measurements
B-2440 Geel
BELGIUM
E-Mail: BASTIAN@CBNM.JRC.RTT.BE

Brian Broadhead
Oak Ridge National Laboratory
P. O. Box 2008
Bldg. 6011, MS-6370
Oak Ridge, Tennessee 37831-6370
U.S.A.
Telephone: 615-576-4476

Satoshi Chiba
Japan Atomic Energy Research Institute
Tokai Research Establishment
319-11 Tokai-mura, Naka-gun
Ibaraki-ken
JAPAN
Telephone: 81-292-82-5483
FAX: 81-292-82-5927
E-Mail: J4013@JPNJAERI

Eric Fort
DRNR/SPCI/LEPh - Bat. 230
Centre d'Etudes Nucleaires
de Cadarache
F-13108 Saint-Paul-lez-Durance CEDEX
FRANCE

Srinivasan Ganesan
International Atomic Energy Agency
RIPC - Nuclear Data Section
A 2317, P. O. Box 100
A-1400 Vienna
AUSTRIA
Telephone: 43-1-2360-1713
FAX: 43-1-23.45.64
E-Mail: EARN-bitnet: RNQ@IAEA1

David Hetrick
Engineering Physics and Mathematics Div.
Bldg. 6010, MS-6356
Oak Ridge Nat. Laboratory, P.O.Box 2008
Oak Ridge, Tennessee 37831-6356,
U.S.A.
Telephone: 615-574-6131
FAX: 615-576-8746

Yukinori Kanda
Dept. of Energy Conversion Engineering
Kyushu University
Kasuga Fukuoka 816
JAPAN
Telephone: 81-92-573-9611
FAX: 81-92-575-1352

Nancy M. Larson
Engineering Physics and Mathematics Division
Oak Ridge National Laboratory
P. O. Box 2008
Oak Ridge, Tennessee 37831-6356
U.S.A.
Telephone: 615-574-4659
FAX: 615-576-8746

Richard E. Maerker
Oak Ridge National Laboratory
P. O. Box 2008
Bldg. 6025, MS-6364
Oak Ridge, Tennessee 37831-6356
U.S.A.
Telephone: 615-574-4659
FAX: 615-576-8746

Wolf Mannhart
Physikalisch-Technische Bundesanstalt
Lab. 7.23
Bundesallee 100
W-3300 Braunschweig
FED. REP. OF GERMANY
Telephone: 49-531-592-7230
FAX: 49-531-592-4006
BITNET: MANNH620@DBSPTB

Douglas W. Muir
T2, MS B243
Los Alamos National Laboratory
Los Alamos, New Mexico 87545
U.S.A.
Telephone: 505-667-1207

Vladimir Pronyaev
Fiziko-Energeticheskij Institut
Bondarenko sq. 1
249020 Obninsk
Kaluga Region
RUSSIA
Telephone: 007-08439-05494
FAX: *
E-Mail: IGNATYUK@CJD.FEI.OBNIN.SU

Nikolai S. Rabotnov
Prof. of Physics
Institute of Physics and Power Engineering
249020, Bondarenko Sq. 1
Obninsk, Kaluga Region
RUSSIA
Telephone: 007-08439-986-85
FAX: *
E-Mail: IGNATYUK@CJD.FEI.OBNIN.SU

Enrico Sartori
OECD NEA Data Bank, Bat 45
91191 Gif-sur-Yvette
Cedex
FRANCE

Donald L. Smith
Engineering Physics Division, Bldg. 314
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60544-4841
U.S.A.
Telephone: 708-252-6021
FAX: 708-252-6022
E-Mail: B18245@ANLOS.BITNET

Siegfried Tagesen
University of Vienna
Institut für Radiumforschung und Kernphysik
Boltzmanngasse 3
A-1090 Wien, AUSTRIA
Telephone: 43-1-31-91-366
FAX: 43-1-31-91-458 - 482
E-Mail: TAGESEN@AIRK.RAD.UNIVIE.AC.AT

Herbert K. Vonach
University of Vienna
Institut für Radiumforschung und Kernphysik
Boltzmanngasse 3
A-1090 Wien, AUSTRIA
Telephone: 43-1-34-72-05
FAX: 43-1-31-91-458 - 482

Zhao Zhixiang
Chinese Nuclear Data Center
Institute of Atomic Energy
P. O. Box 275(41)
Beijing, P. R. CHINA
Telephone: 935-7830

---

* FAX to: Dr. Yu. Lipatov
Ministry of Atomic Power and Industry
Staromonetny Perculole 26
109180 Moskow, Russian Federation
FAX No.: 095-2302420 (include notation to direct to Obninsk, to the attention of...)

NEEDS FOR EVALUATED COVARIANCE DATA FOR REACTOR PRESSURE VESSEL DOSIMETRY

R. E. Maerker and B. L. Broadhead
Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA
and
J. J. Wagschal
Racah Institute of Physics, The Hebrew University, Jerusalem, Israel

A new methodology for quantifying and then reducing uncertainties in the calculated pressure vessel fluences of a pressurized water reactor (PWR) is reviewed. The technique involves combining the integral results of the calculated and measured PWR surveillance dosimetry activities with the differential data used in the calculations, along with covariances of all the quantities, into a generalized linear least-squares adjustment procedure. Based on analysis of both PWRs and test reactor benchmarks, substantial evidence now exists to support the conclusion that, of all the nuclear as well as non-nuclear differential data considered, ENDF/B-V values of the total inelastic iron cross sections and their covariances are the most important data controlling the outcome of the adjustment procedure. Predicted adjustments in these cross sections provided the stimulus for new measurements, the results of which impacted the ENDF/B-VI evaluation of iron 56.

I. INTRODUCTION

The lifetime of a PWR is usually determined by embrittlement of the pressure vessel (PV) that is caused by neutron-induced displacements of the atoms constituting the steel. This decrease in the fracture toughness reduces the ability of the PV to withstand cracking from effects caused by a rapid change in temperature followed by application of pressure such as would occur in response to a loss of coolant accident (pressurized thermal shock), as well as to arrest the propagation of a flaw inward (end-of-life rupture). Updated estimates of the state of the PV have been based in the past on analysis of passive dosimetry and metallurgical specimens extracted from capsules located in the downcomer region in front of the PV. Recently, however, the depletion of these capsules and the desire to extend the lifetime of these reactors have created a need for the installation of additional dosimetry in the reactor cavity behind the PV. This location has the advantage of being readily accessible but the disadvantage of not being able to provide an accelerated monitoring of the accumulated PV damage. For either the in-vessel or ex-vessel dosimetry, the information concerning the spectrum and fluence at these surveillance locations must be translated to the PV, both in space and in time, to determine the accumulated fluence on it and project the time when the PV begins to exceed the screening criteria. After this point is reached, the reactor is then decommissioned or subjected to some form of annealing process.

It is apparent that this procedure for determining a plant's lifetime can be subject to rather large uncertainties and that because of these uncertainties the conservatism required by imposing safety margins may shorten the lifetime considerably. Each step in this prescribed procedure introduces a non-trivial uncertainty - the measurements of the activities, the flux calculations at the dosimetry locations and throughout the PV, the flux adjustments at the dosimetry locations, extrapolation of the adjustments to the PV in space and to future exposures in time, the determination of the fluence level beyond which embrittlement is severe enough to necessitate shutdown - and each of these makes its own contribution to the penalties of a premature reactor shutdown.

Historically, adjustment methods (which are also referred to as unfolding or data combination processes depending on the particular direction of emphasis) have not considered effects of uncertainties in the calculation of the trial spectrum, in the dosimetry measurements, or in the final results. An example is the SAND-II code(1), still used by a large fraction of the international dosimetry community. Although later versions of this code contain some "error" estimation procedures, they are not central to the method. More recently, the codes LSL-M2 (2), STAYS'L (3), and FERRET (4), to name a few, have appeared and which possess the potential for consideration of not only standard deviations but correlations as well. Even for these codes, however, nonrigorous methods for covariance estimation must be employed, since no appropriate methodology is developed

to supply them. In addition, none of these more sophisticated codes, with the exception of LSL-M2, is capable of unfolding fluxes at other than at dosimetry location without resorting to the use of simplifying assumptions which break down completely for ex-vessel dosimetry.

This paper reviews a methodology that has been packaged into a computer software system called LEPRICON (5), which can be used to quantify and subsequently reduce uncertainties in several of the steps in the surveillance dosimetry procedure, namely, in those steps linking the measurements with the determination of PV flux and spectral information. A successful implementation of this method would then leave as the only remaining major source of uncertainty the one involving the prediction of existing PV damage susceptibility from analysis of in-vessel capsules and/or reference to the latest revision of the U.S. Nuclear Regulatory Commission (NRC) Regulatory Guide 1.99, which gives the relationships between fast fluence and several measures of radiation-induced damage in low-alloy steels for various concentrations of residual elements such as copper and nickel (6).

Taking full advantage of the theory reviewed in the next section, the LEPRICON system has the following capabilities that render it unique in the field of few-channel unfolding:

1. It solves the extrapolation problem necessitated by use of ex situ measurements.
2. It is capable of unfolding spectral fluences simultaneously at both a PV location and one or two dosimetry locations, and the dosimetry locations can be either in-vessel, ex-vessel, or a combination. However, if two, they must have been performed at the same time.
3. It unfolds PWR dosimetry measurements in conjunction with measurements previously performed and analyzed using simpler geometries. These benchmarks were calculated with the same cross section library and transport methods and approximations used in the PWR analysis. Thus the PWR multi-location unfolding procedure is performed simultaneously using all available PWR dosimetry data pertinent to a given cycle along with the data for the "cleaner" benchmarks.
4. In order to satisfy the requirement of using a transport procedure common to both the analysis of PWRs and benchmarks, and the desirability of making it as accurate as possible so that method uncertainties can be reduced to a minimum, the LEPRICON system provides a state-of-the-art capability for calculating the dosimeter activities and PV spectral fluences.
5. It incorporates the basic sensitivity and covariance data necessary for estimates of the flux uncertainties. These data are included as part of the default data base, along with the calculated and measured values of the benchmarks. Uncertainties in the mandatory transport method from various approximations are also part of the covariance data base.
6. It produces adjustments to the calculated fluxes along with covariances that are reduced by factors of between two and four from preadjusted values for the PV group fluxes.

In Section II the main features of the theory are reviewed.

Section III describes the benchmark experiments and agreement between the calculations using ENDF/B-IV and -V data and the measurements. In Section IV a description of the methods used in developing the covariances and flux sensitivities of the differential data is presented, including the manner in which flux uncertainties from approximations in the transport methods and in the as-built reactor geometry are defined and evaluated. The results from applying the entire LEPRICON procedure to an analysis of the H. B. Robinson-2 reactor are summarized in Section V. The important role played by the iron total inelastic cross section and its covariance is discussed in Section VI.

II. THEORY

We define a data combination process as one in which various types of data used to define a database are altered in such a fashion as to produce a more consistent data base. The general types of data involved in our present application can be integral measurements (e.g., dosimeter reaction rates or end of irradiation activities, spectrum-averaged cross sections or ratios of these cross sections) or differential data (e.g., dosimetry cross sections, partial cross sections involved in neutron transport, fission spectra, source distributions, and correction factors that account for methods approximations and geometrical assumptions in the transport modeling, i.e., "flux bias factors"). Any or all of these data types can be used to define the data base. The combination procedure must make use of calculations of the experiments using the differential data, have a criterion that defines "consistency" in a mathematical sense, and operate within the limitations imposed by estimated uncertainties of the data.

The particular adjustment procedure adopted for this study is a generalized linear least-squares technique introduced by Gandini (7) and others, and more recently refined and expanded by Wagschal and Yeivin (8) and Bahren (9). In this method, the consistency is expressed mathematically as maximizing the joint probability distribution of the data base subject to the relationships between the differential and integral data. Our problem to be solved is: Given a series of dosimetry experiments performed at an accessible (i.e., surveillance) PWR location, together with a calculation of the group fluxes and activities at this location and the group fluxes at another location that is inaccessible to dosimetry (i.e., in the PV), what are the "best" estimates of these PV group fluxes, and what are the "best" estimates of their corresponding uncertainties?

The adaptation of the least-squares technique to the problem of dosimetry unfolding is originally due to Petilli (10) and to Perey (11), who derived expressions for the flux unfolding at the surveillance location. With these identifications as points of departure, elaboration of the method to include effects of any correlations between the differential and integral data, to accommodate simultaneously in the PWR unfolding the results of earlier analyses of existing benchmarks that take advantage of simpler geometries and better known sources to provide more

definitive testing of sensitive differential data, and finally but most importantly, how to calculate the correlations between the fluxes at two locations such as at the dosimeter and in the PV, or what amounts to the same thing, the relative adjustments in the group fluxes at the two locations.

The following formulation and derivation of the expressions for the adjustment procedure are necessarily incomplete because of space limitations. For a more detailed presentation, the interested reader is referred to the literature (12,13). Let the column vector $r=(r_i)$, $i=1,2,..,I$ represent a series of dosimetry measurements in various fields, i.e., at a PWR surveillance location or at locations in standard or reference benchmark fields, Crr its corresponding IxI covariance matrix, and $\bar{r}=(\bar{r}_i)$ represent the calculations of these same experiments. Let the column vector $p=(p_n)$, $n=1,2,..,N$, with its corresponding NxN covariance matrix Cpp, represent the differential data (i.e., energy dependent parameters) used in the calculations, where $N=PG$, the product of the number of parameter types and number of groups used to define the energy dependence. Any covariances between the integral measurements and the differential data are denoted by the NxI matrix Cpr. If we denote the sensitivities of the calculated responses $\bar{r}$ to each of the parameters p by a IxN matrix $Sr=(d\bar{r}_i/dp_n)$, and impose the linearity restriction

$$\bar{r}(p+\delta p)=\bar{r}(p)+\bar{r}=\bar{r}(p)+(Sr)(\delta p), \qquad (1)$$

then the covariance matrix of the calculated responses becomes

$$C\bar{r}\bar{r}=(Sr)(Cpp)(Sr)^{\top}, \qquad (2)$$

where "δ" in Eq.(1) represents a finite difference and "T" in Eq.(2) the transpose. If the deviations of the measured and corresponding calculated responses are denoted by $d=(d_i)=\bar{r}-r$, then Cdd, the covariance matrix for d, becomes

$$Cdd=(Sr)(Cpp)(Sr)^{\top}+Crr-(Sr)(Cpr)-(Crp)(Sr)^{\top}, \qquad (3)$$

where Crp is the transpose of Cpr. Let the (unknown) adjusted parameter vector be $p'=(p_n')$ and adjusted calculated response vector be $\bar{r}'(p')$. By imposing the condition $r'=\bar{r}'(p')$, where r' is the adjusted measured response, the adjusted values p' and r' are forced to be consistent. If we further denote the actual adjustments by $x=p'-p$ and $y=r'-r$, Eq.(1) becomes

$$r'=\bar{r}+(Sr)(x), \qquad (4)$$

leading to

$$y=d+(Sr)(x). \qquad (5)$$

The generalized linear least-squares procedure involves minimizing the quadratic loss function

$$Q(x,y)=(y,x)^{\top}\begin{pmatrix} Crr & Crp \\ Cpr & Cpp \end{pmatrix}^{-1}(y,x), \qquad (6)$$

where $(y,x)^{\top}\equiv(y_1,\ldots,y_I,x_1,\ldots,x_N)$, subject to the constraint expressed in Eq.(5). Adopting the procedures in Refs. 7, 8, and 9, this formulation is equivalent to unconditionally minimizing the function $R(x,y)$, where

$$R(x,y)=Q(x,y)+(2\lambda^{\top})[(Sr)(x)-(y)] \qquad (7)$$

and 2λ is a column vector of Lagrange multipliers. After some matrix algebra manipulations, the solution for x and y becomes

$$x=[(Cpr)-(Cpp)(Sr)^{\top}]\lambda, \qquad (8a)$$

and

$$y=[(Crr)-(Crp)(Sr)^{\top}]\lambda, \qquad (8b)$$

reflecting the driving influence of the vector λ. Substitution

of these values of x and y into Eq.(4) yields

$$\lambda = (Cdd)^{-1}(d), \qquad (9)$$

with

$$C_{\lambda\lambda} = (Cdd)^{-1} \qquad (10)$$

The adjusted values p′ and r′ are found from Eqs.(8) to be

$$p' = p + [(Cpr) - (Cpp)(Sr)^{T}](Cdd)^{-1}(d) \qquad (11a)$$

and

$$r' = r + [(Crr) - (Crp)(Sr)^{T}](Cdd)^{-1}(d), \qquad (11b)$$

where $(Cdd)^{-1}$ is obtained by taking the inverse of Eq.(3) and is a matrix of dimensions IxI. The covariances of the adjusted differential and integral data are obtained from Eqs.(11) to be

$$Cp'p' = Cpp - [(Cpr) - (Cpp)(Sr)^{T}](Cdd)^{-1}[(Crp) - (Sr)(Cpp)] \qquad (12a)$$

and

$$Cr'r' = Crr - [(Crr) - (Crp)(Sr)^{T}](Cdd)^{-1}[(Crr) - (Sr)(Cpr)]. \qquad (12b)$$

Since the term following the first minus sign on the R.H.S. of these equations is positive, the conclusion can be drawn that the uncertainties in both the measurements and the differential data are reduced by the combination procedure. Furthermore, the cross covariances between all the adjusted data become

$$Cp'r' = Cpr - [(Cpr) - (Cpp)(Sr)^{T}](Cdd)^{-1}[(Crr) - (Sr)(Cpr)]. \qquad (13)$$

Thus, even if no á priori correlations between the differential and integral data exist, an á posteriori correlation does exist by virtue of the combination procedure.

The minimum value of Q in Eq.(6), found by substituting the expressions for x and y from Eqs.(8), is denoted by the symbol χ^2, which is a measure of the adjustments made in units of the (combined) á priori standard deviations summed over all the participating integral and differential data:

$$\chi^2 = Q\min(x,y) = (d)^{T}(Cdd)^{-1}(d). \qquad (14)$$

Values of χ^2/I, named chi-square per degree of freedom, should lie near unity for a meaningful adjustment (i.e., adjustments in each integral experiment and each participating differential datum should lie within one standard deviation with about a two thirds probability). This quantity, which can be considered a figure of merit of the adjustment, can perhaps surprisingly be calculated without actually performing the adjustment, since all the ingredients in Eq.(14) are known beforehand and merely reflect the consistency of the available data. For the case of a single measurement in which there is no correlation between the integral and differential data, Eq.(14) reduces to

$$\chi^2_{IND} = (\bar{r} - r)^2 / [(Crr) + (Sr)(Cpp)(Sr)^{T}], \qquad (15)$$

which is just the square of the discrepancy between the measured quantity r and the calculated quantity $\bar{r}$ using the differential data p expressed in units of the combined variances of r and $\bar{r}$.

In the particular application to the dosimetry problem under consideration, the only adjusted data at the dosimetry location necessary for the PV flux adjustments are the differential data determined from Eq.(11a). For if we denote by the column vector $\phi = (\phi_g)$, $g = 1,2,..,G$ the calculated PV flux and by $S_\phi = d\phi_g/dp_n$ the GxN sensitivity matrix of the group fluxes to the differential data, then again to within the limits of a linear approximation

$$\phi' = \phi + (S_\phi)(p' - p) = \phi + (S_\phi)[(Cpr) - (Cpp)(Sr)^{T}](Cdd)^{-1}(d). \qquad (16)$$

Eq.(16) applies equally well to adjusted fluxes at dosimetry as well as PV locations, providing, of course, that sensitivities appropriate to the particular location are used. The importance of Eq.(16) lies in the fact that it reveals as the cause of the PV flux adjustments just those sources of uncertainty in the

differential data that the dosimetry and PV fluxes share common sensitivities to. These sensitivities need not be the same at the two locations, only large enough to be able to affect both the S_ϕ and $(p-p')$ terms in Eq.(16). The sharing of mutual sources of data uncertainty is what gives rise to correlations between the fluxes at the two locations A and B:

$$C_{\phi_A \phi_B} = (S_{\phi_A})(Cp'p')(S_{\phi_B})^T, \quad (17)$$

and without the existence of these correlations the dosimetry would not provide any useful information about the PV fluences. Since, for either location, the adjusted flux covariances are

$$C_{\phi'\phi'} = (S_\phi)(Cp'p')(S_\phi)^T, \quad (18)$$

then substituting from Eq.(12a) leads to

$$C_{\phi'\phi'} = (S_\phi)\{(Cpp) - [(Cpr) - (Cpp)(Sr)^T](Cdd)^{-1}[(Crp) - (Sr)(Cpp)]\}(S_\phi)^T. \quad (19)$$

Although Eqs.(1-19) have been developed using absolute quantities, they remain unchanged and are far more useful if relative quantities are substituted instead. Hence, covariances may be replaced by relative covariances, sensitivities by such normalized quantities as $(p/\bar{r})(d\bar{r}/dp)$, and the corresponding adjustments become $(p'/p)-1$ and $(\bar{r}'/\bar{r})-1$.

III. THE BENCHMARK INTEGRAL EXPERIMENTS

One of the advantages of this methodology is its capability for simultaneously combining the results of simpler dosimetry-oriented benchmark experiments with those performed in the PWR. The advantage in including these data is that, if properly chosen, the benchmark and PWR calculations will be sensitive to some of the same differential data, but the less complicated benchmark experiments, having fewer sources of uncertainties, will tend to establish these data adjustments more accurately. This procedure thus leaves the PWR measurements primarily with the task of determining the adjustments in the data that are unique to the reactor calculations such as, for example, in the as-built dimensions and physical properties of the various reactor components and the spatial distributions of the source.

The differential data usually shared by the benchmarks are nuclear in nature, and an early exploratory analysis indicated the most important data to be, in order, the total inelastic cross sections of iron, the spectrum above 6 MeV arising from thermal-neutron induced fission in U235, and the cross sections for the dosimetry reactions. These data were determined to be the most influential in affecting the accuracy of the transport calculations because of their relatively large uncertainties and the high sensitivities of the measurements to them.

Table I identifies the 34 experiments adopted as benchmarks together with descriptive information of each measurement and its calculation. Eight were performed in Cf252 driven fields (14,15,16), four in the Intermediate-energy Standard Neutron Field (17), eight in a prototypic PCA mockup of pressure vessel transport geometry (18), and 14 in the prototypic PSF "startup" mockup of another pressure vessel transport geometry (19,20). The PCA and PSF experiments included measurements inside the simulated pressure vessel as well as at surveillance locations,

thus providing invaluable information not normally available in PWR dosimetry. These supplementary PV dosimetry sites included one-quarter depth (T/4) locations in both mockups and a (3T/4) location in the PSF mockup.

TABLE I

Integral Experiment Data Base Adopted for the LEPRICON Adjustment Procedure

Reaction	Field	Measured Quantity	Values		$E/C-1$ (%)	Standard Deviations		
			E	C		E[a] (%)	C (%)	Combined (%)
$^{235}U(n,f)$	^{252}Cf	$\bar{\sigma}$ (b)[b]	1.205	1.236	−2.51	2.05	1.54	2.56
$^{237}Np(n,f)/^{235}U(n,f)$	^{252}Cf	$\bar{\sigma}/\bar{\sigma}$	1.105	1.094	1.01	2.10	9.31	9.54
$^{249}Pu(n,f)/^{235}U(n,f)$	^{252}Cf	$\bar{\sigma}/\bar{\sigma}$	1.500	1.447	3.66	1.38	2.03	2.45
$^{238}U(n,f)/^{235}U(n,f)$	ISNF	$\bar{\sigma}/\bar{\sigma}$	0.0919	0.0910	0.99	0.69	4.24	4.30
$^{238}U(n,f)/^{235}U(n,f)$	ISNF	$\bar{\sigma}/\bar{\sigma}$	0.0926	0.0910	1.76	1.41	4.24	4.47
$^{237}Np(n,f)/^{235}U(n,f)$	ISNF	$\bar{\sigma}/\bar{\sigma}$	0.510	0.513	−0.58	2.02	10.28	10.48
$^{249}Pu(n,f)/^{235}U(n,f)$	ISNF	$\bar{\sigma}/\bar{\sigma}$	1.155	1.143	1.05	1.29	2.67	2.97
$^{27}Al(n,\alpha)$	^{252}Cf	$\bar{\sigma}$ (mb)	1.006	0.984	2.24	2.19	8.70	8.97
$^{58}Ni(n,p)$	^{252}Cf	$\bar{\sigma}$ (mb)	118	114.3	3.24	2.43	3.82	4.53
$^{115}In(n,n')$	^{252}Cf	$\bar{\sigma}$ (mb)	196.4	182.8	7.44	2.45	4.64	5.25
$^{46}Ti(n,p)$	^{252}Cf	$\bar{\sigma}$ (mb)	138	129	6.98	2.54	6.45	6.93
$^{63}Cu(n,\alpha)$	^{252}Cf	$\bar{\sigma}$ (mb)	0.709	0.689	2.90	2.44	8.43	8.78
$^{27}Al(n,\alpha)$	PCA SP	RR[c]	3.06−34[d]	2.90−34	5.52	7.99	11.31	13.85
$^{58}Ni(n,p)$	PCA SP	RR	2.40−32	2.36−32	1.69	7.70	7.83	10.98
$^{115}In(n,n')$	PCA SP	RR	3.64−32	3.51−32	3.70	7.85	7.48	10.84
$^{237}Np(n,f)$	PCA SP	RR	2.88−31	2.75−31	4.73	7.93	10.58	13.22
$^{58}Ni(n,p)$	PCA T/4	RR	5.45−33	4.92−33	10.77	7.70	11.12	13.53
$^{115}In(n,n')$	PCA T/4	RR	1.07−32	1.02−32	4.90	7.29	9.93	12.32
$^{237}Np(n,f)$	PCA T/4	RR	1.16−31	1.14−31	1.75	7.36	12.74	14.71
$^{238}U(n,f)$	PCA T/4	RR	1.80−32	1.63−32	10.43	10.14	9.03	13.58
$^{63}Cu(n,\alpha)$	PSF SSC	RR	1.33−33	1.12−33	18.75	6.34	14.22	15.57
$^{46}Ti(n,p)$	PSF SSC	RR	2.65−32	2.16−32	22.69	6.34	13.53	14.94
$^{54}Fe(n,p)$	PSF SSC	RR	2.02−31	1.76−31	14.77	5.85	12.22	13.55
$^{58}Ni(n,p)$	PSF SSC	RR	2.79−31	2.41−31	15.77	8.29	12.17	14.73
$^{63}Cu(n,\alpha)$	PSF T/4	RR	9.08−35	8.21−35	10.60	5.91	16.40	17.43
$^{46}Ti(n,p)$	PSF T/4	RR	1.75−33	1.43−33	22.38	6.33	16.15	17.35
$^{54}Fe(n,p)$	PSF T/4	RR	1.19−32	1.05−32	13.33	5.78	14.69	15.79
$^{58}Ni(n,p)$	PSF T/4	RR	1.69−32	1.45−32	16.55	6.14	14.49	15.74
$^{237}Np(n,f)$	PSF T/4	RR	6.05−31	5.80−31	4.31	7.84	15.32	17.21
$^{238}U(n,f)$	PSF T/4	RR	6.74−32	6.01−32	12.15	10.55	13.12	16.84
$^{63}Cu(n,\alpha)$	PSF 3T/4	RR	1.21−35	1.06−35	14.15	6.10	20.09	21.00
$^{46}Ti(n,p)$	PSF 3T/4	RR	2.29−34	1.73−34	32.37	6.84	20.23	21.36
$^{54}Fe(n,p)$	PSF 3T/4	RR	1.62−33	1.29−33	25.58	6.41	18.27	19.36
$^{58}Ni(n,p)$	PSF 3T/4	RR	2.40−33	1.86−33	29.03	6.80	17.76	19.02

[a]Experimental standard deviations have been multiplied by E/C to put them on the same relative basis as those of the calculation.

[b]The symbol $\bar{\sigma}$ should not be confused with the symbols σ_i and σ_o introduced later, which represent input and output standard deviations.

[c]Units of reaction rates are reactions per second per atom per source neutron per second.

[d]Read 3.06×10^{-34}.

Inspection of Table I reveals that all but two experiments are undercalculated using the ELXSIR library (21) which was derived from ENDF/B-IV for the cross sections involved in the transport process and from an update of the ENDF/B-V dosimetry cross sections (22), with a strong implication that similar underpredictions of PWR measurements and PV fluxes probably would occur as well. It is also evident from Table I that the uncertainties in the calculations are significantly higher than those of the measurements, particularly for those experiments involving transport through iron. If this were not the case, then there would obviously be little need for the measurements.

The covariances of the benchmark measurements are shown in Table II in the form of a correlation matrix. The covariances of the benchmark calculations are developed in the next section.

IV. DEVELOPMENT OF THE DIFFERENTIAL DATA BASE

The benchmark data base, in addition to the data presented in Tables I and II, also must contain a selection of parameters determined to be of particular importance to the calculations, their values, covariances, flux sensitivities, and ultimately, the covariances of the calculated benchmark responses. For the benchmarks as well as for subsequent PWR calculations, these parameters consist of two basic types: nuclear data that is differential in the energy, and non-nuclear data that involves geometric and physical properties of the reactor components, source distributions, and transport method approximations. The propagation of nuclear data uncertainties through the transport calculations to uncertainties in the dosimetry responses and/or fluxes was handled by means of sensitivities [viz., Eq.(2) in Section II] which were calculated using the FORSS code. (23) The non-nuclear data assume the form of group-dependent flux bias factors. These bias factors provide a means for correcting the calculations for a given datum perturbation or a method approximation. Often the values of these bias factors may be assumed originally to be unity, since the most probable values of the data are used in the reference calculation, but their uncertainties will dictate, in general, values different from unity after adjustment. The sensitivities no longer need to be calculated, however, for if a corrected flux is written as

$$(\phi c)g = \phi g \prod_j (BFj')g, \qquad (20)$$

then

$$S=[d(\phi c)g/(\phi c)g]/[d(BFj')g/(BFj')g]=1. \qquad (21)$$

The benchmark parameters consist of three spectral shapes, i.e., normalized fission spectra for U235, Cf252, and the ISNF, two types of flux bias factors of unit magnitude (the first is due to the effect of a finite core height in the PCA and PSF 2-D calculations, the second arises from the magnitude of the PSF source as calculated by diffusion theory), and 13 partial cross sections (three total inelastic cross sections for the major components in stainless steel and ten dosimetry reaction cross sections). Most of these parameters are uncorrelated, the exceptions being the ISNF field which contains a U235 component, the spatial correlations among the bias factors of a given type,

TABLE II

Correlation Matrix of the Measurements in the LEPRICON Dosimetry Benchmark Data Base*

Reaction	PSD (%)	^{252}Cf			ISNF				^{252}Cf					PCA 12/13 SP				PCA 12/13 T/4				PSF SSC				PSF T/4						PSF 3T/4			
		25	37/25	49/25	28/25	28/25	37/25	49/25	Aluminum	Nickel	Indium	Titanium	Copper	Aluminum	Nickel	Indium	37	Nickel	Indium	37	28	Copper	Titanium	Iron	Nickel	Copper	Titanium	Iron	Nickel	37	28	Copper	Titanium	Iron	Nickel
^{252}Cf																																			
25	2.10	100																																	
37/25	2.08	−9	100																																
49/25	1.33	−19	32	100																															
ISNF																																			
28/25	0.68	14	9		100																														
28/25	1.39	2	15	3	7	100																													
37/25	2.03	−14	98	32	4	14	100																												
49/25	1.28	−21	32	95		4	33	100																											
^{252}Cf																																			
Aluminum	2.14								100																										
Nickel	2.35								75	100																									
Indium	2.28								77	70	100																								
Titanium	2.37								74	68	70	100																							
Copper	2.37	34											100																						
PCA SP																																			
Aluminum	7.57													100																					
Nickel	7.57													75	100																				
Indium	7.57													75	75	100																			
37	7.57													75	75	75	100																		
PCA T/4																																			
Nickel	6.95													64	90	64	64	100																	
Indium	6.95													64	64	90	64	70	100																
37	7.23													62	62	62	86	67	67	100															
28	9.18													49	49	49	49	53	53	60	100														
PSF SSC																																			
Copper	5.34													13	13	13	13	14	14	14	11	100													
Titanium	5.17													14	14	14	14	15	15	14	11	79	100												
Iron	5.10													14	14	14	14	15	15	14	11	80	82	100											
Nickel	7.16													33	58	33	33	63	36	34	27	56	58	58	100										
PSF T/4																																			
Copper	5.34													13	13	13	13	14	14	14	11	82	79	80	56	100									
Titanium	5.17													14	14	14	14	15	15	14	11	79	84	82	58	79	100								
Iron	5.10													14	14	14	14	15	15	14	11	80	82	83	58	80	82	100							
Nickel	5.27													13	16	13	13	17	14	14	11	77	79	80	59	77	79	80	100						
37	7.52													9	9	9	11	10	10	19	16	56	56	56	40	56	56	56	55	100					
28	9.41													7	7	7	7	8	8	17	49	44	45	45	32	44	45	45	44	40	100				
PSF 3T/4																																			
Copper	5.34													13	13	13	13	14	14	14	11	82	79	80	56	82	79	80	77	56	44	100			
Titanium	5.17													14	14	14	14	15	15	14	11	79	84	82	58	79	84	82	79	56	45	79	100		
Iron	5.10													14	14	14	14	15	15	14	11	80	82	83	58	80	82	83	80	56	45	80	82	100	
Nickel	5.27													13	16	13	13	17	14	14	11	77	79	80	59	77	79	80	81	55	44	77	79	80	100

*Matrix is symmetric; only the lower half is shown. Values of zero can be assumed if no entry is given. All correlations have been multiplied by 100.

and the dosimetry cross sections of Ref. 22. Inelastic cross-section covariances for iron, chromium, and nickel were taken from ENDF/B-V using the PUFF code (24), as were fission cross-section covariances for Np237 and Pu239. Covariances for the fission spectra were developed from suggestions by Perey and Marable (25), and covariances for the two types of bias factors were estimated by Maudlin and Maerker in Reference (26).

The sensitivities of the dosimeter reaction rates to the bias factors, dosimetry cross sections, and calculated fluxes at the dosimeter location are all identical. For dosimeter d, since

$$\bar{r}d = \sum_g (\sigma d)g\ (\phi g) \prod_j (BFj)g = \sum_g (\sigma d)g\ (\phi c)g, \quad (22)$$

it follows that, for each of the three terms $(X)g$ in Eq.(22),

$$S = d(\bar{r}d)/(\bar{r}d)/[d(X)g/(X)g] = (\sigma d)g\ (\phi c)g/(\bar{r}d). \quad (23)$$

These reaction rate sensitivities are thus the fractional contributions of each group to the corrected reaction rate. By invoking the chain rule for sensitivities, these dosimeter sensitivities to nuclear data $(p)g$ used in the transport become

$$S[\bar{r}d \text{ to } (p)g] = S[\bar{r}d \text{ to } (\phi c)g'] \cdot S[(\phi c)g' \text{ to } (p)g],\ g' \geq g. \quad (24)$$

By combining the sensitivities and covariances for each of the parameters involved in each benchmark and summing, the resulting correlation matrix of the calculated values may be obtained and is shown in Table III. Comparison of corresponding entries in Tables II and III shows that more of the experiments are correlated (albeit rather weakly) in the calculations and that the correlations among the calculated responses are also generally higher. However, as was pointed out earlier, the most significant difference lies in the fact that the uncertainties in the calculations are also consistently higher. For the PCA and PSF experiments in the pressure vessel, the differences become even more apparent, and suggest that the increasing contribution from uncertainties in the inelastic cross sections of iron are beginning to dominate. Since the data in Table I indicate a growing tendency of the calculations to underpredict the measurements as more iron is penetrated, a conclusion that is difficult to avoid is that the iron ENDF/B-IV inelastic data (and also that of ENDF/B-V, since there is very little if any difference between them) is deficient and should be remeasured. An application of the LEPRICON methodology to the on-line PWR H.B. Robinson-2, the results of which will be summarized in the following section, reinforces this tentative conclusion with additional data on the size of the adjustments in this cross-section that are required to effect agreement with measurement.

V. APPLICATION TO CYCLE 9 OF H.B. ROBINSON-2

The entire LEPRICON procedure has been applied to the first cycle of an older PWR in which the distribution of fresh and burned fuel was altered from that of previous cycles in order to provide lower leakage from the core to reduce the rate of accumulated PV fluence. (27) This PWR contains a 24.15cm-thick pressure vessel which is thicker than average and should serve as a severe test of the accuracy of the iron cross sections since dosimetry was located in the cavity behind the vessel as

TABLE III

Correlation Matrix of the Calculations in the LEPRICON Dosimetry Benchmark Data Base*

Reaction	PSD (%)	^{252}Cf			ISNF				^{252}Cf					PCA 12/13 SP				PCA 12/13 T/4				PSF SSC				PSF T/4						PSF 3T/4			
		25	37/25	49/25	28/25	28/25	37/25	49/25	Aluminum	Nickel	Indium	Titanium	Copper	Aluminum	Nickel	Indium	37	Nickel	Indium	37	28	Copper	Titanium	Iron	Nickel	Copper	Titanium	Iron	Nickel	37	28	Copper	Titanium	Iron	Nickel
^{252}Cf																																			
25	1.54	100																																	
37/25	9.31	-17	100																																
49/25	2.03	21	-3	100																															
ISNF																																			
28/25	4.24	-5	1	4	100																														
28/25	4.24	-5	1	4	100	100																													
37/25	10.28	-11	93	-1	33	33	100																												
49/25	2.67	10	-2	59	55	55	20	100																											
^{252}Cf																																			
Aluminum	8.70	1	6	4					100																										
Nickel	3.82	19	1	-10	-3	-3	-1	-4	72	100																									
Indium	4.64		1	1					19	14	100																								
Titanium	6.45	1	5	3					87	77	17	100																							
Copper	8.43	1	6	4					91	71	19	86	100																						
PCA SP																																			
Aluminum	11.31				50	50	10	6	7	3		3	1	100																					
Nickel	7.83	7	-1	-6	42	42	8	3	3	22		7	2	87	100																				
Indium	7.48				33	33	7	3			59			69	74	100																			
37	10.58		82		23	23	82	2						48	51	44	100																		
PCA T/4																																			
Nickel	11.12	5	-1	-4	29	29	6	2	2	15		5	1	68	86	65	44	100																	
Indium	9.93				24	24	5	2			45			57	66	85	40	82	100																
37	12.74		72		19	19	73	2						44	49	43	91	60	59	100														
28	9.03	10	-2	3	28	28	5	5						66	75	65	45	93	88	66	100														
PSF SSC																																			
Copper	14.22				34	34	7	4	1	2		2	6	63	60	46	31	53	41	31	48	100													
Titanium	13.53				28	28	6	3	2	7		11	1	54	58	43	29	55	41	30	47	95	100												
Iron	12.22	3	-1	-2	22	22	4	2	2	7		4	1	44	50	37	25	49	38	28	44	93	96	100											
Nickel	12.17	5	-1	-4	21	21	4	1	2	15		4	1	42	51	36	25	50	37	27	42	92	95	98	100										
PSF T/4																																			
Copper	16.40				31	31	6	4	1	2		1	5	66	65	51	35	62	49	36	57	96	91	88	87	100									
Titanium	16.15				26	26	5	3	1	6		9	1	57	65	50	33	67	50	36	58	90	96	91	90	94	100								
Iron	14.69	3		-2	21	21	4	1	2	6		3	1	48	60	47	32	64	50	36	57	88	93	95	93	91	97	100							
Nickel	14.49	4	-1	-3	20	20	4	1	1	12		4	1	47	61	46	31	64	50	36	57	88	93	94	96	90	96	99	100						
37	15.32		61		12	12	60	1						27	31	28	71	33	32	70	36	66	68	72	72	65	66	71	71	100					
28	13.12	7	-1	2	18	18	3	3						40	46	40	28	50	47	35	54	85	87	92	92	85	88	94	94	77	100				
PSF 3T/4																																			
Copper	20.09				26	26	5	3	1	2		1	4	64	64	51	35	70	57	42	66	88	83	80	78	95	89	85	84	58	78	100			
Titanium	20.23				22	22	4	2	1	4		7	1	55	66	51	34	77	60	42	68	82	88	83	81	89	95	92	91	59	80	93	100		
Iron	18.27	2		-2	17	17	3	1	1	5		2	1	46	61	49	33	75	62	44	70	79	85	87	85	85	92	95	94	64	87	88	96	100	
Nickel	17.76	3	-1	-2	17	17	3	1	1	10		3	1	45	62	48	33	75	62	45	70	79	85	86	87	84	91	94	95	66	89	87	95	99	100

*Matrix is symmetric; only the lower half is shown. Values of zero can be assumed if no entry is given. All correlations have been multiplied by 100.

well as in front of it.

The bias factors invoked for this PWR appear in Table IV, only one of which (BF 5) is common to the benchmark data base. Covariances of these bias factors were based on uncertainties in geometric and materials data estimated from our own limited experience, discussions with others qualified in the field, and as a result of an ad hoc specialists meeting convened in 1980. (28) Table V presents the flux uncertainties at the in-vessel dosimeter location arising from both the nuclear data and the pertinent bias factors, and Tables VI and VII show similar information for the cavity dosimeter and PV locations.

TABLE IV

Flux Bias Factors Assumed in the Calculations

Bias Factor	Source of Bias Factor Uncertainty	Locations
1	Dosimetry capsule location	Downcomer only
2	Finite capsule perturbation	Downcomer only
3	Pressure vessel out-of-roundness	Cavity and pressure vessel
4	Coolant density	Downcomer, cavity, and pressure vessel
5	Three-dimensional flux synthesis	Downcomer, cavity, and pressure vessel
6	Steel density	Downcomer, cavity, and pressure vessel

TABLE V

Standard Deviations in the Fluxes at the Downcomer Dosimeter Location Arising from Parameter Uncertainties

Flux Group	Lower Energy (MeV)	Standard Deviation (%)							
				Bias Factor					
		χ_{25}	$\sigma_{steel}(n,n')$	1	2	4	5	6	Total
1	11.1	14.1	13.2	10.9	1.0	3.1	1.5	3.0	22.7
2	8.2	10.6	13.7	12.1	1.0	3.4	1.5	3.1	21.7
3	6.1	8.1	13.3	13.3	1.0	3.8	1.5	3.4	21.2
4	4.1	6.4	14.3	14.7	1.0	4.2	1.5	3.6	22.3
5	3.0	6.1	13.2	17.0	2.0	5.0	1.5	3.5	23.3
6	2.6	5.5	9.7	17.8	2.5	5.3	1.5	3.3	22.1
7	2.1	5.1	9.5	18.0	3.0	5.7	1.5	3.2	22.2
8	1.8	5.2	9.2	18.3	3.5	6.0	1.5	3.1	22.5
9	1.5	5.2	8.8	19.3	3.5	6.3	1.5	3.0	23.3
10	1.2	5.1	8.9	19.5	4.0	6.5	1.5	2.9	23.5
11	0.9	5.2	8.0	20.3	4.5	6.9	1.5	2.6	24.1
12	0.6	5.1	5.4	20.5	5.0	7.2	1.5	2.4	23.7
13	0.4	5.1	5.4	20.2	5.5	7.6	1.5	2.1	23.6
14	0.2	5.1	5.4	19.8	6.0	7.7	1.5	1.9	23.4
15	0.1	5.1	5.3	18.4	6.5	7.5	1.5	1.9	22.3

TABLE VI

Standard Deviations in the Fluxes at the Cavity Dosimeter Location Arising from Parameter Uncertainties

Flux Group	Lower Energy (MeV)	Standard Deviation (%)						
				Bias Factor				
		χ_{25}	$\sigma_{steel}(n,n')$	3	4	5	6	Total
1	11.1	14.1	29.6	6.7	3.7	2.5	5.5	34.3
2	8.2	10.6	30.8	7.3	4.0	2.5	5.8	34.3
3	6.1	8.1	29.8	7.9	4.4	2.5	6.3	32.9
4	4.1	6.4	32.2	8.6	4.9	2.5	6.6	35.0
5	3.0	6.1	29.8	9.2	5.5	2.5	6.4	33.0
6	2.6	5.5	21.8	9.6	5.7	2.5	6.2	26.0
7	2.1	5.1	21.3	9.9	6.0	2.5	6.0	25.6
8	1.8	5.2	20.6	9.9	6.0	2.5	5.8	25.0
9	1.5	5.2	19.9	10.1	6.2	2.5	5.5	24.5
10	1.2	5.1	20.0	10.2	6.3	2.5	5.2	24.6
11	0.9	5.2	18.0	10.3	6.5	2.5	4.5	22.9
12	0.6	5.1	12.0	10.5	6.4	2.5	3.8	18.5
13	0.4	5.1	12.0	10.6	6.9	2.5	3.4	18.7
14	0.2	5.1	12.2	10.7	6.9	2.5	2.8	18.7
15	0.1	5.1	12.0	10.7	7.1	2.5	2.8	18.7

TABLE VII

Standard Deviations in the Fluxes at the Critical LCW and T/4 Pressure Vessel Locations Arising from Parameter Uncertainties

Flux Group	Lower Energy (MeV)	Standard Deviation (%)									
			$\sigma_{steel}(n,n')$		Bias Factor					Total	
							5				
		χ_{2s}	LCW	T/4	3	4	LCW	T/4	6	LCW	T/4
1	11.1	14.1	11.4	15.9	6.8	3.7	5.0	1.5	3.0	20.6	22.9
2	8.2	10.6	11.9	16.5	7.4	4.1	5.0	1.5	3.1	19.0	21.7
3	6.1	8.1	11.5	16.0	7.9	4.5	5.0	1.5	3.4	17.8	20.4
4	4.1	6.4	12.4	17.3	8.6	5.0	5.0	1.5	3.6	18.2	21.3
5	3.0	6.1	11.4	15.9	9.5	5.7	5.0	1.5	3.5	18.1	20.7
6	2.6	5.5	8.4	11.7	10.0	6.0	5.0	1.5	3.3	16.5	17.8
7	2.1	5.1	8.2	11.4	10.2	6.3	5.0	1.5	3.2	16.5	17.7
8	1.8	5.2	8.0	11.0	10.3	6.3	5.0	1.5	3.1	16.5	17.5
9	1.5	5.2	7.7	10.7	10.5	6.5	5.0	1.5	3.0	16.5	17.4
10	1.2	5.1	7.7	10.7	10.6	6.5	5.0	1.5	2.9	16.5	17.5
11	0.9	5.2	6.9	9.6	10.6	6.6	5.0	1.5	2.6	16.2	16.9
12	0.6	5.1	4.7	6.5	10.9	6.5	5.0	1.5	2.4	15.5	15.4
13	0.4	5.1	4.7	6.5	10.9	7.0	5.0	1.5	2.1	15.7	15.6
14	0.2	5.1	4.7	6.6	10.9	7.0	5.0	1.5	1.9	15.6	15.6
15	0.1	5.1	4.6	6.4	10.9	7.2	5.0	1.5	1.9	15.7	15.6

The LCW location refers to the lower circumferential weld in Table VII above. These tables show that the contribution from the iron inelastic uncertainty is significant at the in-vessel location, a major contributor at the critical PV locations, and dominates in the reactor cavity. The advantages of cavity over downcomer dosimetry are apparent since the cavity activities possess higher sensitivities to the same sources of uncertainty that influence the PV fluxes, such as the iron cross sections and the PV out-of-roundness, and at the same time no sensitivity to the location of the downcomer dosimetry to which the PV flux is also insensitive.

The complete correlation matrix of the calculated activities is shown in Table VIII, where high degrees of correlation are seen to exist both among the activities at a given dosimetry location (the auto-correlations) and between the activities at different locations (the cross-correlations). This is primarily

TABLE VIII

Complete Correlation Matrix of the Calculated Activities*

Target Atom	Standard Deviation (%)	Downcomer Location						Cavity Location					
		^{63}Cu	^{46}Ti	^{54}Fe	^{58}Ni	^{238}U	^{237}Np	^{63}Cu	^{46}Ti	^{54}Fe	^{58}Ni	^{238}U	^{237}Np
Downcomer Location													
^{63}Cu	19.7	100[a]											
^{46}Ti	20.3	96	100										
^{54}Fe	20.9	93	98	100									
^{58}Ni	21.0	93	97	99	100								
^{238}U	21.2	89	92	96	97	100							
^{237}Np	23.9	79	82	86	87	90	100						
Cavity Location													
^{63}Cu	30.6	87	82	76	75	69	59	100					
^{46}Ti	31.7	84	87	83	82	74	62	95	100				
^{54}Fe	32.0	80	86	87	86	80	68	87	96	100			
^{58}Ni	31.4	80	86	88	87	82	69	86	95	100	100		
^{238}U	30.0	78	82	86	86	86	74	80	88	95	96	100	
^{237}Np	29.0	76	80	83	83	83	89	73	80	85	87	89	100

*Matrix is symmetric; only the lower half is given.

[a]All elements have been multiplied by 100.

due, of course, to the significant uncertainties in the iron inelastic data that are propagated to all flux groups by the transport process, and hence represent a strong source of correlation among the calculated fluxes.

Covariances of the 12 dosimeter measurements were estimated with the help of the experimentalists. (29) Four sources of uncertainty were identified and quantified: random counting statistics, gamma-ray counter efficiency calibrations, bias factors arising from contributions of competing reactions, and normalization of the measured activities during exposure to one core neutron/second as required by the LEPRICON adjustment module. The major contributors were the counter calibration and source normalization, both of which produce correlations among the measurements. The complete correlation matrix of the measured activities appears in Table IX below.

TABLE IX

Complete Correlation Matrix of the Measured Activities*

Target Atom	Standard Deviation (%)	Downcomer Location						Cavity Location					
		^{63}Cu	^{46}Ti	^{54}Fe	^{58}Ni	^{238}U	^{237}Np	^{63}Cu	^{46}Ti	^{54}Fe	^{58}Ni	^{238}U	^{237}Np
Downcomer Location													
^{63}Cu	6.72	100[a]											
^{46}Ti	6.16	31	100										
^{54}Fe	6.16	31	64	100									
^{58}Ni	6.16	31	55	72	100								
^{238}U	8.00	24	26	26	26	100							
^{237}Np	6.65	29	32	32	32	78	100						
Cavity Location													
^{63}Cu	6.72	54	31	31	31	24	29	100					
^{46}Ti	6.16	31	64	44	42	26	32	31	100				
^{54}Fe	6.16	31	44	64	47	26	32	31	64	100			
^{58}Ni	6.16	31	42	47	64	26	32	31	55	72	100		
^{238}U	.11.79	16	18	18	18	26	24	16	18	18	18	100	
^{237}Np	7.93	24	27	27	27	29	46	24	27	27	27	84	100

*Matrix is symmetric; only the lower half is given.

[a]All elements have been multiplied by 100.

Comparison of Tables VIII and IX again shows that both the standard deviations and the correlations of the calculations are higher than corresponding values of the measurements, thus increasing the covariances of the calculations in two ways. The similarity to the comparisons obtained in Section IV for the PCA and PSF benchmarks reinforces the earlier conclusion that the dosimetry is of critical importance in directing the course of the adjustment procedure.

As a final illustration of the results of the procedure for estimating the á priori covariances for this reactor, the cross-correlation matrix between both sets of important PV fluxes and both sets of dosimeter activities is presented in Table X. As has been already mentioned in Section II in the derivation of Eq.(17), the effectiveness of the adjustment procedure (i.e., of the dosimetry) is determined by the elements of just such a matrix as the one shown here. Reasonably high values for these cross-correlations are sine qua non to the success of the whole methodology. The entries in Table X are in the vicinity of 0.5, which, while not overwhelming, are deemed adequate. It should also be noted that the cavity location is clearly superior in

providing information about the PV flux levels.

TABLE X

Cross-Correlation Matrix Between the Calculated Critical Pressure Vessel Fluxes and the Dosimeter Activities

Flux Group	Lower Energy (MeV)	Downcomer Location						Cavity Location					
		^{63}Cu	^{46}Ti	^{54}Fe	^{58}Ni	^{238}U	^{237}Np	^{63}Cu	^{46}Ti	^{54}Fe	^{58}Ni	^{238}U	^{237}Np
1	11.1	58[a] (59)[b]	46 (46)	36 (35)	35 (34)	31 (31)	25 (24)	67 (72)	53 (56)	40 (41)	40 (40)	37 (37)	33 (31)
2	8.2	56 (56)	44 (43)	33 (32)	33 (32)	29 (28)	23 (22)	69 (74)	54 (57)	40 (40)	40 (40)	38 (37)	33 (31)
3	6.1	59 (62)	61 (66)	57 (62)	56 (60)	47 (49)	36 (38)	69 (74)	76 (82)	75 (82)	73 (80)	65 (69)	57 (60)
4	4.1	53 (55)	58 (62)	56 (60)	55 (59)	45 (48)	35 (36)	64 (67)	74 (79)	76 (82)	74 (80)	65 (69)	58 (60)
5	3.0	51 (54)	56 (60)	54 (59)	53 (57)	44 (47)	34 (36)	62 (66)	71 (77)	73 (80)	72 (78)	64 (69)	58 (60)
6	2.6	44 (48)	46 (51)	45 (51)	45 (50)	42 (47)	32 (36)	55 (60)	59 (66)	63 (71)	64 (72)	64 (72)	54 (58)
7	2.1	41 (44)	42 (46)	42 (46)	41 (46)	40 (45)	31 (34)	51 (56)	54 (61)	59 (66)	60 (67)	63 (70)	52 (56)
8	1.8	42 (45)	43 (47)	42 (48)	42 (47)	41 (45)	32 (35)	52 (57)	55 (62)	59 (67)	60 (68)	63 (70)	53 (57)
9	1.5	42 (45)	42 (47)	42 (47)	42 (47)	40 (45)	32 (35)	52 (57)	55 (62)	58 (66)	60 (67)	62 (70)	53 (57)
10	1.2	42 (46)	43 (48)	42 (48)	42 (47)	40 (45)	32 (35)	52 (58)	55 (62)	59 (67)	60 (68)	62 (70)	53 (57)
11	0.9	43 (48)	44 (50)	43 (49)	43 (48)	40 (45)	32 (35)	53 (60)	57 (65)	59 (68)	60 (68)	60 (68)	54 (58)
12	0.6	39 (44)	40 (47)	39 (45)	38 (44)	34 (39)	28 (32)	47 (54)	51 (59)	52 (61)	52 (61)	51 (57)	51 (56)
13	0.4	39 (44)	40 (46)	39 (45)	38 (44)	34 (39)	28 (32)	47 (53)	51 (59)	52 (61)	52 (60)	51 (57)	50 (55)
14	0.2	39 (44)	41 (47)	39 (45)	38 (44)	34 (39)	28 (32)	47 (54)	51 (59)	52 (61)	53 (61)	51 (58)	50 (55)
15	0.1	39 (43)	40 (46)	38 (44)	38 (43)	34 (38)	28 (31)	47 (53)	51 (59)	52 (61)	52 (60)	51 (57)	50 (55)

[a]All elements have been multiplied by 100.

[b]The LCW flux cross correlations appear first, followed by the T/4 flux cross correlations in parentheses.

A summary of the comparisons between measured and calculated activities before any adjustment (cols. 2 and 4) and between the measured and adjusted activities (cols. 3 and 5) are shown in Table XI. The important things to observe are the magnitudes of the disagreement in cols. 2 and 4, the close proximity of the adjusted to the measured values, and the reductions by factors of about 4 in the standard deviations of the pre- and post-adjusted differences. It is also of interest to observe that the disagreements between calculations and measurements in the cavity exceed the standard deviations by about 50%, thus suggesting a possible underestimate in the iron uncertainties. Combining all 12 HBR-2 measurements and the 34 benchmarks leads to a value of chi-square per degree of freedom of 1.15. When the Np237 cavity measurement is "deactivated" (i.e., prevented from being included in the adjustment procedure), the resulting value of chi-square per degree of freedom for the remaining 45 measurements becomes, almost unbelievably, 1.00 - a dramatic and significant change. Consequently, until this discrepancy is eventually resolved, adjustments are based on only 11 of the HBR-2 experiments.

TABLE XI

Comparison of Calculated C and Adjusted A HBR-2 Activities with Measurement E

Reaction	Downcomer Dosimeter		Cavity Dosimeter	
	$(C/E-1) \pm \sigma_i$[a]	$(A-E)/E \pm \sigma_0$	$(C/E-1) \pm \sigma_i$	$(A-E)/E \pm \sigma_0$
$^{63}Cu(n,\alpha)^{60}Co$	−17.3% ± 17.6%	−3.6 ± 4.2[b]	−27.9 ± 23.1	−3.7 ± 5.2
$^{46}Ti(n,p)^{46}Sc$	−19.2 ± 17.5	0.6 ± 4.2	−34.5 ± 21.7	−1.1 ± 4.5
$^{54}Fe(n,p)^{54}Mn$	−17.4 ± 18.3	0.0 ± 4.5	−32.2 ± 22.6	2.8 ± 5.0
$^{58}Ni(n,p)^{58}Co$	−13.3 ± 19.2	5.5 ± 4.7	−33.9 ± 21.7	−0.3 ± 4.8
$^{238}U(n,f)^{137}Cs$	−20.0 ± 18.8	−7.1 ± 4.8	−34.8 ± 22.8	−8.7 ± 5.7
$^{237}Np(n,f)^{137}Cs$	−15.0 ± 21.4	−4.3 ± 5.4	−39.0 ± 19.4	−18.5 ± 5.8[c]

[a]The values of σ_i, the relative standard deviations of $(C-E)$, are calculated as $(\sigma_E^2 + \sigma_C^2 C^2/E^2)^{1/2}$, where σ_E and σ_C are the standard deviations of the measured and calculated activities, respectively.

[b]Read as −3.6% with a relative standard deviation in A of 4.2%.

[c]This experiment was adjusted on the basis of sensitivity to the adjusted parameters only. It did not actively participate in the adjustment procedure and is included only for completeness.

The covariances of the adjusted activities appear in Table XII. Comparison of the correlations with those in Tables VIII and IX shows that they are smaller than those of the original calculations, but larger than those of the measurements. The standard deviations, of course, are smaller than either.

TABLE XII

Complete Correlation Matrix of the Adjusted Activities*

Target Atom	Standard Deviation (%)	Downcomer Location						Cavity Location					
		^{63}Cu	^{46}Ti	^{54}Fe	^{58}Ni	^{238}U	^{237}Np	^{63}Cu	^{46}Ti	^{54}Fe	^{58}Ni	^{238}U	^{237}Np
Downcomer Location													
^{63}Cu	4.2	100[a]											
^{46}Ti	4.2	90	100										
^{54}Fe	4.5	82	91	100									
^{58}Ni	4.7	81	91	96	100								
^{238}U	4.8	73	74	84	87	100							
^{237}Np	5.4	67	68	76	79	90	100						
Cavity Location													
^{63}Cu	5.2	73	62	54	54	50	46	100					
^{46}Ti	4.5	67	76	68	67	53	49	85	100				
^{54}Fe	5.0	57	67	75	72	62	55	65	87	100			
^{58}Ni	4.8	56	65	71	74	66	59	64	84	97	100		
^{238}U	5.7	47	48	56	59	74	63	53	60	78	85	100	
^{237}Np	5.8	40	44	50	52	53	65	43	53	66	70	73	100

*Matrix is symmetric; only the lower half is given. The ^{237}Np cavity dosimeter was deactivated.
[a]All elements have been multiplied by 100.

Table XIII presents a summary of the flux adjustments with their reduced uncertainties at the LCW pressure vessel location for several combinations of active HBR-2 experiments but always including the benchmarks. The column headed "none" represents the a priori standard deviations. The last four columns give results of the adjustment when (a) only the in-vessel dosimetry is activated, (b) only the cavity dosimetry including Np237 is activated, (c) only the cavity dosimetry but excluding Np237 is activated, and (d) both the in-vessel and cavity dosimetry save for the Np237 cavity are simultaneously activated. Comparison of the a priori column with the last column (the most consistent combination) shows the standard deviations are about halved for fluxes above 3 MeV. Adjustments are observed to be considerable.

TABLE XIII

Flux Adjustments and Standard Deviations at the Critical LCW Pressure Vessel Location as Functions of HBR-2 Measurements Activated

Flux Group	Lower Energy (MeV)	None	34 Benchmarks +			
			6 Downcomer Only	6 Cavity Only	5 Cavity Only	6 Downcomer + 5 Cavity
1	11.1	0 ± 20.6[a]	−0.5 ± 12.5	4.5 ± 11.2	5.7 ± 11.3	8.2 ± 11.0
2	8.2	0 ± 19.0	−3.5 ± 12.4	2.1 ± 10.9	3.3 ± 10.9	6.3 ± 10.5
3	6.1	0 ± 17.8	22.9 ± 12.1	26.7 ± 10.8	27.5 ± 10.8	29.9 ± 10.3
4	4.1	0 ± 18.2	25.3 ± 12.9	29.0 ± 11.4	29.5 ± 11.4	32.0 ± 10.8
5	3.0	0 ± 18.1	23.2 ± 13.5	27.3 ± 12.1	27.4 ± 12.1	30.1 ± 11.5
6	2.6	0 ± 16.5	12.2 ± 13.8	15.5 ± 12.4	16.7 ± 12.4	20.3 ± 11.8
7	2.1	0 ± 16.5	9.2 ± 14.2	12.4 ± 12.7	13.9 ± 12.7	17.9 ± 12.1
8	1.8	0 ± 16.5	9.9 ± 14.1	13.5 ± 12.7	14.6 ± 12.7	18.4 ± 12.2
9	1.5	0 ± 16.5	9.7 ± 14.2	13.5 ± 12.9	14.6 ± 12.9	18.4 ± 12.3
10	1.2	0 ± 16.5	9.6 ± 14.3	13.8 ± 12.9	14.5 ± 12.9	18.3 ± 12.3
11	0.9	0 ± 16.2	10.4 ± 14.1	15.9 ± 12.8	15.2 ± 12.8	18.7 ± 12.3
12	0.6	0 ± 15.5	11.4 ± 13.9	19.0 ± 12.8	15.5 ± 12.9	18.2 ± 12.5
13	0.4	0 ± 15.7	11.5 ± 14.1	18.8 ± 13.0	15.5 ± 13.1	18.3 ± 12.7
14	0.2	0 ± 15.6	11.6 ± 14.0	18.5 ± 13.0	15.7 ± 13.0	18.5 ± 12.7
15	0.1	0 ± 15.7	11.4 ± 14.1	18.2 ± 13.0	15.5 ± 13.1	18.5 ± 12.7

[a]Read as a change of 0% with a standard deviation of 20.6%.

VI. CONCLUSIONS

It has been demonstrated that PWRs are amenable to prediction of pressure vessel fluence and its uncertainties by an in-depth analysis of the differential data used in the calculations in conjunction with an uncertainty analysis of existing dosimetry. Although not all bias factors were considered in the present analysis (for example, uncertainties in the composition of the concrete biological shield, in particular its water content and whether or not a steel liner is used, both of which might affect the cavity measurements, and in the radial source distributions which would affect all flux levels in the reactor beltline), subsequent consideration of these omissions in HBR-2 have not altered the main conclusions to be drawn from this paper.

The first of these important conclusions is that the use of ad hoc cavity dosimetry is preferable to the earlier more conventional in-vessel location where it was placed along with metallurgical specimens for early monitoring of any PV damage. In the determination of damaging fluence within the pressure vessel, the proximity of this latter location to the PV is outweighed by the greater sensitivity to the iron penetration afforded by the cavity location.

The second important conclusion is that accuracy in the iron total inelastic cross section is a requirement for an adequate estimate of the PV fluence, and this accuracy is not available in either the ENDF/B-IV or ENDF/B-V evaluations. Worse, these data underestimate the PV fluences, necessitating the use of conservative safety margins. The consistency of the benchmark and HBR-2 analyses in estimating the adjustments to these data in the important energy region between 3 and 8 MeV is shown in Table XIV below of the results from sequential addition of the iron-sensitive measurements. Notice should be taken of the reduction in the uncertainties as more of the experiments are considered.

TABLE XIV

Summary of Present and Past Adjustments in the Total Inelastic Cross Section of Iron in the 3- to 8-MeV Region

Energy Group	Energy Range (MeV)	ENDF/B[a]	PCA	+ PSF	+ HBR-2[b]
3	6.1 to 8.2	0.0 ± 5.4[c]	−8.9 ± 3.7	−8.7 ± 2.7	−9.4 ± 2.2
4	4.1 to 6.1	0.0 ± 5.5	−9.0 ± 3.7	−9.2 ± 2.7	−9.7 ± 2.2
5	3.0 to 4.1	0.0 ± 5.6	−8.9 ± 3.9	−9.0 ± 2.8	−9.7 ± 2.3

[a]The *a priori* values were taken from ENDF/B-V.
[b]The HBR-2 results include approximate contributions from chromium and nickel as well.
[c]Read as an adjustment of 0% with a standard deviation of 5.4%.

Expectations are high that the use of updated inelastic iron data in ENDF/B-VI, the need for which was first suggested as a consequence of these LEPRICON analyses, will result in improved agreement between calculation and measurement with the eventual adoption of less restrictive margins. Some preliminary evidence using an update to Mod-3 of ENDF/B-V (30) of such an improvement has been encouraging. (31)

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COVARIANCE DATA REQUIREMENTS

E. FORT, J. ROWLANDS and M. SALVATORES

SUMMARY

The question of covariance data requirements is dependent on the energy schemes used for application. It is concentrated here on the needs related to energy schemes in current use at present.

It is argued that for many cross sections it is not necessary to have uncertainty information for the resonance parameters but only for the infinite dilution cross sections. This argument is illustrated by calculations for ^{238}U for both fast and thermal reactors.

Nevertheless a limited number of resonances have been identified for which covariance data are required for further investigation of the general problem of resonance parameter adjustment, especially in the case where the self shielding factor is dependent on the resonance parameter.

It is proposed that the requirement is for the uncertainties in cross sections averaged over intervals of the order of E to 3E plus uncertainty correlation between these intervals. The requirements for fast reactors are illustrated by the results of a cross section adjustment study.

It is shown how the adequacy of the choice of covariance data can be verified in the course of an adjustment study and the information which is gained by varying the covariance parameters.

INTRODUCTION

Predictions of the neutronics characteristics of reactors are made using evaluated nuclear data libraries taking into account the results of analyses of integral measurements. Estimation of the accuracy of reactor neutronics predictions is an essential requirement and the reliability of these accuracy estimates depends on the quality of the covariance data, or uncertainty information, for both the evaluated nuclear data libraries and the integral measurements.

It is now usual to produce nuclear data libraries for reactor applications which have been adjusted to give a simultaneous best fit to the basic evaluations and the integral measurements. This fitting procedure produces a covariance matrix for the adjusted library which can then be used to estimate the accuracy of reactor parameter predictions. When the first adjusted cross-section sets were produced, in the mid 1960's and early 1970's, the uncertainties in the evaluated differential cross-sections were much larger than they are today and the covariance matrices for the adjusted cross-section sets were determined mainly by the integral measurement uncertainties.

The estimated uncertainties on reactor parameters calculated using the adjusted cross-sections were not so sensitive to the uncertainties assumed for the evaluated differential cross-sections. However, we find much closer agreement now between calculations made using the current

unadjusted nuclear data libraries (such as JEF-2) and integral measurements, in many cases within the uncertainties of these measurements. The accuracies of the calculations of many characteristics, such as reaction rate ratios, are comparable with those of the integral measurements, although the accuracies of Keff measurements remain significantly higher. The covariance data for the evaluated nuclear cross-sections now play a much more important role in determining the cross-section adjustments and the accuracy of reactor parameter predictions.

Also, it is possible to identify more clearly discrepant items of data, both differential cross-sections and integral measurements, but this identification depends on the reliability of the covariance data for the evaluated differential cross-sections and for the integral measurements.

Underestimation of the systematic error uncertainties associated with a particular type of integral measurement can result in an accuracy estimate for predictions of related reactor parameters which is too high and the adjustment made to related cross-sections is too large. Recent reaction rate ratio intercomparisons have shown some surprisingly large differences between results obtained using different techniques. Some fission ratio measurements depend on the relative values of the yields of selected fission products and the differences between the yield ratios found in different evaluations are as high as 3 %, introducing a systematic error uncertainty of this magnitude into the fission rate ratio measurements made using this technique. Small sample reactivity worth measurements are also subject to systematic errors. Approximations in the calculational methods used to analyse integral measurements also introduce systematic errors which must be estimated. In the analysis of buckling measurements the treatment of leakage and the assumption of an asymptotic spectrum might introduce uncertainties in some cases. However, measurements of simple geometry critical systems, such as the homogeneous Los Alamos spheres, provide Keff values which are significantly more accurate than the values which can be calculated using unadjusted nuclear data and so are very important in cross-section adjustment studies.

In order to improve the accuracy of reactor predictions and resolve discrepancies, and also to provide nuclear data for new applications, further differential and integral measurements are required. The accuracies required in the measurements depend on the balance between the two types of measurement and the accuracy of existing data. Strategies for deciding the optimum balance have been discussed, for example, by Usachev and Bobkov (1973) [1]. The accuracies required depend on the correlations which will be present in the measurements, the greater the energy correlations of the uncertainties the higher the accuracy requirement.

Although the need for covariance data is generally accepted, due to a lack of resources the provision of covariance data in evaluated nuclear data files is far from complete. There are some areas where the data are available, in particular the ENDF/B-VI standards and in files of dosimetry cross-sections, and some other evaluations (particularly in ENDF/B-VI). Work is also being undertaken by the International Cooperation on Evaluation, with the aim of identifying more precisely the requirements as well as studying ways of providing the data.

Part of the problem is deciding on the level of detail to be included in the covariance files, in particular when there is a resonance structure, and this paper discusses this question.

For reactor applications, we consider that there are two priorities for the provision of covariance data :

(a) Data for the major actinides suitable for both fast and thermal reactor studies. In the latter case, the data for Pu isotopes in the epithermal range can be of particular importance. Covariance data is also required for the structural materials, but possibly limited to the major isotopes.

(b) Data for extended isotope burn-up/build-up chains to be used in connection with fuel cycle studies, in particular those which can arise from radioactive waste transmutation strategies (capture, fission and (n,2n) cross-sections).

In terms of data types particular attention should be given to the representation of covariances in resonance regions and this question is discussed in the paper. Data for secondary energy and angular distributions of scattered neutrons should also be given consideration.

THE TYPES OF UNCERTAINTY INFORMATION TO BE DERIVED FROM THE DIFFERENTIAL CROSS-SECTION COVARIANCES

In broad terms it is the uncertainties in spectrum averaged values of cross-sections which it is required to calculated. These uncertainties can be separated into components - the uncertainties in the values of cross-sections averaged in known spectra, the relative uncertainties in the cross-sections averaged in different spectra, and the effects of uncertainties in the calculation of spectra on the spectrum averaged cross-section values. The spectrum uncertainty includes the uncertainties in the calculation of resonance shielding effects, which is considered here as a separate component. These components are now discussed in a little more detail :

1. The uncertainties in the spectrum averaged values of the important fission and capture cross-sections including the cross-sections of the secondary actinides (the spectra being specified). Also the uncertainties in ratios of spectrum averaged cross-sections are required. For shielding applications the requirement relates to the total, or transport cross-section (or the reciprocal of the total cross-section) average over a specified spectrum.
   It is clearly a requirement that the uncertainties in these spectrum averaged values should not be dependent on the group structure used to represent or process the data. A broad group representation of the covariances (E to 3E, for example) with simple covariance relations between these groups, should be a satisfactory representation.
2. Requirements relating to the differences in the values averaged over different spectra, and in the changes in values with changes in spectra (such as the changes in the thermal neutron spectrum with temperature, and, in fast reactor spectra, with sodium density) and more generally in the values calculated in different spectra. The requirements relate to the dominant fission and capture cross-sections, (^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{56}Fe). For this requirement it is necessary to take more care over the representation of covariances. It might even be preferable to give the uncertainty in the gradient of the cross-section directly. However, it should still be acceptable to use the broad group representation (E to 3E) with correlations between these group averaged uncertainties. For the interpretation of dosimetry

measurements a finer energy group structure could be required.

3. For the uncertainties in the spectrum averaged values of the dominant fission and capture reactions (as well as Doppler effects and shielding transmission) due to uncertainties in calculated spectra the inelastic and elastic scattering cross-sections play the dominant role (these being the major sources of uncertainty in calculations of the spectra, although the dominant absorption reactions also play a part). Again uncertainties in the average values of the inelastic and elastic cross-sections over energy ranges of the order of (E to 3E), plus covariances between these, should suffice. In addition to the uncertainties in the primary cross-sections the uncertainties in the mean energy (or lethargy) change and the mean cosine of scattering are required.
4. Resonance shielding effects must be treated and, for these, in principle, a separation between the uncertainty in the infinite dilution cross-section and the shielding factor is required. This information is required only for the dominant individual resonances, or for averages over energy ranges of the order of (E to 3E) (eg for the first 3 resonances in ^{238}U, the first resonance in ^{240}Pu and averages for ^{238}U in wide energy ranges, (E to 3E) at higher energies). For ^{235}U and ^{239}Pu the resonance shielding is small and is probably not a significant source of uncertainty. In fact, even for ^{238}U it is possible that, for fast reactor applications the main source of uncertainty is in the infinite dilution cross-sections, and this question is discussed further. For the uncertainties in the calculation of Doppler effects the requirements relate more directly to the resonance parameters.

COVARIANCES FOR RESONANT CROSS-SECTIONS

To illustrate the questions which have to be considered when the cross-sections have a resonance structure we look at the form of the expression for the effective cross-section averaged over a broad energy group with the resonance shielding treated in a simple way.

The effective cross-section can be written in the form :

$$\sigma^{iJ}_{eff,g} = \sigma^{iJ}_{\infty,g} \cdot f^{iJ}_{g}\,(\sigma^{J}_{o})$$

where i denotes the reaction type
J the isotope
and g the energy group

$\sigma^{iJ}_{\infty g}$ is an average value of the cross-section obtained by integration with a smooth flux through the group, ie the infinite dilution value

and $f^{iJ}_{g}\,(\sigma^{J}_{o})$ is the factor which corrects for the flux perturbations caused by the resonances in the isotope J

here σ^{J}_{o} is the background cross-section per atom of isotope J. In the general case it takes into account the heterogeneity of the composition.

When the narrow resonance approximation applies, we have :

$$f^{iJ}_{g}\,(\sigma^{J}_{o}) = \left\{ \frac{\int_{g} \frac{\sigma^{iJ}(E) \cdot C(E)\,dE}{(\sigma^{tJ}(E) + \sigma^{J}_{o})}}{\int_{g} \sigma^{iJ}(E) \cdot C(E)\,dE} \right\}$$

and $\sigma^{iJ}_{\infty.g} = \int_g \sigma^{iJ}(E) \,.\, C(E)\, dE \Big/ \int_g C(E)\, dE$

where C(E) is a smoothly varying weighting spectrum.

Is it necessary to calculate the sensitivities of effective cross-sections to changes in resonance parameters, and adjust these, or can a simpler approach be adopted ?

If we consider separating the sensitivities into two components, the sensitivities to changes in the infinite dilution cross-sections and to the shielding factors we have the complication that the changes in the shielding factors could be dependent on the values of σ_0. If this is the case, we must derive the sensitivities of the effective cross-sections to resonance parameter changes for each system studied (or as a function of σ_0). Is this really necessary, or is the sensitivity independent of σ_0 for the ranges of σ_0 values of practical interest ?

The question whether it is necessary to have covariance data for resonance parameters or whether it is sufficient to have covariance data only for the infinite dilution cross-sections has been considered by making calculations of the changes in the ^{238}U capture cross-section (or resonance integrals) with changes in the resonance parameters. The changes in cross-section have been calculated for a range of background cross-sections covering the range of practical interest. If the same percentage change is found throughout the range of background cross-sections then it is not necessary to work in terms of the resonance parameters, the same adjustment factor will apply throughout the range of background cross-sections.

In Table 1 the results of calculations for the first three resonances of ^{238}U are presented. A typical value of the background cross-section for a PWR fuel pin cell is 50 barns and the range covered is 10 barns to 150 barns. The resonance parameter changes studied are 2 % for Γ_γ and 1 % for Γ_n these values being larger than the quoted uncertainties on the evaluated data. We see that the percentage changes in the shielded resonance integrals are essentially the same throughout the range of background cross-sections, from 10 barns to 150 barns. Consequently we can assume the same percentage uncertainty and adjustment factor throughout the range and consider only the uncertainty in the capture resonance integral rather than in the individual parameters. In fact, taking the uncertainties in the resonance parameters quoted by Moxon and Sowerby [2] one would conclude that the uncertainty in the calculated resonance integral is negligibly small. However, they point out that one must be cautious about the cross-section values between resonances, which are not well determined by the measurements and could be a source of uncertainty. Also one must consider uncertainties in the influence of solid state effects on Doppler broadening.

For fast reactor applications a typical background cross-section for ^{238}U is 30 barns and the range 5 barns to 200 barns has been considered.

Considering the ^{238}U shielded capture cross-section at 10 KeV, which is representative of the average value in a fast reactor spectrum, we see from Table 2 that, apart from the changes due to changes in Γ^o_n for s-wave resonances, the effects of 5 % changes do not vary strongly about the value for a 30 barns background cross-section. The effect of variations in the value

of Γ_n^o for s-waves is small and so the assumption of a constant value for the uncertainty in the capture cross-section is acceptable for a range of background cross-sections from 5 to 200 barns.

At 4 keV, an energy representative of the Doppler effect in a fast reactor we see from Table 3 that there is a stronger dependence on the background cross-section. Also the relationship between the change in the capture cross-section and in the Doppler effect depends markedly on the parameter varied. However, the changes are, in fact, small compared with the target accuracy for the prediction of Doppler effects, which we take to be ± 5 % (1 σ) in the ^{238}U contribution. (In fact, we find satisfactory agreement for the JEF-2 analyses of the SEFOR Doppler effect measurements and the SPX measurement, which have accuracies of about ± 10 % to ± 15 %). It seems probable that the major source of uncertainty in Doppler effect calculations arises from uncertainties in the spectrum rather than the changes in cross-sections with temperature.

Table 1
Percentage increases in shielded resonance integrals

For changes in resonance parameters

Change in Γ_γ + 2 %.
Change in Γ_n + 1 %.

Background cross-sections

50 barns (reference value for PWR)	10 barns (lower limit oxide fuel)	150 barns (approximate practical upper limit)

Changes in capture resonance integrals

6.67 eV resonance

	Γ_γ increased 2 %	
1.00 %	1.04 %	0.91 %
	Γ_n increased 1 %	
0.44 %	0.46 %	0.41 %

20.871 eV resonance

	Γ_γ increased 2 %	
1.27 %	1.30 %	1.20 %
	Γ_n increased 1 %	
0.30 %	0.32 %	0.25 %

36.682 eV resonance

	Γ_γ increased 2 %	
1.59 %	1.60 %	1.57 %
	Γ_n increased 1 %	
0.16 %	0.18 %	0.13 %

Table 2
Effects of changes in mean resonance parameters on the ^{238}U capture cross-section at 10 keV

5 % changes in mean resonance parameters

Background cross-sections

30 barns	5 barns	200 barns	Infinite dilution
$\overline{\Gamma}_\gamma$ increased by 5%			
2.61 %	2.49 %	2.73 %	2.77 %
$\overline{D}$ increased by 5%			
- 4.88 %	- 4.94 %	- 4.80 %	- 4.76 %
S-wave Γ_n^o increased by 5%			
0.16 %	0.06 %	0.29 %	0.37 %
P-wave Γ_n^o increased by 5%			
1.79 %	1.73 %	1.79 %	1.78 %

Table 3
Effects of changes in mean resonance parameters on the ^{238}U Doppler effect at 4 keV

Effects of 5 % changes in mean resonance parameters.

Temperature change 300 K to 1500 K

Background cross-sections Γ_γ increased by 5 %	30 barns	5 barns	200 barns
Change in σ_c at 300 K	2.30 %	2.07 %	2.60 %
Change in Doppler change	3.68 %	3.29 %	4.07 %
$\overline{D}$ increased by 5 %			
Change in σ_c at 300 K	- 4.93 %	- 5.00 %	- 4.82 %
Change in Doppler change	- 5.50 %	- 5.82 %	- 5.02 %
p-wave Γ_n^o increased by 5 %			
Change in σ_c at 300 K	1.78 %	1.84 %	1.61 %
Change in Doppler change	0.87 %	1.24 %	0.48 %

The maximum difference, for these changes in parameters, between the % change in the capture cross-section and the % change in the Doppler effect is 2.5 %.

The here above example based on ^{238}U illustrates a simple case since the capture cross-section even described in multichannel formation is not sensitive to the effects of the interference between resonances of a same channel. In the REICH-MOORE formalism for example, the interference effect is proportional to :

$$\frac{(\Gamma_{n\lambda}.\Gamma_{\alpha\lambda})^{1/2}(\Gamma_{n\lambda'}.\Gamma_{\alpha\lambda})^{1/2}}{D^2_{\lambda\lambda'}}$$ where $\Gamma_{n\lambda}$ and $\Gamma_{\alpha\lambda}$ refer to the partial widths of a resonance λ and $D_{\lambda\lambda'}$ to the spacing of the interfering resonances λ and λ'.

Although we don't have any practical experience of resonance parameter adjustment, we suspect that the general case will not be so simple. The requirements for covariance data can be stated only after explanatory studies to prepare adjusted resonance parameter sets, but to have a starting point to allow reactor Physicists to make more refined requests covariance data are needed for a few low lying resonances of the major actinide isotopes and for oxygen, sodium and iron, provided it is possible to identify the major resonances which interfere with the resonances of interest and for which the uncertainty information would be also required. Simplifications are obvious if one considers that the interference effects don't exist for the capture cross section and for resonances not belonging to the same channel.

That is why the requests limited to the three first resonances of ^{238}U (although this nucleus can be treated more simply as demonstrated above) to the first resonances of ^{239}Pu (resonance 1^+ not interfering with the O^+ resonance) and ^{240}Pu (capture

resonance which could be an ideal simple case to check the methodology of resonance parameter adjustment) are reasonable in size.

For ^{235}U the assessment of the uncertainty needs requires a full study which has still to be made.

In the unresolved range the problem doesn't seem to be redhibitory.

USE OF COVARIANCE DATA IN CROSS-SECTION ADJUSTMENT STUDIES

Covariance data requirements can perhaps be illustrated by describing how they are currently being used in a study to validate the JEF-2 library. The validation is being made using the techniques of nuclear data adjustment, and the chosen example is a study relating to fast spectrum systems.

The study begins with the following two steps :

1. Processing the evaluated data into parameter or group constants in a way that preserves the quality and the integrity of the information. This requires that fully validated tools are used for the processing and that methods sophisticated enough exist to use the processed data.
2. A choice of integral data according to criteria of cleanness of the experimental environment. The integral data should be derived from the raw data by applying corrections of small amplitude so that the integral values are not sensitive to uncertainties in the corrections (Doppler, heterogeneity, self-shielding, ...) nor to the methods used to calculate them. It has to be noted that in recent years these methods have received considerable improvements so that a number of additional experiments can be considered now as valuable benchmarks.

On the other side, in order to obtain the energy dependence of the nuclear data corrections the integral data should have differing energy dependent sensitivities.

This is the reason why the benchmark integral data set should contain as many experiments with different spectra as possible, and for a given integral experiment as many parameters (K_{eff}, $B^2_{m'}$, reaction rate ratios) as possible in order to separate the effects of the different cross-section types.

Neutronics calculations must be as exact as possible so that the calculated integral parameters are not dependent on the calculational method nor on the calculational scheme. If these conditions are satisfied the differences between experimental data and calculated data are the exact measures of the imperfect quality of the input data (both differential and integral).

The sensitivity coefficient calculations are based on perturbation theory or variational methods. Both types of methods are equivalent provided that the amplitude of the nuclear data modification in the adjustment is small enough for the linearity principle to apply.

But here again the condition of exact calculations imposes an energy scheme that is adapted to the fine structure of the flux $\phi(E)$ as a function of energy.

This condition is easily satisfied with fast and very fast systems, but one has to be careful in analysing thermal and epithermal systems.

The main objective in nuclear data adjustment is to check the consistency of integral and microscopic data so as to create a data set able to calculate any integral parameter with the best reliability and with

an accuracy at least equal that of the measurements.

Everything has already been said about adjustments, their general theoretical bases, and the conditions and limitations in application.

We will incidentally recall some special features of relevance to the present topics and used in the work described here below as an illustration.

A set of measured integral quantities, combined in a vector E with covariance matrix V is considered. The nuclear data implied in these integral parameters are combined also in a vector T with a covariance matrix M. The integral parameters calculated from T are denoted by the vector C.

If the sensitivity matrix S expresses the dependence of C on relative variations of T one has :

$$\frac{dC}{C} = S\frac{dT}{T}$$

The use of such logarithmic variates (with possibility of variation between $-\infty$ and $+\infty$) is the most appropriate to be used in the operation of entropy maximisation.

Actually, in the adjustment the objective is to minimise the quantity :

$$\sum_{JI}\left(\frac{E_I - C_I}{C_I}\right)\left(\frac{E_J - C_J}{C_J}\right)V_{IJ}^{-1} + \sum_{ij}\frac{dTi}{Ti}\frac{dTj}{Tj}M_{ij}^{-1}$$

A vector T' is obtained. This vector is recommended as the best estimate of the unknown true vector since it minimises the expected consequences of choosing a vector deviating from the true vector [3].

T' needs to be close to T in order to satisfy the linearity assumption. Statistical adjustments are meaningful only when the a priori evaluated data are of sufficient quality, i.e. when non excessive values are obtained for any component of :

$$\frac{E-C}{C}$$

(let us say less than 4% - 5%).

The final vector C' for the integral data is :

$$C' = C + S\left(\frac{T'-T}{T'}\right)$$

with a new covariance matrix V', while the covariance matrix for T' is denoted by M'.

Simplifications are obtained if the assumption is made that the probability distributions for T and E are Gaussian. The Gaussian distributions are kept in the adjustment for T' and C' and it is supposed that the true unknown distributions are also Gaussian.

Significant deviations from this assumption (existence of systematic errors) are detected by large :

$\left(\frac{E-C'}{C'}\right)$ values, or/and by adjustments to cross-sections much greater than the assigned standard deviations. The existence of such deviations leads to a deviation of the χ^2 parameter from its expected normal value that should equal N, the number of integral data (whether they are correlated or not).

If $\chi^2 > N$ the consistency between integral and microscopic data is not good. It is well known that the solution is to correct the discrepant data when possible, or to increase by judgement the related uncertainties or to reject the data when justified.

Finally, to keep the goodness of the fit all the "a posteriori" standard deviations have to be enhanced by the factor :

$$\left(\frac{\chi^2}{N}\right)^{1/2}$$

that will be referred to in the following as the enhancement factor.

It follows that, for a given integral observable i the standard deviation after adjustment is :

$$\left(V_{ii}\frac{\chi^2}{N}\right)^{1/2} = \left[S_i\, M'\, S_i^T \cdot \frac{\chi^2}{N}\right]^{1/2} \text{ when } \chi^2 > N.$$

For more details concerning the practical conditions of JEF2 validation data processing, choice of integral experiments, neutronics calculations one can refer to [4].

ADJUSTMENTS :

The adjustments have been performed using the code AMERE [5].

The "a posteriori" χ^2 parameter value has been used as a test of goodness of the fit, and consequently as a test of reliability of integral parameter prediction, by the adjusted data set.

The "a posteriori" average uncertainty on integral parameters served as measure a criterion of accuracy of prediction.

In practice a sequential procedure has been adopted to implement the system of integral data so as to detect the introduction of any inconsistent integral datum by a sharp increase of the χ^2 value.

The different experimental programs have been considered first separately (i.e., the "LOS ALAMOS spheres" data only, or the "MASURCA" data only, ...) in order to test their internal consistency. Some experiments have been rejected on a statistical criterion, but the elimination has been found justified by arguments of experimental techniques. Finally a system of N=50 integral data has been selected.

The JEF2 evaluations are not provided with covariance matrices, with the exception of ^{239}Pu [6] and ^{238}U [7]. Covariances have been generated on the basis of personal judgement for what concerns both the standard deviations and the range of correlations (medium range). (A covariance matrix can be written as $B = \Sigma P \Sigma$ in a way that displays explicitly the standard deviations (diagonal matrix Σ) and their correlations (matrix P).

As a compromise between constraints relevant to physics and to have common boundaries with the schemes in current use (1968, 172 and 33 g) a 15 group scheme has been established to perform the sensitivity calculations and the cross-section adjustments (see the table 4). The covariance matrices have been collapsed into this 15 group scheme.

Table 4 - 15 group scheme used for adjustment calculations

Group boundaries upper limit (eV)	Group	Scheme 1968 g	Scheme 172 g	Scheme 33 g	Lethargy
19.64033 +6	1	1	1	1	-0.675
6.06531 +6	2	142	9	3	0.500
2.231302 +6	3	262	15	5	1.500
1.353353 +6	4	322	18	6	2.000
4.978707 +5	5	442	26	8	3.000
1.831564 +5	6	664	32	10	4.000
6.737947 +4	7	686	36	12	5.000
2.478752 +4	8	808	42	14	6.000
9.118820 +3	9	928	46	16	7.000
2.034684 +3	10	1108	53	19	8.500
4.539993 +2	11	1268	61	22	10.000
2.260329 +1	12	1648	80	28	13.000
4. +0	13	1837	93		14.731
5.3158 - 1	14	1920	137	33	16.75
1. - 1	15	1952	156		18.42068
1.1 - 4		1968	172		

This system was well adapted for systematic studies so as to define the optimal conditions for the JEF2 validation.

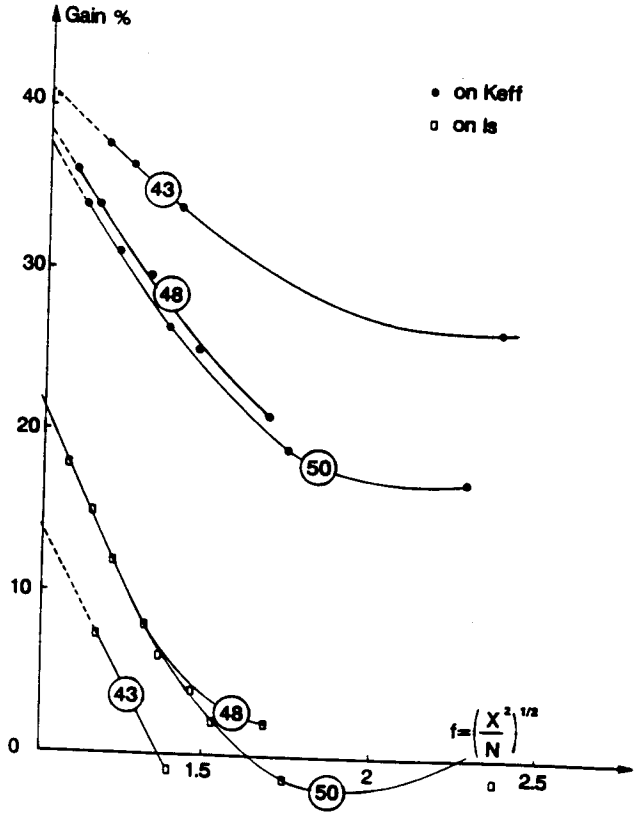
The gains (expressed in percent) on the accuracy of K_{eff} and the spectral indices I_s resulting from adjustments are defined as :

$$\left(1 - \frac{<\Delta K_{eff}>^*}{<\Delta K_{eff}>}\right) \times 100 \text{ and } \left(1 - \frac{<\Delta I_s>^*}{<\Delta I_s>}\right) \times 100$$

respectively. The brackets denote the average value and the star * distinguishes the "a posteriori" value from the "a priori" value. The variations in the gains have been investigated as functions of the enhancement factor for different standard deviations obtained from the nominal "a priori" values by a multiplication by factors 0.3, 0.6, 1.3, 1.5, and for different values of the range of the "a priori" correlations labelled by R = 1, 2, ..., 15.

Figure 1 shows that the gains are generally improved by an increase of the standard deviations in the case of no energy correlation (R=0). This situation is practically unchanged by introducing correlations of any range (R = 1, 2, ..., 12).

Figure 1- Gains (%) in accuracy on K_{eff} and I_S resulting from changes in a priori standard deviations



Two experiments have been rejected from the N = 50 system because of discrepancies which are too large after adjustment $\left(\left|\frac{E-C'}{C'}\right| > 3\sigma\right)$.

With this new system of N=48 experiments the situation is globally improved : better consistency with integral experiments is obtained with the nominal "a priori" standard deviations $\left(\frac{\chi^2}{N}\right)^{1/2} = 1.314$, against $\left(\frac{\chi^2}{N}\right)^{1/2} = 1.37$ in the case of N=50). Both gains in K_{eff} and I_S are increased but the importance of "a priori" correlations remains small (effect of ~ 5% on $<\Delta K_{eff}>$ * for example).

If one reduces the system to the N = 43 integral data such that $\left|\frac{E-C'}{C'}\right| < 1.5\,\sigma$, one notes (see fig. 1) when using the nominal "a priori" standard deviations :

- an equally good consistency :

$$\left(\left(\frac{\chi^2}{N}\right)^{1/2} = 1.39\right)$$

- a large improvement in accuracy of K_{eff} and a worsening in accuracy of I_S.

In addition, the cross-section adjustments are different in sign and amplitude if one compares them to the adjustments with N = 48 or N = 50. This suggests some inconsistency between K_{eff} and I_S data. This is confirmed if one considers the systems of K_{eff} data (N=28) or spectral index I_S data (N=20) separately.

One observes a good consistency between microscopic and integral data since good $\left(\frac{\chi^2}{N}\right)^{1/2}$ values are obtained with "a priori" nominal uncertainties [$\left(\frac{\chi^2}{N}\right)^{1/2} = 1.11$ in the case of the K_{eff} data system; $\left(\frac{\chi^2}{N}\right)^{1/2} = 1.043$ in the case of Is data]. For these configurations the importance of the off diagonal terms is more significant (14% on K_{eff} calculation, 10% on spectral index calculation).

Finally some general conclusions can be drawn.

To avoid the problem of different adjustment configurations corresponding to similar $\frac{\chi^2}{N}$ values one has to consider on the same footing additional parameters such as the gain in accuracy for the prediction of any integral parameter. In these conditions :

1. The optimum system for data validation is the one which simultaneously exhibits :
   - Good consistency between integral and microscopic data (enhancement factor $\left(\frac{\chi^2}{N}\right)^{1/2}$ as close to 1 as possible).
   - Most accurate prediction for each integral parameter (However, one must have good reasons for omitting any measurement).
2. Concerning the microscopic data, the very sophisticated covariance matrices with very small standard deviations, which can be found in some evaluations, are not of practical use, at present, because of the existence of some degree of inconsistency between integral and microscopic data, which limits the importance of the "a priori" off diagonal terms.
   In inconsistent situations the weight of the integral data is dominant in the "a posteriori" microscopic correlations. This is visible since the accuracies on the integral parameters are improved when the "a posteriori" standard deviations are increased.
   This suggests :
   - The correlations existing between integral data of the same type (I_S essentially), in a given experimental program should be taken into account in the adjustment. In the present study their effects have not been investigated.
   - Uncertainty calculations for practical configurations should be performed only with adjusted data sets.

- **RESULTS :**

According to the conclusions of the systematic studies the system of N = 48 experiments is better adapted, for the moment, to validate JEF2. For what concerns the microscopic data the range of the correlations has been limited to 3 groups, unless it has been differently assigned in the evaluated covariances (^{238}U, ^{239}Pu).

We have considered as valuable adjustments only those which are greater than the "a posteriori" standard deviations. As demonstrated in the systematic study, the sign and the energy range of these adjustments are independent of the input standard deviations, so that they can be considered as significant.

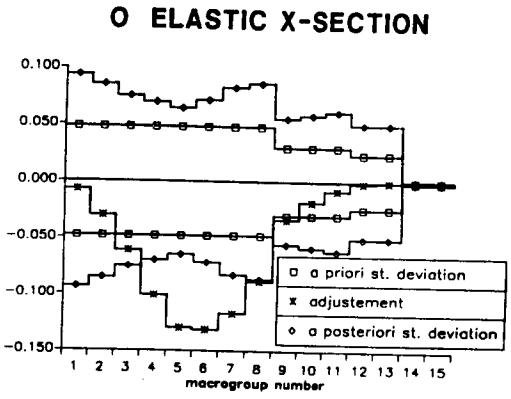
For this first approach in the general process of JEF2 validation, 5 nuclear constants have been considered :

- the average number of neutrons emitted per fission : ν,
- the fission cross-section : σ_f,
- the neutron absorption cross-section : $\sigma_a = \sigma_c + \sigma_{n,p} + \sigma_{n,\alpha} + \ldots$,
- the elastic and the inelastic scattering cross-sections : $\sigma_{n,n}$ and $\sigma_{n,n'}$.

For these 2 last nuclear constants the sensitivity coefficients correspond to the global energy transfer so that both the cross-sections and the secondary angular and energy distributions are involved by the adjustments.

The most significant adjustment found in the study so far completed is to the oxygen elastic scattering cross-section. The adjustment is shown in Figure 2.

Figure 2 - Adjustment of the elastic cross-section of ^{16}O as required by the benchmarking



CONCLUSIONS

The importance of the estimation of systematic uncertainties in integral data measurements is emphasized.

It is shown that the impact of the self shielding factor is, in most cases, extremely modest and it is argued, from calculations made for ^{238}U that, in general, it is sufficient to have covariance data for the cross sections calculated for a representative level of self shielding. In a first step and to take into account the fine group calculation the covariance data requirements are for a few low lying identified resonance parameters of major substances in reactors (^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, O, Na, Fe).

For higher energy cross section data it is argued that the requirements is not for a high level of detail in the covariances but for uncertainties in average over energy ranges of the order of E to 3E together with the correlations between ranges. A fast reactor cross section adjustment study is described and a number of conclusions are drawn from this.

It is shown that the results are not very sensitive to the correlations in the uncertainties between the energy groups, due to the relative inconsistency of the analysed integral data.

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GENERATION OF COVARIANCE DATA AMONG VALUES FROM A SINGLE SET OF EXPERIMENTS

DONALD L. SMITH
Engineering Physics Division, Argonne National Laboratory
9700 South Cass Avenue, Argonne, Illinois 60439, U.S.A.

ABSTRACT

Modern nuclear data evaluation methods demand detailed uncertainty information for all input results to be considered. It can be shown from basic statistical principles that provision of a covariance matrix for a set of data provides the necessary information for its proper consideration in the context of other included experimental data and/or a priori representations of the physical parameters in question. This paper examines how an experimenter should go about preparing the covariance matrix for any single experimental data set he intends to report. The process involves detailed examination of the experimental procedures, identification of all error sources (both random and systematic), and consideration of any internal discrepancies. Some specific examples are given to illustrate the methods and principles involved.

1. Introduction

A collection of measured physical parameters is of limited value unless some specification is made of the associated errors.[1] However, mere specification of total errors for individual quantities from the collection is generally inadequate because various components of these errors can have origins common to more than one member. This important information must be conveyed. Provision of useful, reliable error information for his experimental results clearly places rather heavy demands upon an experimenter to understand and document the results, thereby revealing the intimate details of his work. Of course, such effort is clearly beneficial to the community of his peers and to posterity which must eventually pass judgment on the work. The objectives of this paper are: i) to indicate the significance of covariance information, ii) to explore the statistical origins of error formalism, iii) to discuss the details of providing such information, iv) to offer some suggestions for simplification of the process, and v) to touch upon some problem areas, e.g., discrepancies.

2. Why Covariance Information is Required

The purpose of providing error information is, quite simply, to quantify the confidence to be accorded to each data point of a set and, thereby, establish how it is to be weighted in various analyses which

incorporate these data (e.g., in evaluations). If we possess estimates for the mean values and a covariance matrix for a set of physical quantities (i.e., the "results" of an experiment and their "errors"), then a fundamental principle of information theory[2] tells us that we are justified in proposing a normal (Gaussian) probability distribution to describe our current state of understanding of these physical quantities. This is a convenient result since Gaussians are simple and widely accepted localized distributions for expressing knowledge of physical quantities. Finally, there are philosophical justifications for considering errors: "..if a man will begin with certainties, he shall end in doubts; but if he will be content to begin in doubts, he shall end in certainties..." (Francis Bacon, *Novum Organum*), and "...it is only in the realm of doubt that we engage in the pursuit of truth..." (Mortimer Adler, *Six Great Ideas*).

3. Some Basic Attributes of Measurable Parameters

The entity in question should be sufficiently well defined to be acceptable as worthy of determination (e.g., speed of light, neutron total cross section of ^{12}C at 2.75 MeV, monthly income of a governor from one of the 50 U.S. states, height of male U.S. citizens over age 20, etc.). All measurable parameters belong to one or the other of the following two categories: i) the quantity itself has natural variance (e.g., the weight of a Valencia orange, the height of male citizens of Paris, France, with ages exceeding 30 years, etc.) or it is assumed to have a precise and immutable value, except possibly on a cosmic time scale (e.g., mass of the proton, speed of light, reaction cross sections, etc.). The physical parameters with which we are concerned belong almost invariably in the second category. Regardless of the category to which any measurable quantity might belong, the process of measurement introduces dispersion in the outcomes and, therefore, uncertainty in our knowledge of that quantity.

4. Statistical Considerations for a Single Parameter

Let p be a single measurable quantity. We suppose that outcomes from measurements of p are governed by the univariate probability function f[3]. Furthermore, we consider f to be normalized, i.e., $\int f(p)dp = 1$. Here, and in all following equations, we assume that integration extends over the range of possible values of the variable(s) of integration. The quantity $\langle p \rangle = \int pf(p)dp$ is the mean value. We assume that the value p_e from a single measurement of p is an approximation to $\langle p \rangle$, thus, $\langle p \rangle \approx p_e$. If f is fairly localized, this is the only reasonable assumption we can make when no other data are available. The variance is given by $var(p) = \int (p-\langle p \rangle)^2 f(p)dp$. Then, $\sigma_p = [var(p)]^{1/2}$ is the standard deviation, i.e., the "error" or "uncertainty" we should attribute to our measurement. Since f is generally not known, we need to estimate σ_p too. Let σ_e be that estimate, thus, $\sigma_p \approx \sigma_e$. Based on this available information, p_e and σ_e, we are justified, from information theory, in supposing that $f(p) \approx \exp[-(p-p_e)^2/(2\sigma_e^2)]/(2\pi\sigma_e^2)^{1/2}$ is our best possible choice for f. Knowledge of f can be refined by acquisition of additional data and applications of Bayes theorem.

5. Statistical Considerations for Several Parameters

Let $\underline{p}$ be a collection of n measured quantities, with f as the corresponding multivariate probability function governing the measurement process[3]. Again, assume f is normalized, i.e., $\int f(\underline{p})d\underline{p} = 1$. The quantity $\langle p_i \rangle = \int p_i f(\underline{p})d\underline{p}$, $[i=1,n]$, defines the mean value for the i-th component of $\underline{p}$. A single experiment yields $\underline{p}_e = (p_{e1}, p_{e2}, \ldots, p_{en})$. Thus, $\langle p_i \rangle \approx p_{ei}$ is the only reasonable assumption when no other data are available to consider. We are then led to examine the quantity $\mathrm{var}(p_i) = \langle (p_i - \langle p_i \rangle)^2 \rangle = \int (p_i - \langle p_i \rangle)^2 f(\underline{p})d\underline{p}$, $[i=1,n]$. Then, $\sigma_{pi} = [\mathrm{var}(p_i)]^{1/2}$, $[i=1,n]$, defines the i-th standard deviation. For the multivariate case, we also have to consider the i,j-th covariance, i.e., $\mathrm{cov}(p_i,p_j) = \langle (p_i - \langle p_i \rangle)(p_j - \langle p_j \rangle) \rangle = \int (p_i - \langle p_i \rangle)(p_j - \langle p_j \rangle) f(\underline{p})d\underline{p}$, $[i,j=1,n; i \neq j]$. Then, the n x n array of elements, $V_{pij} = \langle (p_i - \langle p_i \rangle)(p_j - \langle p_j \rangle) \rangle$, $[i,j=1,n]$, defines the variance-covariance (or simply covariance) matrix $\underline{V}_p$. It provides complete "uncertainty" information for $\underline{p}$. Likewise, the n x n array of elements. $C_{pij} = V_{pij}/(V_{pii}V_{pjj})^{1/2}$, $[i,j=1,n]$, defines the correlation matrix $\underline{C}_p$. Note that $C_{pii} = 1$, $[i=1,n]$. Since f is not known, we need to estimate $\underline{V}_p$ corresponding to our single experiment which produced $\underline{p}_e$. Let $\underline{V}_e$ be that estimate. Correspondingly, one obtains the estimated correlation matrix. Thus, $\underline{V}_p \approx \underline{V}_e$ and $\underline{C}_p \approx \underline{C}_e$. Based on this available information ($\underline{p}_e$ and $\underline{V}_e$, as best estimates of $\langle \underline{p} \rangle = (\langle p_1 \rangle, \langle p_2 \rangle, \ldots, \langle p_n \rangle)$ and $\underline{V}_p$ from one experiment), it is suggested that $f(\underline{p}) \approx (2\pi)^{-n/2}[\det(\underline{V}_e)]^{-1/2}\exp[-(1/2)(\underline{p}-\underline{p}_e)^+\underline{V}_e^{-1}(\underline{p}-\underline{p}_e)]$, directly from information theory ("+" implies matrix transposition). Knowledge of f can be refined by acquisition of additional data sets and applications of Bayes theorem. The emphasis in this paper is on procedures for estimating $\underline{V}_e$ for a single data set. Attention is given primarily to those physical considerations which govern the estimation procedure, but the mathematical principles which must be observed are also indicated.

6. Law of Error Propagation

Let $\underline{x}$ be a collection of q measurable quantities, with a q x q covariance matrix $\underline{V}_x$. Then, let $\underline{p}$ be a collection of n derived quantities based on $\underline{x}$, namely, $p_i = p_i(\underline{x})$, $[i=1,n]$. Finally, let $T_{ki} = \partial p_i/\partial x_k$, $[i=1,n; k=1,q]$. These elements form a q x n matrix $\underline{T}$. Then, $\underline{V}_p = \underline{T}^+\underline{V}_x\underline{T}$ yields the covariance matrix for $\underline{p}$ in terms of that for $\underline{x}$. The elements of $\underline{T}$ are sensitivity coefficients. The expression which relates $\underline{V}_p$ and $\underline{V}_x$ is called the Law of Error Propagation. Actually, This transformation of $\underline{V}_x$ to $\underline{V}_p$ is based upon an assumption that the distribution function for $\underline{x}$ is quite well localized and, thus, that a Taylor series expansion of p_i as a function of $\underline{x}$ can be truncated beyond first order, i.e., that $\delta p_i \approx \Sigma_{k=1,q}\, T_{ik}\delta x_k + O(2)$, with $O(2)$ terms being negligible. It is very important to keep in mind the fact that the relationship between p and x has been linearized, when considering error propagation. For very large errors, a different approach based on transformation of probability would have to be considered. Such transformations are difficult to do in analytical form for all but the simplest cases, but they can be readily handled by Monte Carlo methods.

7. Derivation of a Basic Formula Used in Constructing Estimates of Covariance Matrices for Sets of Measured Data

Suppose that a particular experiment can be characterized completely by a collection $\underline{x}$ of q measurable quantities (distances, masses, detector yields, calibration parameters, etc.). It is important that these be viewed as the most elementary quantities of the experiment, not higher-level, derived parameters (e.g., cross sections). Let $\underline{V}_x$ be the corresponding covariance matrix. Then, let $\underline{p}$ represent the derived quantities (e.g., cross sections) that are functionally related to $\underline{x}$, i.e., $p_i = p_i(\underline{x})$, $[i=1,n]$. From error propagation we have that $\underline{V}_p = \underline{T}^+\underline{V}_x\underline{T}$, as described above. Ideally, all the components x_k of $\underline{x}$ would be independent, yielding in a diagonal $\underline{V}_x$. For practical reasons, this is seldom observed. However, it is frequently the case (either rigorously or to a good approximation) that $\underline{x}$ can be partitioned into w distinct subvectors $\underline{x}_r$, $[r=1,w]$, such that $\underline{x} = (\underline{x}_1,\underline{x}_2,\ldots,\underline{x}_r,\ldots,\underline{x}_w)$, and that these $\underline{x}_r$ can be treated as mutually independent[4]. These w subvectors correspond to distinct attributes of the experiment. For example, typical independent attributes of a nuclear experiment are detector calibrations, geometry factors, sample masses, etc. The partitioning of $\underline{x}$ leads to a corresponding partitioning of $\underline{V}_x$:

$$\underline{V}_x = \begin{bmatrix} \underline{V}_{x1} & & & & 0 \\ & \underline{V}_{x2} & & & \\ & & \cdots & & \\ & & & \underline{V}_{xr} & \\ & & & \cdots & \\ 0 & & & & \underline{V}_{xw} \end{bmatrix} .$$

Thus, $\underline{V}_x$ consists of submatrices $\underline{V}_{xr}$ (which are not necessarily diagonal) situated along its diagonal, and zeros elsewhere. Similarly, $\underline{T}$ can be partitioned into submatrices $\underline{T}_r$, which correspond to the $\underline{V}_{xr}$, and the remainder which is essentially without influence.

As a consequence of these assumptions, we obtain for $\underline{V}_p$ the expression $\underline{V}_p = \underline{T}^+\underline{V}_x\underline{T} = \Sigma_{r=1,w}\, \underline{T}_r{}^+\underline{V}_{xr}\underline{T}_r$. It follows that the elements of $\underline{V}_p$ are given by $V_{pij} = \Sigma_{r=1,w}\, (\underline{T}_r{}^+\underline{V}_{xr}\underline{T}_r)_{ij}$, $[i,j=1,n]$. Let us denote e_{ir} as the partial error in the derived quantity p_i due to the attribute r, $[i=1,n;\ r=1,w]$. This error has the same units as p_i. If $p_i \neq 0$, we can express the corresponding fractional error as $f_{ir} = e_{ir}/\mathrm{abs}(p_i)$ and the percent error as $100f_{ir}$. Note that $e_{ir} \geq 0$, always. Furthermore, it is useful to define the parameter $S_{ijr} = (\underline{T}_r{}^+\underline{V}_{xr}\underline{T}_r)_{ij}/(e_{ir}e_{jr})$, so long as both $e_{ir} > 0$ and $e_{jr} > 0$ (as is usually the case). If either equals zero, assume that $S_{ijr} = \delta_{ij}$ (Kronecker Delta). Clearly, all the S_{ijr} are dimensionless quantities. So, we arrive at the very useful formula $V_{pij} = \Sigma_{r=1,w}\, S_{ijr}e_{ir}e_{jr}$ $[i,j=1,n]$. This formula permits us to construct quite readily the covariance matrix, $\underline{V}_p$, from a table of partial errors e_{ir} which are associated with each derived value p_i, $[i=1,n]$, and correspond to various independent experimental attributes, r, $[r=1,w]$. We are led here to approximate only to the extent that very rarely are complex experiments perfectly resolvable into such distinct attributes. By careful choice of $\underline{p}$, such approximations can usually be justified.

8. Micro Correlations and Macro Correlations

The n x n matrices, $\underline{S}_r$, consisting of the parameters S_{ijr}, [i,j=1,n; r=1,w], clearly provide all correlations between the partial error components e_{ir}, [i=1,n; r=1,w]. For lack of a better term, these have been designated as micro-correlation matrices[4]. The n x n correlation matrix, $\underline{C}_p$, derived from $\underline{V}_p$, describes the correlations between the total errors of the parameter set p. For convenience, this is denoted as the macro-correlation matrix[4]. Given the partial errors, e_{ir}, [i=1,n; r=1,w], and the micro-correlation matrices, $\underline{S}_r$, [r=1,w], derivation of $\underline{V}_p$ and $\underline{C}_p$ is a straightforward, objective application of the formulas derived earlier. Subjectivity - when it becomes unavoidable - enters only into the estimation of e_{ir} and $\underline{S}_r$. In general, estimation of the component errors e_{ir}, [i=1,n; r=1,w], is far less difficult than estimation of the correlations appearing in the matrices $\underline{S}_r$ [r=1,w]. So, how sensitive are the elements of $\underline{V}_p$ to ambiguities in these $\underline{S}_r$? A study of this effect has been reported[4]. It was found that the sensitivity decreases with increasing w according to the factor $w^{-1/2}$, i.e., consistent with the Law of Large Numbers from statistics[3].

9. Some Fundamental Constraints on Generation of Covariance Matrices for Data Sets

The method described here aims at providing for an objective determination of $\underline{V}_p$, based on detailed analysis of partial errors and their correlations. However, no matter how $\underline{V}_p$ is determined, it must end up being a positive definite matrix, e.g., it cannot predict zero total error for any single data point of a set or 100% correlation between the total errors of any two particular data points. Therefore, $\underline{V}_p$ must be tested for positive definiteness after its generation. It follows that when $\underline{V}_p$ is positive definite, then $\underline{C}_p$ is also. However, individual $\underline{S}_r$ need not be positive definite. As an example, consider three data points (n=3) corresponding to measurements of a particular neutron activation cross section at three different energies. The activities are all measured by observing the same emitted gamma ray with one detector. Clearly, the detector calibration is the source of a fully correlated error component for these points. Thus, $S_{ijr} = 1$ for this particular r and [i,j=1,3]. Such a matrix $\underline{S}_r$ is obviously not positive definite.

10. The Need for a Mathematical Model of an Experiment as a Condition for the Estimation of a Data Covariance Matrix

A mathematical model of the experiment is necessary in order for the experimenter to be able to identify the q-fold collection of characteristic parameters, $\underline{x}$, even if some of them remain implicit and not directly manipulated. Only if such a model is developed can the distinct, and presumably independent, attributes of the experiment be identified. These attributes are characterized by w subvectors $\underline{x}_r$. A model is required in order to consider (possibly implicitly) the relationships $p_i = p_i(\underline{x}_1, \underline{x}_2, \ldots, \underline{x}_r, \ldots \underline{x}_w)$, [i=1,n]. In practice, there is usually a great deal of variability from one attribute to another in

regard to an experimentalist's understanding of the quantitative dependence of each p_i on the individual $\underline{x}_r$ for his measurements. For example, if $\underline{x}_1$ relates to detector calibration, knowledge of the functional relationship between any p_i and $\underline{x}_1$ is generally very explicit. However, if $\underline{x}_2$ relates to neutron multiple scattering, the functional relationship to any p_i will likely be virtually impossible to express. Then, estimation of the partial cross errors e_{i2}, [i=1,n], and the micro-correlation matrix $\underline{S}_2$ will be far more subjective.

11. Relative Covariance Matrix

Let $\underline{V}_p$ be a covariance matrix for the data set $\underline{p}$. Suppose that all $p_i > 0$, [i=1,n]. Then, we can define the relative covariance matrix, $\underline{R}_p$, by the formula $V_{pij} = p_i p_j R_{pij}$, [i,j=1,n]. From the basic expression for deriving V_{pij}, we have that $R_{pij} = \Sigma_{r=1,w} S_{ijr} (e_{ir}/p_i)(e_{jr}/p_j)$. The quantity $f_{ir} = e_{ir}/p_i$ is the fractional error in p_i. We could also work with percent errors, namely, $100f_{ir}$. Clearly, $\underline{C}_p$ can be derived directly from $\underline{R}_p$. Thus, $C_{pij} = V_{pij}/(V_{pii}V_{pjj})^{1/2} = R_{pij}/(R_{pii}R_{pjj})^{1/2}$, since the factors p_i and p_j cancel. There is a very important reason why it is preferable to work with $\underline{R}_p$ and $\underline{C}_p$ rather than $\underline{V}_p$ and $\underline{C}_p$. It has to do with an issue that has acquired the label "Peelle's Pertinent Puzzle (PPP)"[5]. It will be mentioned briefly in Section 18 of this paper.

12. Requirements for the Tabulation of Errors and Techniques for Reducing the Volume of Error Information to be Recorded

It is suggested that what ought to be required of an experimenter who reports an individual data set is that he provide a table of estimated error components (preferably fractional), as follows:

$$
\begin{array}{ccccccc}
f_{11} & f_{12} & \cdots & f_{1r} & \cdots & f_{1w}, \\
f_{21} & f_{22} & \cdots & f_{2r} & \cdots & f_{2w}, \\
 & & & \vdots & & \\
f_{i1} & f_{i2} & \cdots & f_{ir} & \cdots & f_{iw}, \\
 & & & \vdots & & \\
f_{n1} & f_{n2} & \cdots & f_{nr} & \cdots & f_{nw},
\end{array}
$$

plus a set of w estimated micro-correlation matrices, i.e.,

$$
\underline{S}_r = \begin{pmatrix}
S_{11r} & S_{12r} & \cdots & S_{1jr} & \cdots & S_{1nr} \\
S_{21r} & S_{22r} & \cdots & S_{2jr} & \cdots & S_{2nr} \\
 & & & \vdots & & \\
S_{i1r} & S_{i2r} & \cdots & S_{ijr} & \cdots & S_{inr} \\
 & & & \vdots & & \\
S_{n1r} & S_{n2r} & \cdots & S_{njr} & \cdots & S_{nnr}
\end{pmatrix}, \qquad [r=1,w].
$$

Given this information, $\underline{R}_p$ and $\underline{C}_p$ can always be derived when needed and, if demanded, also $\underline{V}_p$ through knowledge of $\underline{p}$. There are opportunities to reduce the number of values f_{ij}, [i,j=1,n], and S_{ijr}, [i,j=1,n; r=1,w], that need to be reported. These should be exploited. Let us consider two brief examples. First, Suppose n=10 and w=5. Also, suppose that for r=3, f_{i3} represents a detector calibration error of 5%, regardless of the

data point, [i=1,10]. Then, $f_{i3} = 0.05$, [i=1,10]. One can simply express this fact. Actually, explicit tabulation of each f_{ir}, for fixed r, [i=1,10], is necessary only when these errors are distinct for each i. Certain blocks of data points might have equal errors; e.g., $f_{i2} = 0.04$, [i=1,3]; $f_{i2} = 0.05$, [i=4,6]; $f_{i2} = 0.08$, [i=7,10]. Next, consider the situation above where $f_{i3} = 0.05$, [i=1,10]. Suppose this error source is attributable to a common origin which afflicts each data point in a 100%-correlated manner. Then, $S_{ij3} = 1$, [i,j=1,10]. Obviously, there is no need to write down an explicit matrix consisting entirely of "ones"! A similar approach is sometimes used to represent components of covariance matrices in the widely applied ENDF formats[6].

Let us discuss a somewhat more detailed example to illustrate the present approach. We shall consider providing errors associated with a Ge photon detector calibration procedure[7]. The calibration is carried out using standard point gamma-ray sources situated at a distance d ≈ 20 cm from the Ge detector. The formulas (model) used in this analysis are $C = AB\epsilon$ and $A = A_0\exp(-\lambda t)$, where C is the gamma-ray peak count, B is the branching factor, ϵ is detector efficiency, A is the source activity at the time of the count, A_0 is the same activity at the time of source calibration, λ is the decay constant and t is the time elapsed between the source calibration and the detector calibration. The sources employed and their activities are: ^{60}Co [3.193×10^5 (± 0.9%) on 1 February 1984], ^{137}Cs [1.565×10^5 (± 1.5%) on 1 January 1985], and ^{152}Eu [4.208×10^5 (± 1.5%) on 20 April 1979]. Twelve gamma-ray lines were measured and analyzed from these sources, each identified by a line number (LN). Here are the specifics:

Source	LN	Gamma-ray Energy (keV)	Gamma-ray Branch (%)
^{60}Co	1	1173	100.0
	2	1333	100.0
^{137}Cs	3	662	85.0
^{152}Eu	4	245	7.42
	5	344	26.4
	6	444	3.08
	7	779	13.0
	8	867	4.16
	9	964	14.5
	10	1086	11.8
	11	1112	13.6
	12	1408	20.7

Using this information and the observed yields of the full-energy peaks it is possible to deduce the efficiency of the detector at each of the indicated energies. The following table provides the various errors needed for a complete analysis. Associated with each data point is the line number (LN), efficiency multiplied by 10^4 (Eff), four error components (r = 1 to r = 4), and total error (Tot Err). These errors are

given in percent:

LN	Eff	r = 1	r = 2	r = 3	r = 4	Tot Err
1	3.089	0.4	0.0	0.9	0.0	1.0
2	2.783	0.4	0.0	0.9	0.0	1.0
3	5.016	0.3	0.0	1.5	0.6	1.6
4	12.69	0.2	0.1	1.5	2.1	2.6
5	9.278	0.1	0.1	1.5	1.5	2.1
6	7.337	0.4	0.1	1.5	1.6	2.2
7	4.315	0.3	0.1	1.5	1.7	2.3
8	4.031	0.4	0.1	1.5	1.3	2.0
9	3.681	0.2	0.1	1.5	1.6	2.2
10	3.320	0.3	0.1	1.5	2.2	2.7
11	3.284	0.2	0.1	1.5	1.5	2.1
12	2.683	0.2	0.1	1.5	1.3	2.0

The correlations involved can be expressed as follows: the statistical error in C is uncorrelated (r = 1), the half-life uncertainty is 100% correlated for all lines from the same source and uncorrelated otherwise (r = 2), the uncertainty in A_0 is 100% correlated for all lines from the same source and is uncorrelated otherwise (r = 3), and the uncertainty in B is uncorrelated for all lines from different sources and is effectively uncorrelated for ^{152}Eu lines because the errors are largely due to peak yields and, thus, are mainly statistical (r = 4). Combining this information according to the standard prescription given in Section 7 leads to the following macrocorrelation matrix:

	1	2	3	4	5	6	7	8	9	10	11	12
1	1											
2	.84	1										
3	0	0	1									
4	0	0	0	1								
5	0	0	0	.41	1							
6	0	0	0	.39	.48	1						
7	0	0	0	.38	.46	.44	1					
8	0	0	0	.43	.52	.50	.49	1				
9	0	0	0	.40	.48	.46	.45	.51	1			
10	0	0	0	.33	.40	.38	.37	.42	.38	1		
11	0	0	0	.41	.50	.47	.46	.52	.48	.40	1	
12	0	0	0	.44	.53	.51	.49	.56	.51	.42	.53	1

13. Objective Estimation of Errors and Correlations

Suppose we choose to fit an empirical curve to the set of detector efficiency values, with associated errors and correlations, as given in Section 12 above. The least-squares fitting process will generate a covariance matrix for the fitted parameters[3]. Through error propagation,

errors and their correlations for derived values at arbitrary energy points along the curve can be deduced objectively. For example, if we decide to fit the formula $ln\ \epsilon = a_1 + a_2\ ln\ E_g$ (where ϵ if the efficiency and E_g is photon energy) to the calibration data given in Section 12, and derive efficiency (Eff) from the fitted curve at E_g = 300, 500, 700, 900, 1100 and 1300 keV, we obtain the following results:

ID	E_g (keV)	Eff (x 10^4)	Total Error (%)
1	300	10.28	1.3
2	500	6.552	1.0
3	700	4.870	0.8
4	900	3.902	0.7
5	1100	3.270	0.7
6	1300	2.822	0.8

Associated with this solution is the error correlation matrix:

	1	2	3	4	5	6
1	1					
2	.96	1				
3	.84	.96	1			
4	.65	.83	.96	1		
5	.44	.67	.86	.97	1	
6	.26	.51	.74	.90	.98	1

Clearly this approach offers a relatively objective means for estimating errors and correlations for these derived physical results.

14. Subjective Estimation of Errors and Correlations

Often, errors and their correlations can be estimated only on rather subjective grounds. Experience is an important consideration here. Let us consider the fairly common situation where we encounter a number of small error components of complex origin. Then, it may suffice to assign as the correlations one or more of the following values, based on qualitative considerations:

S_{ijr}*	Strength
± 1.00	Full correlation
± 0.75	Strong correlation
± 0.50	Moderate correlation
± 0.25	Weak correlation
0	Negligible correlation

* Negative values imply anti-correlation.

Another frequently observed occurrence can be illustrated by the following example. Let us suppose that a set of neutron activation cross sections has been measured in the range E = 2-10 MeV. Each data point has an uncertainty due to multiple scattering of ~ 3%. It is reasonable to assume that the error correlation is strong for neighboring points (in neutron energy) and progressively weaker if the energy separation is large. It is not unrealistic to assume that $S_{ijr} \sim 1\text{-abs}(E_i\text{-}E_j)/(10\text{-}2)$. This ad hoc assumption can be defended only in that it is "plausible" under the circumstances.

15. Some Typical Attributes of Neutron Nuclear Data Experiments

It was pointed out earlier that one needs to consider for each experiment the various independent or nearly independent attributes which contribute error to the results. In the case of nuclear data experiments, the following are commonly considered: i) event statistics, ii) background corrections, iii) event determination procedures, iv) event determination calibration standards, v) sample assay parameters, vi) decay activity half lives, vii) decay activity branching parameters, viii) elemental isotopic abundances, ix) geometry factors, x) neutron source parameters, xi) absolute or relative neutron fluences, xii) neutron absorption, xiii) neutron scattering, xiv) absorption and scattering of secondary radiations, and xv) standard cross sections (for ratio measurements). There are many other factors, often quite specific to particular measurement techniques, which might have to be considered in individual experiments. It is up to the responsible experimenter, who ought to be well informed about all the details of his measurement procedures, to insure that each "significant" attribute of his experiment is considered in the modeling and error analysis.

16. The Virtues of Redundancy and Data Averaging

Whenever possible, it is worthwhile incorporating as much redundancy into an experiment as time and circumstances allow. For example, the cross section at a particular energy might be measured several times, perhaps with some variations of the experimental details (sample size, geometry, etc.) in order to test for reproducibility, to uncover systematic error sources and improve statistical accuracy. Multiple values for a single physical quantity generally ought to be averaged to produce a single "best" number for reporting purposes. A procedure for doing this, with full consideration of data covariances, has been developed and reported[8]. The method involves transformation from data vector $\underline{x}$ to a "collapsed" vector $\underline{y}$ by least squares, and application of the law of error propagation, $\underline{V}_y = \underline{T}^+\underline{V}_x\underline{T}$.

The process of data averaging can be thwarted by unresolved discrepancies. Actually, this procedure forces upon the experimenter the necessary discipline to face up to and, ultimately, either resolve the discrepancies, increase the errors or reject certain values. This issue is discussed in the next section.

17. Data Discrepancies

Discrepancies in data are the nemesis of all research endeavors. Evaluators must deal routinely with discrepant data from diverse experiments. For all the concern, there are no foolproof techniques for handling discrepant data. Here, we are involved with discrepancies amongst data from a single experiment. Discrepancies cannot arise in an individual experiment unless enough data are acquired to signal the presence of a systematic deviation of some result(s) from what was anticipated. For example, repeated measurements of a particular quantity under fixed conditions may lead to a flyer . Another possibility is that measurements of a physical parameter with systematic changes of a variable, e.g., cross section versus energy, may suddenly produce anomalous departure from a smooth curve trend. Discrepancies arise from two basic origins: i) systematic experimental errors or blunders, or ii) a real, but previously unanticipated physical phenomenon (e.g., discovery of an unexpected resonance). It is hard to identify the real cause in any single instance. Further investigation is usually required.

There are several ways to deal with a discrepancy. In order of descending preference they are as follows: Method 1: Identify and eliminate the source of the discrepancy. Method 2: Increase the error of the afflicted data point if the origin of discrepancy is elusive. Method 3: Average a collection of comparable values if several are available - including the discrepant value - and increase the error of the average accordingly. This effectively "dilutes" the effect of the discrepancy. Method 4: Discard the discrepant value outright. The hazard of this method is that the "discrepancy" could be indicative of new knowledge (e.g., a previously unsuspected resonance). Method 5: Keep the discrepant value and live with the full consequences without dilution.

The best way to search for the source of discrepancy (if there is one) is to examine all of the measured or standard parameters which enter into the derivation of a result, in the context of the model which is employed to compute this result and/or estimate its error. This approach will eliminate many possibilities and focus attention on a few critical areas of the experiment. The "detective" work just described may narrow the problem to a single aspect of the experiment, yet still not resolve the issue. Nevertheless, the experimenter will be in a better position to judge which of the Methods 2-5 might best be invoked in order to deal with the problem.

When a discrepancy is not outrageous, and there are several comparable data values available, then Method 3 (averaging the results and enhancing the error) is probably the best practical approach, whenever the origin of the discrepancy cannot be identified. For example, suppose there are five comparable measurements of count yield (with statistical error) as follows: Count 1 - 10250 ± 101.2; Count 2 - 10138 ± 100.7, Count 3 - 9987 ± 99.9, Count 4 - 10649 ± 103.2; Count 5 - 10069 ± 100.3. Count No. 4 looks discrepant in this data collection. Let

us average the results using two methods. Method 3: <N> = 10213 ± 45.2 (0.4%), (χ^2/f) = 6.43 (f=4), "enhanced" error = 114.6 (1.1%); Method 4: <N> = 10110 ± 50.3 (0.5%), (χ^2/f) = 1.22 ≈ 1 (f=3), "enhanced" error = 55.6 (~0.5%). Here, <N> signifies average counts and (χ^2/f) is the chi square per degree of freedom, a test of statistical significance. Both results are consistent with the errors of the majority of the data points. However, Method 3 is the most conservative approach.

18. The Issue of "Peelle's Pertinent Puzzle"

Under certain conditions, covariance matrices generated directly from experimental data lead to anomalous results when employed in analyses involving the least squares method. A symptom of the problem is the emergence of values that are "too low" in evaluations of such data. The problem is particularly acute when there are seriously discrepant data but, in fact, is present to some degree under any circumstances.

For practical reasons, there is a great advantage in expressing the uncertainties for a set of experimental data in terms of a relative covariance matrix. This provides an evaluator or other user of such information with possibilities for adjusting input values (to account for revisions in the experimental data for objective reasons as well as subjective ones) in order to circumvent discrepancies. With relative covariance matrices, this can be done without altering the fundamental uncertainty information content provided by the author of the data set.

One empirical approach which has been suggested to deal with the "Peelle Puzzle" issue is to alter $\underline{p}$ and, thus, $\underline{V}_p$, but not $\underline{R}_p$. This may be required if there are hidden variables involved in a transformation of the raw data to derived parameters (with loss of information)[5].

19. Summary

The formalism needed to generate the covariance matrix for an experimental data set follows from general statistical principles and application of the Law of Error Propagation. In practice, it is essential to develop a mathematical model for the experiment and identify the essentially independent attributes of the measurement process. Certain aspects of every experiment can be analyzed quite rigorously (statistics, calibration standards, etc.) while others can be approached only with considerable subjectivity (radiation absorption and scattering, etc.). One separates the various attributes of the experiment and does the best one can to attend to each distinct issue. There are certain advantages to dealing with relative covariance matrices, $\underline{R}_p$, rather than the explicit covariance matrices, $\underline{V}_p$, in this context. Discrepancies are the nemesis of both producers and users of nuclear data. When they occur, it is best to try to identify and eliminate them. If this is not possible, then there are some compromise approaches that can be used to dilute the negative impact.

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COVARIANCE DATA EVALUATION FOR EXPERIMENTAL DATA

LIU TINGJIN
China Nuclear Data Center, CIAE,
Beijing, P. R. China

ABSTRACT

Some methods and codes have been developed and used for covariance data evaluation of experimental data, they are parameter analysis, physical analysis, spline fitting etc.. These methods and codes can be used in different cases.

Introduction

Recent ten years, with the developing of the reactor physics and computer technique, the covariance matrix of nuclear data becomes more and more important for nuclear engineering. For evaluators and experimenters, the data information is given out completely only in the case that the data themselves and their covariance matrix are given, because the error, as traditionally given, is only the diagonal elements of the covariance matrix and describes the accuracy of the data, nothing about the correlation of the data is given. However, to give out the covariance matrix is not easy, because the matter itself is more complicated and the methods for this are being developed.

Some methods and codes for covariance data evaluation of experimental data have been developed and used for last few years, which are parameter analysis, physical analysis, spline function fitting etc.. They are suitable in different cases. Using these methods and codes, the experimenters or evaluators can evaluate the covariance data, calculate the covariance matrix from the error information of the experiments.

1 Parameter Analysis

If the conditions of an experiment, especially the information about the error are well known, the covariance matrix can be constructed according to the formula[1]

$$Cov(f_i,f_j) = \sum_k \frac{\partial f}{\partial x_k}\Big|_i \frac{\partial f}{\partial x_k}\Big|_j \rho_{ij}^k \sigma_{ki}\sigma_{kj} \quad (1.1)$$

(Suppose $\rho_{ij}^{kk'} = 0$, when $k \neq k'$)

Where

$\partial f / \partial x_k \mid_{i(j)}$ is the derivative of function f to parameter x_k, taken the value at $X_{ki(j)} = < X_{ki(j)} >$, $\sigma_{ki(j)}$ is the absolute error of kth parameter x_k at energy point i(j); and $\rho_{ji}^{kk'}$ is the correlation coefficient between parameter x_k at energy point i and parameter $x_{k'}$ at energy point j, ρ_{ij}^k is the correlation coefficient of parameter x_k at energy points i and j.

From the Eq. (1.1) it can be seen that the covariance matrix of the indirectly measured data can be constructed if its expression formula and the errors, the correlation coefficients of the directly measured parameters concerned are known.

In general case, it is easier for experimenters themselves to know the expression formula and the errors of the parameters. But for the correlation coefficients of the parameters at different energy points it's more complicated, which has been discussed in many papers[2~4].

If the function f or the errors Δx_k of the directly measured parameters are not known (for example for evaluators), the covariance matrix can be calculated like this :

$$Cov(f_i,f_j)=\sum_{k=1}^{N}\rho_{ij}^{k}\Delta f_{ki}\Delta f_{kj} \qquad (1.2)$$

where, Δf_{ki} (Δf_{kj}) is the error of the indirectly measured data contributed from kth parameter at energy point i(j). So if the partial error contributed from each parameter and their correlation coefficients at different energy points are known, the covariance matrix of indirectly measured data also can be calculated.

In mathematics, it can be proved that the constructed matrix in above way must be symmetric and positive definite[1].

For practical application, a program CMC was developed to calculate the covariance matrix from the error information of the experiment. The calculation is performed in two cases : whether the explicit formula for the indirectly measured quantity is known. If it is know, it is calculated with formula (1.1) and input needed parameters x_{ki}, σ_{ki}, ρ_{ij}^{k}, otherwise calculated with formula (1.2) and input needed parameters Δf_{ki}, ρ_{ij}^{k}. To simplify only one constant is input for some parameter if it is independent on energy.

In the explicit formula case, the following subroutines are included:

1) Total cross section,
2) Nonelastic scattering cross section,
3) Fission cross section,
4) Activation method,
5) Capture cross section,
6) Differential cross section and spectrum with time–of–flight method.

In the implicit case, two subroutines are included :

1) The relative error of each parameters are known
2) The partial percents contributed to the total error of each parameters are known.

To insure the covariance matrix constructed is reasonable in mathematics and physics, the positive definite feature of the constructed matrix is checked by using the method of calculating the eigenvalues of the correlation coefficient matrix.

An example is given for the cross section of $^{23}Na(n,2n)^{22}Na$ reaction in the energy region from 13.0~ 18.0 MeV, measured by Prof. Lu[5] with activation method at six energy points. The measurement was relative one, and $^{93}Nb(n,2n)^{92}Nb$ cross section was used as standard. The calculation formula is as follows :

$$\sigma_x=\frac{N_x[MI_\gamma f_a f_e \varepsilon K(1-e^{-\lambda T})]_s}{N_s[MI_\gamma f_a f_e \varepsilon K(1-e^{-\lambda T})]_x} \qquad (1.3)$$

where N is neutron count, M is the weight of the sample, I_γ is γ count, f_a is γ–ray correction factor in the radial direction, ε is the detector efficiency for the full energy peak, K is the correction factor for neutron flux fluctuation, and f_e is γ–ray self–absorption factor (it contributes very little, so it is neglected in the calculation). The footnote 0 and x represent the standard sample and the sample to be measured

respectively.

The measured values and their errors of above quantities at different energy points are given in Table 1.

The correlation coefficients for each parameter at different energy points ρ_{ij}^{k} are given in Table 2.

The calculated results are shown in Table 3. The errors and correlation coefficient matrix are given (the error σ^{*} were given by authors).

From Table 3, it can be seen that the results are reasonable :

1) The errors calculated in this work are in good agreement with the ones given by the authors.

2) The correlation between first 4 points is larger, the same situation for last two points. But the correlation is smaller between first four and last two points (ρ_{15},ρ_{16},ρ_{25}, ··· etc.). This is corresponding to the situation that the measurements for first four points and last two points were completed with the same devices respectively.

2 Physical Analysis

The data that their covariance is not given and the error information is not well known, which is usual case faced by the data evaluators, must be analyzed carefully in physics, and the total error, especially the main contributions for the systematic error should be found out as much as possible based on the realistic situations. Some examples, selected from the complete neutron data evaluation of Oxygen by author[6], are given as follows, which illustrate some typical cases.

2.1 Total Cross Section

In the evaluation, only one set of data[7] was taken in the energy region from 3 to 20 MeV. The information about the error given in the paper is : statistical, 0.3~ 1%; background correction, 1~ 3%; dead time<0.1%; multi–scattering, negligible and sample error, no information. The data were normalized to their early measured data[8, 9] at 3.5 MeV. It is clear that the main systematic error comes from the normalization, which is depended on the error of their early work. But there is no exact information about the data error at 3.5 MeV, in the paper only saying that it is less than 3%. Comparing this data around 3.5 MeV with F. G. Perey's[10] and R. B. Schrack's[11] data, it can be seen that the statistical error is 1.3% and the systematic difference between this data and Perey's data is 1.1%, which can be regarded as systematic error. So the total, used as normalization error, is 1.7%.

2.2 (n,p) Cross Section

According to the situation, as shown in Fig. 1, it is divided into three regions :

1) 16.5~20 MeV

In this region, there are two sets of data, and there are systematic differences between them. Drawing lines through each set of data, the average distance between them

(divided by 2) was taken as systematic error in this region.

2) 12.6～16.5 MeV

In this region, there are 8 sets of data, but only three of them were measured in whole region, five of others only around 14 MeV, and there is no systematic difference among them. Carefully analyzing the data shows that Seeman's[12] data have not only more energy points, but also smaller error 4% (others 8%, 10% respectively). So the curve is mainly determined by this set of data, and so the covariance. Analyzing this data shows that the total error is about 4.5% and the systematic component is 1.5% for detector efficiency and 1.0% for sample volume, so the total systematic error is 1.8%.

For convenience, a processing code CMP was written. With the code, explicit covariance matrix can be calculated and output in the ENDF / B–6 format, using the systematic error information given through above analysis in physics and the evaluated total or statistical error (for example through curve fitting), taking into account whether the systematic error needs to be added to the diagonal elements.

3 Spline Function Fitting

For cross section or other quantities, if there are multi–sets of measured (correlative) data and their covariance matrices are all known, the data can be fitted and the fit values and their covariance matrix can be calculated with spline function. The fit values

$$\hat{Y} = EY$$

and their covariance matrix

$$V_{\hat{Y}} = EV_Y E^T$$

where

$$E = B^T(W - U^T D U)$$

and Y is the vector of input measured data, V_Y is the covariance matrix of vector Y, B is base spline function matrix, and W, U, D are the matrices concerning different weights respectively[13].

A practical program SPC was developed; using it the multi–sets of correlative data can be fitted, and the covariance matrix of the fit values can be calculated, which is resulted mainly from the propagation of the input covariance matrices, and also some what production in the fitting. In the program, the order of the spline function can be chosen and the spline knots can be optimized automatically[14].

Using the program, the properties of correlative data fitting and their covariance were researched. It was shown that the fit values and their correlation coefficients are systematically changed with increasing the input correlation coefficient (suppose it is the same to all data points). Examples are given in Fig. 2～4. A practical example is given in Fig. 1, which was taken from the evaluation of Oxygen complete data for CENDL–2.

It was also found that the PPP problem[15] happened when the data to be fitted are in large discrepancy and the correlation is strong (see Fig. 2, curves No. 5, 6). In this case, the fit

values are outside the input experimental data and are not reasonable. To solve this problem, the input absolute covariance matrix is iterated, keeping the input relative covariance matrix unchanged and replacing the input experimental data by fit values. An example is given in Fig. 5, the start curve is the curve No. 6 in Fig. 2. As a practical example, the change of output covariance matrix with iteration is given in Fig. 6.

Conclusion Remarks

The methods and codes for covariance data evaluation of experimental data described above can be used in different cases and for different purpose. The parameter analysis can be used for experimenters to construct the covariance matrix of their measured data, because they well know the experiment conditions, especially the information about the error. The evaluators usually have to do physical analysis, because they face large amount of data and not well know the measurement conditions. The spline fit is suitable for both experimenters and evaluators to process their correlative data : calculate the fit values and their covariance matrix, but it can be used only in the case that the covariance matrices of input data are all already known.

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Table 1 The measured values and their errors of the quantities concerned

quan. x_k, Δx_k \ E_n	13.5		14.1		14.64	
	Value	error	Value	error	Value	error
N_x	3.85×10^{-3}	0.92%	1.1825×10^{-2}	1.2%	2.5259×10^{-2}	0.43%
M_o	2.01882×10^{21}	0.2%	1.6409×10^{21}	0.2%	1.3553×10^{21}	0.2%
$I_{\gamma o}$	0.990		0.990		0.990	
f_{ao}	0.995	0.1%	0.996	0.1%	0.998	0.1
ε_o	0.03248	1.2%	0.03248	1.2%	0.03248	1.2%
K_o	1.0147	0.1%	1.0147	0.1%	1.0147	0.1%
$(1-c)_o^{-\lambda T}$	0.2365		0.2365		0.2365	
σ_o	448	7.4	456.7	4.7	459	5.0
N_o	90.22	0.5%	69.602	0.5%	64.690	0.5%
M_x	3.1769×10^{22}	0.4%	3.0507×10^{22}	0.4%	2.9441×10^{22}	0.4%
$I_{\gamma x}$	0.9994		0.9994		0.9994	
f_{aX}	0.9635	0.4%	0.9650	0.4%	0.9664	0.4%
ε_x	0.0005783	0.8%	0.0005783	0.8%	0.0005793	0.8%
$(1-c)_x^{-\lambda T}$	2.8773×10^{-3}		2.8773×10^{-3}		2.8773×10^{-3}	

quan. x_k, Δx_k \ E_n	14.87		16.95		17.98	
	Value	error	Value	error	Value	error
N_x	3.0235×10^{-2}	0.7%	0.1231	0.36%	0.2822	0.26%
M_o	1.1914×10^{21}	0.2%	6.4818×10^{18}	0.2%	6.4818×10^{18}	0.2%
$I_{\gamma o}$	0.990		0.990		0.990	
f_{ao}	0.998	0.1%	0.998	0.1%	0.996	0.1
ε_o	0.03248	1.2%	0.03248	1.2%	0.03248	1.2%
K_o	1.0147	0.1%	0.9911	0.1%	0.9933	0.1%
$(1-c)_o^{-\lambda T}$	0.2365		0.1644		0.1043	
σ_o	458	6.0	413	11.0	388	15.0
N_o	57.612	0.5%	0.04729	0.5%	0.09549	0.5%
M_x	3.3073×10^{22}	0.4%	1.4342×10^{22}	0.4%	1.4342×10^{22}	0.4%
$I_{\gamma x}$	0.9994		0.9994		0.9994	
f_{aX}	0.9623	0.4%	0.9869	0.4%	0.9840	0.4%
ε_x	0.0005783	0.8%	0.01509	0.8%	0.01509	0.8%
$(1-c)_x^{-\lambda T}$	2.8773×10^{-3}		1.9163×10^{-3}		1.1754×10^{-3}	

Table 2 The correlation coefficients of directly measured quantities

Measured quantities x_k	Correlation coefficient f_{ij}^{*}	Comments
N_x	0	completely statistical
N_o	0	
M_x	1.0	completely systematical
M_o	1.0	
ε_o	1.0	
f_{ax}	0.7	statistical and systematical, mainly systematical
f_{ao}	0.7	
σ_o	0.5	estimate
ε_x	1.0, i,j = 1～4 or 5,6	same device
	0.7 i = 1～4, j = 5,6	different device

Table 3 The correlation coefficient matrix and error for ^{23}Na(n,2n) reaction

E_n \ ρ	13.5 MeV	14.10 MeV	14.64 MeV	14.87 MeV	16.95 MeV	17.98 MeV
13.50 MeV	1.0000					
14.10 MeV	0.5543	1.0000				
14.64 MeV	0.6398	0.6281	1.0000			
14.87 MeV	0.6423	0.6201	0.7140	1.0000		
16.95 MeV	0.5094	0.4390	0.5122	0.5325	1.0000	
17.98 MeV	0.4720	0.3897	0.4571	0.4834	0.5435	1.0000
σ	0.14	0.45	0.78	0.87	2.69	4.05
σ^{*}	0.16	0.50	0.80	0.90	3.0	4.3

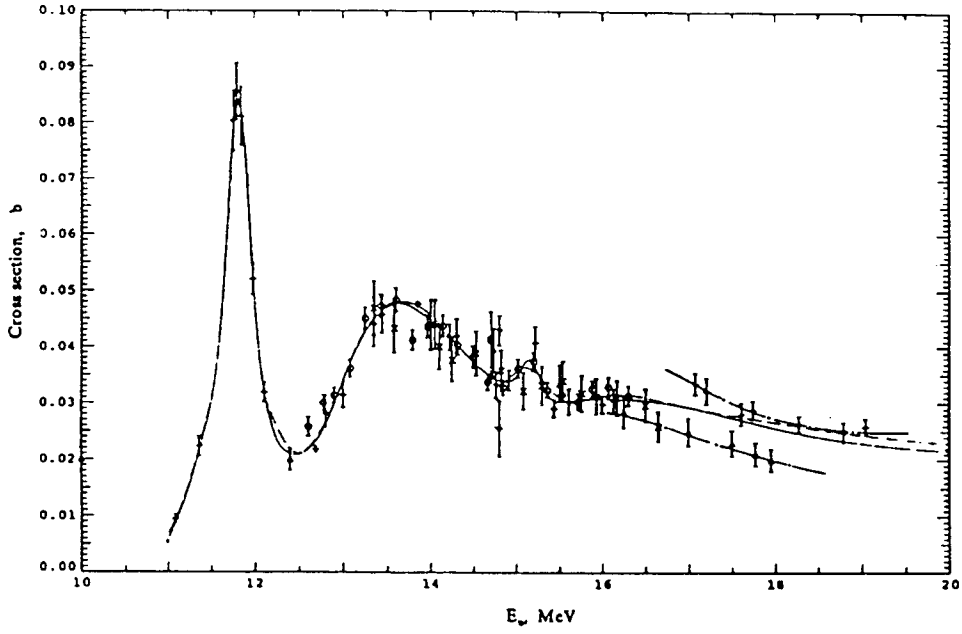

Fig. 1 O(n,p) cross section

Φ etc. exp. data; —— fit curve, $\rho = 0.0$; – – – fit curve, $\rho = 0.5$;
— · — The line to estimate the systematic error in the energy region 16.5 to 20 MeV

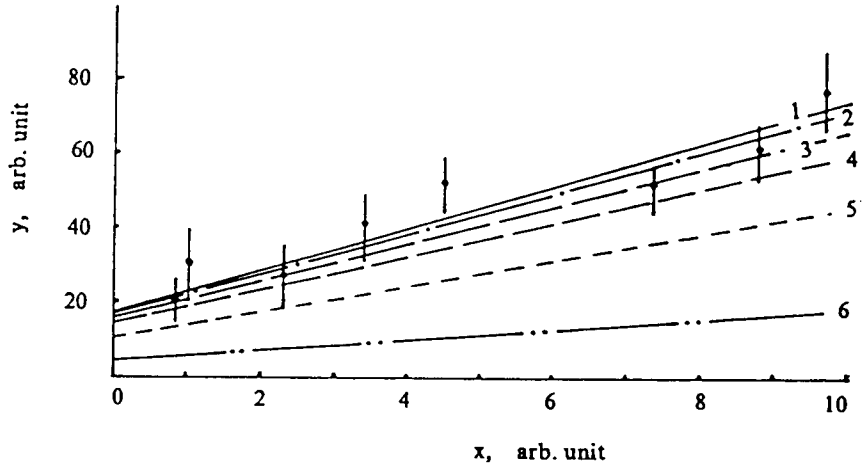

Fig. 2 The changing of fit values with the correlation coefficient ρ of input data
1 – $\rho = 0.0$; 2 $\rho = 0.2$; 3 $\rho = 0.4$; 4 $\rho = 0.6$; 5 $\rho = 0.8$; 6 $\rho = 0.95$;

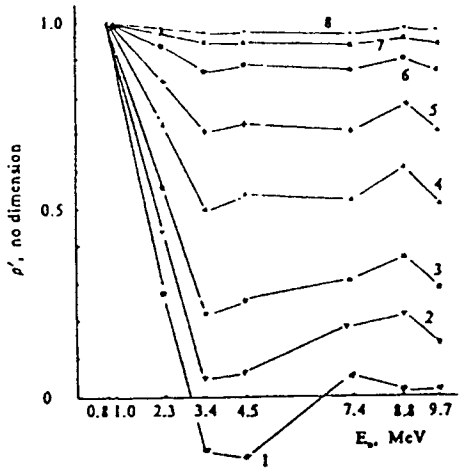

Fig. 3 The effect of the input correlation coefficient ρ on the correlation coefficient ρ' of fit values

1 $\rho=0.0$; 2 $\rho=0.1$; 3 $\rho=0.2$;
4 $\rho=0.4$; 5 $\rho=0.6$; 6 $\rho=0.8$;
7 $\rho=0.9$; 8 $\rho=0.95$

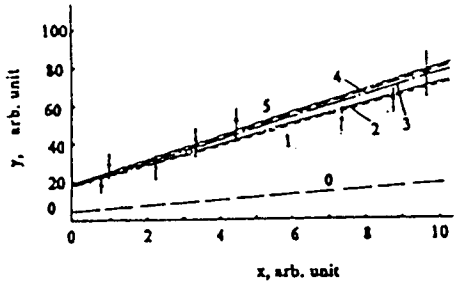

Fig. 5 The changing of fit values with iteration
the numbers in the figure are the iteration times

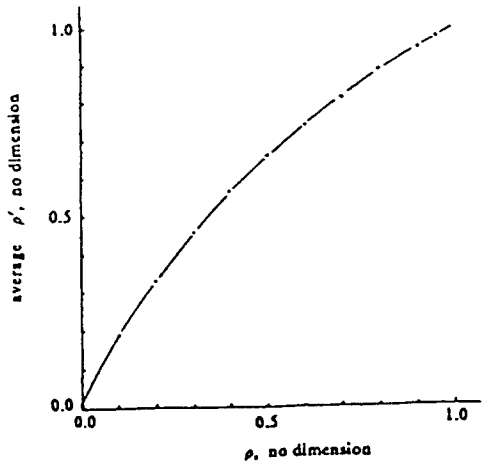

Fig. 4 The changing of average correlation coefficient ρ' of fit values with input correlation coefficient ρ

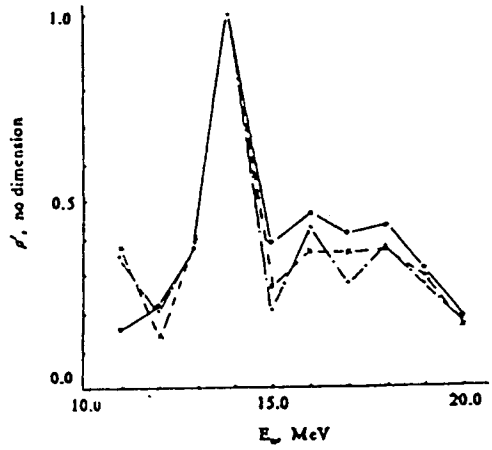

Fig. 6 The effecting of iteration times k on the correlation coefficient ρ' of fit values for O(n,p) cross section
× k = 0; O k = 1; · k = 2

COVARIANCE MATRIX OF MODEL PARAMETERS AND UNCERTAINTIES OF CALCULATED NEUTRON CROSS SECTIONS ON ^{19}F

Zhixiang Zhao
Institute of Atomic Energy, P. O. Box 275 (41), Beijing, China

C. Y. Fu D. C. Larson
ORNL, P. O. Box 2008, Oak Ridge, TN 37831, U. S. A

ABSTRACT: A simplified method to estimate covariance matrix of the model parameters is presented in this work and applied to calculate covariance matrix of calculated cross sections on ^{19}F.

I. Introduction

Theoretical calculation plays an important role in modern nuclear data evaluation. This theoretical calculation may be refered as[1] a " theoretical evaluation " . The procedure of using theory calculation as evaluation can be divided into two steps. Firstly, the measured data available are selected as input data to parameterize the theory formulas for a given nuclei, i. e., to determine the parameters in the formulas through fitting the measured input data. And then the parameters determined in this way are used to compute a complete and consistent data set.

One of the problems evaluators meet with in this kind of theoretical evaluation is how to estimate the uncertainties of calculated quantities. Several methods suggested by different authors have been used in obtaining the covariance matrix of theoretical evaluated quantities[2-7].

A simplified method to estimate covariance matrix of the model parameters is presented in this work and applied to calculate the covariance matrix of calculated cross sections on ^{19}F.

II. Method

The uncertainties of model parameters arise from (1) the uncertaintities of experimental data used to determine model parameters and (2) drawbacks of the model itself. The first type of uncertainties can be derived based on the law of error propagation, and the second one can be estimated from the scatter of experimental data around the calculated values (Moment Method). In fact, we only need to known the long-range components of experimental uncertainties when the Moment Method is used to estimate the uncertainties of model parameters because the scatter of measured data around calculated values reflect not only the drawbacks of model

used in the analysis, but also the fluctuation of measured data due to statistical error. In the present work, a simple method given in the following was used to determine the covariance matrix of the model parameters.

Let

$$Y_k(E_i) = f_k(E_i, C) \qquad (1)$$

where $Y_k(E_i)$ is a measurable physical quantity such as a cross section; the subscript k denotes a specific type of physical quantity (for example, the (n,p) reaction cross section); E_i represents the argument (for example, incident neutron energy) which is assumed to have no uncertainties , and $f_k(E_i,C)$ gives the relation between $Y_k(E_i)$ and the model parameter vector C. In general, many types of measured data (for example, cross section, angular distribution and spectra of different reaction channels can be used to determine a set of model parameters simultaneously. Assuming that no correlation exists between two different types of data, the covariance matrix, $V_c(M \times M)$, of the M– dimension parameter vector C can be written as

$$\begin{aligned} V_c(M \times M) &= [\Sigma_k (F_k(NK \times M)^t V_k^{-1}(NK \times NK) F_k(NK \times M)]^{-1} \\ &= [\Sigma_k W_k(M \times M)]^{-1} \end{aligned} \qquad (2)$$

according to the least squares method. In the equation above, F_k represents the so–called sensitivity matrix for k–th type of data

$$F_k(i,j) = \frac{\partial f_k(E_i, C)}{\partial C_j} \qquad (3)$$

and $V_k(NK \times NK)$ is the covariance matrix of measured values $Y_k = (Y_k(E_1), Y_k(E_2), \ldots\ldots, Y_k(E_{nk}))$. The deviations of measurement here is defined as the differences between measured values and the calculated values, that means V_k should include not only the uncertainties of experimental data but also the drawbacks of the model and can be written as

$$V_k = P_k(NK \times NK) R_k(NK \times NK)(P_k(NK \times NK)) \qquad (4)$$

where

$$P_k = \begin{bmatrix} f_k(E_1, C) & 0 & \ldots & 0 \\ 0 & f_k(E_2, C) & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & f_k(E_{nk}, C) \end{bmatrix} \qquad (5)$$

and R_k is the relative covariance matrix

$$R_k(i,j) = \frac{Cov(Y_k(E_i), Y_k(E_j))}{f_k(E_i, C) f_k(E_j, C)} \qquad (6)$$

If only long–range correlations are important, R_k can be expressed approximatelly as follows

$$R_k(i,i) = [S'_k(E_i) / f_k(E_i, C)]^2 + D_k^2 \qquad (7)$$

and

$$R_k(i,j) = D_k^2 \qquad (i \neq j) \qquad (8)$$

where D_k^2 is the long–range component of the relative uncertainty of the k–th data vector Y_k and $S'_k(E_i) / f_k(E_i,C)$ is the short–range component of relative error of $Y_k(E_i)$. In the case of

$$S'_k(E_l) / f_k(E_l,C) = S_k \qquad (9)$$

the elements of inverse of matrix R_k can be simply written as

$$R_k^{-1}(i,i) = a_k = 1 / S_k^2 - 1 / [(NK-1)S_k^2 + (S_k^2 + D_k^2)S_k^2 / D_k^2] \qquad (10)$$

and

$$R_k^{-1}(i,j) = b_k = -1 / [(NK-1)S_k^2 + (S_k^2 + D_k^2)S_k^2 / D_k^2] \qquad (11)$$

so that

$$W_k(i,j) = (a_k - b_k) \sum_{l=1}^{NK} \frac{F_k(l,i)F_k(l,j)}{f_k^2(E_l,C)} + b_k [\sum_{l=1}^{NK} \frac{F_k(l,i)}{f_k(E_l,C)}] \times [\sum_{l=1}^{NK} \frac{F_k(l,j)}{f_k(E_l,C)}] \qquad (12)$$

and finally

$$V_c(M \times M) = [\sum_k W_k(M \times M)]^{-1} \qquad (13)$$

The problem is how to determine D_k^2 and S_k^2. The D_k^2 can be expressed as

$$D_k^2 = D_k^2(exp.) + D_k^2(th.) \qquad (14)$$

where D_k^2(exp.) denotes the component arisen from measurement and can be obtained by analyzing the experimental conditions; D_k^2(th.) represents those from drawbacks of the model and can be estimated by

$$D_k^2(th.) = \frac{1}{NK-M} [\sum_{l=1}^{NK} \frac{Y_k(E_l) - f_k(E_l,C)}{f_k(E_l,C)}]^2 \qquad (15)$$

in the case that the calculated values systematically deviate from the measured one. If the calculated values pass through the k–th type of measured data without systematic deviation, the D_k^2(th.) calculated from the equation above will be close to zero. The short–range component S_k can be estimated by

$$S_k^2 = \frac{1}{NK-M} \sum_{l=1}^{NK} (\frac{Y_k(E_l) - f_k(E_l,C)}{f_k(E_l,C)})^2 \qquad (16)$$

As metioned above, S_k^2 given by the equation above not only includes random uncertainties in measurement but also reflects the uncertainties from the fact that the model used sometimes cannot describe the detailed structure in physical curves very well.

III. Application

Based on the method above, the covariance matrix of a set of the model parameters was obtained. These

parameters were used in TNG for calculating cross sections of the reactions induced by neutrons on F^{19}. This study concerned six types of cross sections including those of (n,n'), (n,2n), (n,p), (n,α), (n,np+pn) and (n,nα+αn) reactions and nine of model parameters such as a_n, a_p, a_α(level density parameters for ^{19}F, ^{19}O and ^{16}N), V_0, W_0(depths for real and imaginary well),R_V,R_d(radius of real and imaginary potential), A_V,A_P(diffuseness of real and imaginary potential).

The partial derivatives of cross sections to parameters as a function of neutron energy were calculated by the difference quotient

$$F_k(i,j) = \frac{\partial f_k(E_i,C)}{\partial C_j} \approx \frac{f_k(E_i,C') - f_k(E_i,C)}{\Delta C_j} \qquad (17)$$

where $C' = (C_1, C_2, ..., C_j + \Delta C_j, ..., C_M)$ and ΔCj was taken as 0.02Cj. From calculated product of partial derivatives and the parameters themselves, it is found that in general the values of this kind of product for a_p,A_V andA_d are much smaller compared to other parameters. This means that these three parameters have less importance than other parameters in calculating uncertainties of the cross sections. Thus, only six most sensitive parameters were considered.

The measured cross sections for (n,2n), (n,p) and (n,α) were used to determine V_c. The long–range components of the relative variance, D_k^2(exp.), were taken from File 33 of ENDF / B–V. The covariance matrix of six parameters is given in Table 1. The covariance matrix of the calculated cross sections for (n,nα+αn) reaction were calculated from the covariance matrix in Table 1 and are given in Table 2.

Table 1 Covariance Matrix of Model Parameters

Parameter	St.Error, %	Correlation Matrix					
a_n = 4.00 MeV	8.12	1.00					
a_α = 3.68 MeV	4.96	−0.10	1.00				
W_o = 6.20 MeV	56.2	−0.67	0.38	1.00			
V_o = 45.8 MeV	29.9	−0.48	0.03	0.68	1.00		
R_v = 1.260 fm	9.39	0.49	−0.20	−0.80	−0.92	1.00	
R_d = 1.300 fm	26.5	0.48	−0.25	−0.92	−0.67	0.79	1.00

Table 2 Covariance Matrix of (n,nα+αn) Cross Sections

E_n MeV	σ mb	St.error %	Correlation Matrix								
6.0	26.8	17.2	1.0								
7.0	122.7	17.2	0.99	1.0							
8.0	218.7	13.8	0.71	.71	1.0						
10.0	412.9	8.29	0.71	.71	.58	1.0					
12.0	439.4	8.29	0.71	.71	.58	.99	1.0				
14.1	381.8	11.6	0.70	.70	.70	.88	.88	1.0			
16.0	333.4	11.6	0.70	.70	.70	.88	.88	.99	1.0		
18.0	273.5	14.4	0.59	.59	.68	.78	.78	.97	.97	1.0	
20.0	242.0	14.4	0.59	.59	.68	.78	.78	.97	.97	.99	1.0

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COVARIANCE OF HISTOGRAMS IN PARALLEL WEIGHTED COUNTING

C.Bastian

CEC-JRC Central Bureau for Nuclear Measurements
B-2440 Geel, Belgium

Abstract

Double differential nuclear cross-sections measurements (neutron energy-emission angle) usually rely on biparametric counting histograms. Alternatively the detector output may be processed on-line to produce the angular distribution as an expansion in Legendre polynomials of cos θ. The Legendre moments are accumulated in a set of single parameter histograms covering the neutron input energy range so they may be visualized during acquisition. Their covariances are accumulated simultaneously in another set of histograms. The multiple weighted counting method producing these data is presented and discussed in comparison with the classical off-line least-squares analysis of biparametric counting spectra.

INTRODUCTION

Some charged particle detectors used in neutron cross-section measurements produce detailed information on the reaction products. This is the case of the Frisch grid detector (Fig.1), by which a combination of the output signals leads to a measurement of the cosine of the angle of emission of every detected particle[1].

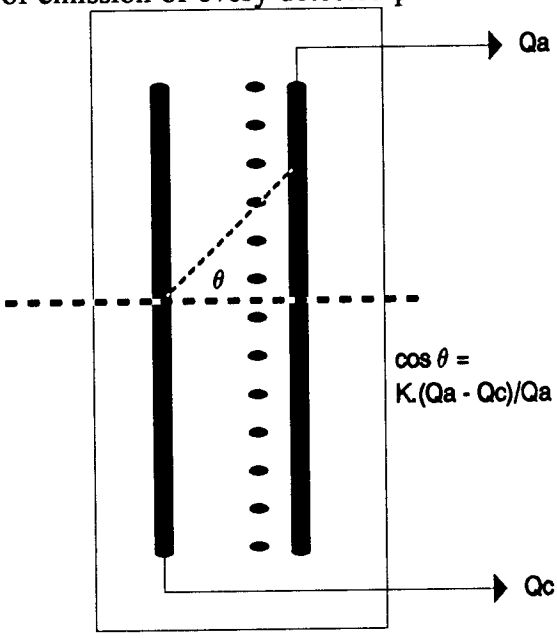

Fig.1 - Frisch grid detector

Every reaction is thus recorded at least as a two-parameter event. Usually the events are sorted and accumulated in biparametric histograms, from which the angular distribution of the emission is deduced as a function of the input energy. For theoretical or numerical application, an angular distribution is best represented as a linear expansion in Legendre polynomials of the cosine of the angle. We will show in the following that a limited set of Legendre moments of the distribution may be accumulated in the form of single-parameter histograms.

1.CLASSICAL DETERMINATION OF THE LEGENDRE MOMENTS

In a double differential cross-section measurement, the detected events are sorted and counted in a histogram matrix M_{ij} where **i** is the running index of counting channels in input neutron energy and **j** the index of counting channels over the range **[-1 , +1]** of the cosine of the emission angle.

Every line of **M** corresponding to a constant input energy channel E_i and the whole range of the emission angle may be expressed as a linear expansion in Legendre Polynomials:

$$M_{ij} = \Sigma_k \alpha_k(E_i).P_{kj} \qquad (1)$$

where P_{kj} is proportional to the L.P. of order **k** of the average value of $\cos\theta$ in the **j**-th counting channel of emission angle. It is advisable to choose the discrete values of P_{kj} such that they fulfil the orthogonality feature of the L.P.'s over the **[-1 , +1]** range, i.e.:

$$\Sigma_r (P_{mr}.P_{nr}) = 0 \text{ if } m \neq n \qquad (2)$$

In the following, we will also assume for the sake of clarity that:

$$\Sigma_r(P_{mr}.P_{mr}) = 1 \qquad (3)$$

(which needs not be always true in applications with integer numerics.)

Orthonormality equations (2,3) allow us to express the Legendre moments by a projection on the base functions:

$$\alpha_k(E_i) = \Sigma_j M_{ij}P_{kj} \qquad (4)$$

Besides, we have here the simplest case of a least squares solution where the design matrix times its transpose is a unit matrix. Eq(4) are the normal equations in their most obvious form.

As our notation suggests, the Legendre moments $\alpha_k(E_i)$ may be seen each as a pseudo-counting distribution over the neutron energy. Altogether they will require less storage space than the original histogram M_{ij} when only a few Legendre moments are needed .

On the other hand, Eq(4) shows that at a constant value E of the neutron energy, all Legendre moments $\alpha_k(E=cst)$ are derived from the same vector of count numbers $M_j(E=cst)$.

The uncertainties on the M_j's are not correlated, their variance is commonly estimated equal to their values. In other words, the covariance matrix of the M_j's is diagonal with values equal to M_j.

On the contrary, the uncertainties on the $\alpha_k(E=cst)$ are not independent. The law of error propagation associated with Eq(4) delivers the covariance of the α_k's in the form:

$$<\Delta\alpha_k.\Delta\alpha_m> = \Sigma_j\ P_{kj}M_jP_{mj} \qquad (5)$$

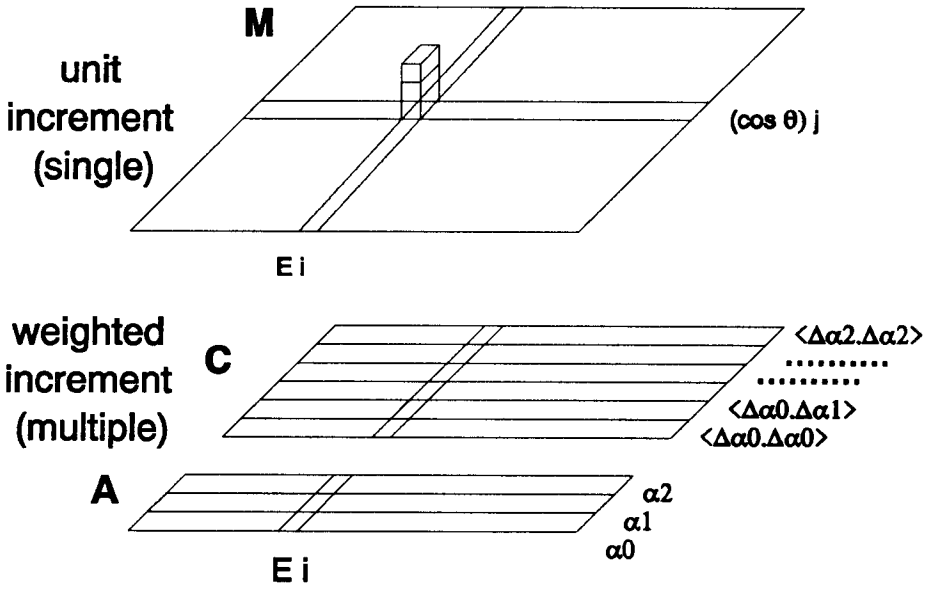

Fig.2 - Direct accumulation of Legendre moments and their covariant counting uncertainties

2. ON-LINE ACQUISITION OF THE LEGENDRE MOMENTS

In the acquisition procedure of Sec.1, for a biparametric event $E_i,(\cos\theta)_j$ M_{ij} is incremented by 1.(See Fig.2).

Alternatively, considering $\alpha_k(E_i)$ as a pseudo-histogram we may use the events to increment a matrix **A** (See Fig.2) where A_{ik} should ultimately contain the values of $\alpha_k(E_i)$ as derived from Eq(4).

The corresponding accumulation scheme bases on the prescription that, for an event input $E_i,(\cos\theta)_j$ all A_{ik}'s (**k** running from **0** to **kmax**) are incremented, each by P_{kj}.(See Fig.2) This multiple accumulation scheme is the event-by-event equivalent of Eq (4).

Further, the covariance of the α's has to be determined for every value of the neutron energy according to Eq(5). This can be done with a subsidiary counting structure C_{ip} (See Fig.2) where the running range of index **p** has enough values to cover all combinations of two values of **k**. The corresponding prescription is that for an event input **(i,j)** the whole column **i** of **C** is incremented by $P_{kj}P_{mj}$ at positions **p** corresponding to the combinations **k,m**. (See Fig 2). This scheme of accumulation is equivalent to Eq(5).

With an acquisition system able to process the double differential detector output at run-time, the accumulation of the Legendre moments obviously simplifies the execution and analysis of an angular measurement. It would for example provide a direct characterisation of the resonances in high resolution time-of-flight measurements.

3. TECHNICALITIES

The accumulation of the Legendre moments reduces the memory requirements on the acquisition system. In the classical approach of Sec.1, the number of rows of histogram **M** should match the angular resolution of the detector. Even with a moderate resolution of .05 in $\cos\theta$,[1] this means 40 or 50 rows times several thousands of energy channels for the histogram **M**. For the accumulation of the first 4 Legendre moments and their covariances, only 14 rows would be required for the matrices **A** and **C**. In general, if **n** Legendre moments are accumulated, the number of independent terms of their covariance matrices is **n.(n+1)/2**, so that the number of rows required for **A** and **C** in live memory will be **n.(n+3)/2 .**

However this acquisition method distinctly requires more real-time computing power : it performs **n.(n+3)/2** additions per event, whereas only one memory position needs to be incremented in the classical method. For computing speed and compatibility with the real-time graphic display, all weighting arithmetics will preferably be done in 4-bytes integers. One will thereby have to respect a prescription on the P_{kj} replacing the simplifying assumption Eq(3) of Sec.1.

Also for real-time speed, the increment weights P_{kj} and $P_{kj}P_{mj}$ would be at best computed once and stored in a lookup-table, **n.(n+3)/2** columns wide and R_θ rows high, where R_θ is the maximum number of angular channels reasonably compatible with the angular resolution of the detector.

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IMPACTS OF ISOMORPHIC TRANSFORMATIONS AND TRUNCATIONS OF DATA SPACES ON THE LEAST-SQUARES SOLUTIONS

S. Chiba

Japan Atomic Energy Research Institute
Tokai-mura, Naka-gun, Ibaraki-ken 319-11, Japan

The least-squares method (LSM) is most commonly used as a tool of statistical inference in nuclear data evaluations and data analyses because its solution (the least-squares solution, LSS) has such desirable properties as indicated by Gauss-Markov theorem. However, in applying the LSM in actual data analyses, the LSS obtained before and after a transformation of the data are often different from each other. Sometimes the impact is very serious, and an example of such anomaly is known as Peelle's Pertinent Puzzle (PPP). In this paper, criterion to obtain the same LSS before and after transformations of data which conserves dimensionality are established, i.e., in order to obtain the same least-squares solution before and after this type of transformation, the data covariance matrix and the design matrix must be transformed in a covariant manner. It is also shown that the Least-squares solution is NOT generally invariant under a truncation of data spaces. This fact also results in the same type of anomaly as PPP. According to these results, the origin of PPP was traced to an improper truncation of a data space and a neglect of the invariance criterion.

1. Introduction

When a researcher performs an experiment, he will not be likely to report the raw data obtained from his measurement. Instead, he will process the data in order to extract information related to the physical quantities under interest. This process is sometimes referred to as "data reduction", "data treatment" or something else. The process of data reduction is roughly classified into two categories. In the first category, a set of data (denoted by a vector y) is converted into another data vector y' having same dimension by using a set of functions f as y' = f(y). In the second category, essence of y' is extracted as y" by truncating a part of y', i.e., y" = a sub-set of y'. Therefore, dimension of y" is less than that of y'. In actual data processing, these two kinds of transformation are often applied simultaneously. However, the classification defined here will still be universally meaningful. These transformations are often applied by evaluators or data analysists also in order to, e.g., linearize the "model" with respect to the parameters to be estimated.

The purpose of this paper is to investigate the relations of the least-squares solutions (LSS) obtained before and after these transformations, based on fundamental thoughts on differentiation and straightforward matrix algebras. In the first part of this paper, the invariance criterion to make invariant the LSS before and after any transformation which conserves dimension of the data are derived, and some examples are given. On the contrary, the LSS is not invariant under truncations. This fact will be illustrated by numerical examples in the later part.

2. Invariance Criterion of the Least-Squares Solutions Under Isomorphic Transformations

Here, the term "isomorphic transformation" is defined as a transformation of a vector y into another as y' = f(y) which conserves number of dimensions, i.e., [dimension of y'] = [dimension of y]. If the dimension of y' is less than that of y, the transformation is referred to as "truncation of data spaces", and is described in Section 4. These transformation need not be linear in y.

Let us suppose a general problem in which a data vector $y = (y_1,y_2,...,y_n)^t$ having covariance matrix V_y is to be fitted according to the LSM with a set of functions $g_i(p)_{(i=1...n)}$, where $p=(p_1,...,p_q)^t$ denote a parameter vector to be estimated ($q < n$). The observation equation of this problem is therefore written down as;

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \cdots \\ y_n \end{bmatrix} - \begin{bmatrix} g_1(p_1,\cdots,p_q) \\ g_2(p_1,\cdots,p_q) \\ \cdots \\ g_n(p_1,\cdots,p_q) \end{bmatrix} \tag{1}$$

The "design matrix a" which contains essence of the "model" g is defined as follows,

$$a = (a_{ij}) = \left(\frac{\partial g_i}{\partial p_j}\right) = \left(\left(\frac{\partial g}{\partial p}\right)_{ij}\right) \tag{2}$$

where the matrix $(\partial g/\partial p)$ is defined by this relation. The design matrix is sometimes referred to as "sensitivity matrix". Then, the least-squares solution vector p is obtained by the following linearized form[1];

$$p = p_0 + (a^t V_y^{-1} a)^{-1} a^t V_y^{-1} [y - g(p_0)] \tag{3}$$

The vector p_0 consists of initial values of the parameters, and the design matrix a should be calculated using p_0. If the function g_i are not linear in p, iterations are needed replacing p_0 and "a" by using the estimated parameters until certain convergence criterion are satisfied. If g's are linear functions, no iterations are required. $(\Delta y) \equiv (y - g(p))$ is referred to as the residual vector.

Let us now transform the data vector y into another designated by y' as $y'_i = f_i(y_1, y_2, .., y_n)$ in an isomorphic way where i=1~n. Then, the model "g" should be also transformed in the same way as $g'_i(p_1, ..., p_q) = f_i[g_1(p_1, .., p_q), .., g_n(p_1, .., p_q)]$ in order to keep the physical meanings of the parameters unchanged.

The residual vector of transformed quantities are calculated as follows;

$$\begin{aligned}
\Delta y'_i &= y'_i - g'_i(p) \equiv f_i(y) - f_i[g(p)] = \Delta f_i \\
&= f_i[g(p)+(y-g(p))] - f_i[g(p)] = \sum_j \frac{\partial f_i}{\partial g_j}(y-g(p))_j = \left(\frac{\partial f_i}{\partial g}\right)\cdot(y-g(p)) \\
&= f_i(y) - f_i[y-(y-g(p))] = \sum_j \frac{\partial f_i}{\partial y_j}(y-g(p))_j = \left(\frac{\partial f_i}{\partial y}\right)\cdot(y-g(p)) \\
&= f_i[\frac{1}{2}(y+g(p))+\frac{1}{2}(y-g(p))] - f_i[\frac{1}{2}(y+g(p))-\frac{1}{2}(y-g(p))] \\
&= \left(\frac{\partial f_i}{\partial y}\Big|_{y=\frac{1}{2}(y+g(p))}\right)\cdot(y-g(p)) \cong \frac{1}{2}\left(\left(\frac{\partial f_i}{\partial y}\right) + \left(\frac{\partial f_i}{\partial g}\right)\right)\cdot(y-g(p))
\end{aligned} \tag{4}$$

The second line of this equation corresponds to a calculation with the forward differentiation, the third line to the backward differentiation, and the fourth and fifth lines to the central differentiation. From the viewpoint of numerical calculation, the central differentiation gives the best result. Let us define matrices $c^{(+)}$, $c^{(-)}$ and $c^{(1/2)}$ as below;

$$c_{ij}^{(+)} \equiv \left(\frac{\partial f_i(g_1,\cdots,g_n)}{\partial g_j}\right) = \frac{\partial f_i}{\partial g_j}, \quad c_{ij}^{(-)} \equiv \left(\frac{\partial f_i(y_1,\cdots,y_n)}{\partial y_j}\right) = \frac{\partial f_i}{\partial y_j}, \quad c^{(1/2)} \equiv \frac{1}{2}(c^{(+)} + c^{(-)}) \tag{5}$$

If the function f(y) is smooth, and if the difference [y−g(p)] is reasonably small, those three matrices become identical by the definition of differentiation. Therefore, they can be designated by a common symbol $c \equiv c^{(+)}$, $c^{(-)}$ or $c^{(1/2)}$. The residual vector $\Delta y'$ is then written as

$$\Delta y' = y' - g'(p) \equiv f(y) - f[g(p)] = \Delta f = c\cdot[y - g(p)] = c\cdot\Delta y \tag{6}$$

In the transformed data space, the observation equation becomes

$$y' = f(y) = \begin{bmatrix} f_1(y_1,..,y_n) \\ ..... \\ f_n(y_1,..,y_n) \end{bmatrix} \sim f[g(p)] = \begin{bmatrix} f_1[g_1(p),..,g_n(p)] \\ ..... \\ f_n[g_1(p),..,g_n(p)] \end{bmatrix} = \begin{bmatrix} g'_1(p_1,..,p_q) \\ ..... \\ g'_n(p_1,..,p_q) \end{bmatrix} \tag{7}$$

By defining a new design matrix a' as,

$$a' = (a'_{ij}) \equiv \left(\frac{\partial g'_i}{\partial p_j}\right) \tag{8}$$

the least-squares solution p' in this transformed data space is written schematically in the same form as Eq. (3);

$$p' = p_0 + (a'^t V_{y'}^{-1} a')^{-1} a'^t V_{y'}^{-1} [y' - g'(p_0))] \tag{9}$$

where

$$V_{y'} \equiv <\Delta y' \cdot \Delta y'^t> = c<\Delta y \cdot \Delta y^t> c^t = c \cdot V_y \cdot c^t \tag{10}$$

is the covariance matrix of the transformed data vector y'. This formula is known as "law of error propagation". More rigorous derivation of this formula is given in Appendix. The same initial value p_0 used in Eq. (3) was also employed in Eq. (9). The new design matrix a' can be rewritten as;

$$a'_{ij} = \frac{\partial g'_i}{\partial p_j} = \frac{\partial (y'_i - \Delta f_i)}{\partial p_j} = -\frac{\partial \Delta f_i}{\partial p_j} = \sum_k c_{i,k} \cdot \frac{\partial g(p)_k}{\partial p_j} \tag{11}$$

where the relation (6) was used. Therefore, a' is obtained by a product of two matrices

$$a' = c\left(\frac{\partial g}{\partial p}\right) = c \cdot a \tag{12}$$

where "a" denotes the design matrix in the original data space defined by Eq. (2). This is the "transformation law of the design matrix". By substituting Eqs. (6), (10) and (12) into (9), p' is written down using the quantities before the transformation;

$$\begin{aligned} p' &= p_0 + (a'^t V_{y'}^{-1} a')^{-1} a'^t V_{y'}^{-1} [y' - g'(p_0))] \\ &= p_0 + \left[(a^t \cdot c^t)(c^t)^{-1} V_y^{-1} c^{-1} (c \cdot a)\right]^{-1} (a^t \cdot c^t)(c^t)^{-1} V_y^{-1} c^{-1} \cdot c[y - g(p_0)] \end{aligned} \tag{13}$$

where each c can take either one of $c^{(+)}$, $c^{(-)}$ or $c^{(1/2)}$ independently in the first order approximation. In the actual data analyses, however, the identicality of those three matrices are often violated. Therefore, if p' is to be equal to p, each c should be replaced by $c^{(-)}$, $c^{(+)}$ or $c^{(1/2)}$ according to either one of the following criterion.

1) Criteria-1 : Backward Differentiation

If all the c's are replaced by $c^{(-)}$, p' = p holds. In this case, the covariance matrix $V_{y'}$ should be calculated as $c^{(-)} V_y c^{(-)t} = (\partial f/\partial y) V_y (\partial f/\partial y)' \equiv V_{y'}^{(-)}$. This is the option usually adopted in applying the law of error propagation. Similarly, the design matrix a' must be calculated as $a' = c^{(-)} \cdot a$

2) Criteria-2 : Forward Differentiation

If all the c's are replaced by $c^{(+)}$, p' = p is also valid. In this case, the covariance matrix $V_{y'}$ should be calculated as $c^{(+)} V_y c^{(+)t} = (\partial f/\partial g) V_y (\partial f/\partial g)' \equiv V_{y'}^{(+)}$. Similarly, the design

matrix a' must be calculated as $a' = c^{(+)}a = (\partial f/\partial g)(\partial g/\partial p) = (\partial f/\partial p) = (\partial g'/\partial p)$, which is equivalent with its definition Eq. (8).

3) Criteria-3 : Central Differentiation

If all the c's are replaced by $c^{(1/2)}$, it will result in a better answer than criterion-1 and -2 in the sense of numerical calculation.

4) Criteria-4 : Mixture of $c^{(+)}$, $c^{(-)}$ and $1/2\cdot(c^{(+)}+c^{(-)})$

In this case, even an "asymmetric law of error propagation", e.g., $V_{y'} = c^{(+)}V_y c^{(-)t}$ or $c^{(-)}V_y c^{(+)t}$, is allowed so long as every pair $c^{-1}c$ appearing in Eq. (13) is kept to be an unit matrix.

If these criterion are neglected, the LSS p' may not be equal to p when $c^{(+)} \neq c^{(-)}$. As will be shown later, this is the reason of an anomaly known as Peelle's Pertinent Puzzle (PPP). Except for the criteria-4 which does not seem to be physically meaningful, the first three criterion claim that the design matrix "a" and covariance matrix "V_y" must be "covariant" under a transformation f. Conversely, if these two quantities are transformed in a covariant way, the least-squares solution becomes invariant under the same transformation. Usually, the covariance matrix in the transformed space is calculated to be $c^{(-)}V_y c^{(-)t}$. Then, the design matrix must be also transformed into $a'=c^{(-)}a$.

In the method proposed by Zhao and Perey[2], the derivative $\partial y'/\partial y$ is evaluated at $y = \langle y \rangle$ which is calculated iteratively from g' as $f^{-1}(g')$. Then, this derivative becomes the matrix $c^{(+)}$ defined in this paper because of the fact that $\langle y \rangle = f^{-1}(g') = f^{-1}(f(g)) = g$ and,

$$\left.\frac{\partial y'_i}{\partial y_j}\right|_{y=\langle y\rangle} = \left.\frac{\partial f_i(y_1,\cdots,y_n)}{\partial y_j}\right|_{y=g} = \frac{\partial f_i(g_1,\cdots,g_n)}{\partial g_j} = c^{(+)}_{i,j} \qquad (14)$$

Therefore, this method can be proved to be equivalent with the criteria-2.

It will be worthwhile to write down the relation between $V_{y'}^{(+)}$ and $V_{y'}^{(-)}$ explicitly:

$$V_{y'}^{(+)} = c^{(+)}(c^{(-)})^{-1}V_{y'}^{(-)}((c^{(-)})^t)^{-1}(c^{(+)})^t \qquad (15)$$

Therefore, if we have a complete knowledge on the transformation f, model g and data y, we can calculate $V_{y'}^{(+)}$ from $V_{y'}^{(-)}$ and vice versa, without knowing the original covariance matrix V_y.

The argument here is based on the Taylor series expansion of the first order. If $\Delta f = f(y) - f[g(p)]$ seriously disagree with $c^{(+)}[y-g(p)]$ and $c^{(-)}[y-g(p)]$, $c^{(1/2)}\cdot[y-g(p)]$ would give a better result from the viewpoint of numerical calculation. If they still disagree, we should have the corrections of higher order which makes the formula non-linear in y. In the problem known as PPP which will be described in Section 3, $\Delta f = c^{(-)}\cdot[y-g(p)] = c^{(+)}\cdot[y-g(p)]$ holds accidentally. Therefore, the results obtained with $c^{(-)}$ (Criteria-1) and $c^{(+)}$ (Criteria-2) become equivalent with the correct answer. This is a fortunate degeneracy resulting from the functional form of f.

If the transformation f is linear in y, i.e., let F be a square matrix so that $y' = f(y) = F\cdot y$, then $g'(p) = f[g(p)] = F\cdot g(p)$. Therefore, a relation $(\partial f/\partial y) = (\partial f/\partial g) = F = c$ is always valid. By putting this result in Eq. (13), we can prove that $p' = p$ without any criteria.

3. Examples of numerical calculations

Example 3-1 (LSS before a transformation of data)

Suppose that we are to estimate a parameter vector $p=(x,c)^t$ from a data vector y and its covariance matrix V_y;

$$y = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 1.5 \\ 1.0 \\ 1.0 \end{bmatrix}, \quad V_y = \begin{bmatrix} 0.15^2 & 0 & 0 \\ 0 & 0.1^2 & 0 \\ 0 & 0 & 0.2^2 \end{bmatrix} \tag{16}$$

according to the following observation equation and the design matrix a;

$$y \sim \begin{bmatrix} g_1(x,c) = x \cdot c \\ g_2(x,c) = x \cdot c \\ g_3(x,c) = c \end{bmatrix}, \quad \rightarrow \quad a = \left(\frac{\partial g_i}{\partial p_j} \right) = \begin{bmatrix} c & x \\ c & x \\ 0 & 1 \end{bmatrix} \tag{17}$$

By taking the initial guess parameter $p_0=(1.1, 1.1)$, the least-squares solution is obtained after 1 iteration as

$$p = \begin{bmatrix} x \\ c \end{bmatrix} = \begin{bmatrix} 1.154 \\ 1.0 \end{bmatrix}, \quad V_p = \begin{bmatrix} 0.06 & -0.046 \\ -0.046 & 0.04 \end{bmatrix} \tag{18}$$

Example 3-2 (Criteria-1)

Next, let us transform the data and the model in an isomorphic way as follows;

$$y' = f(y) = \begin{bmatrix} f_1(y_1,y_2,y_3) = \dfrac{y_1}{y_3} = 1.5 \\ f_2(y_1,y_2,y_3) = \dfrac{y_2}{y_3} = 1.0 \\ f_3(y_1,y_2,y_3) = y_3 = 1.0 \end{bmatrix} \sim g' = f(g) = \begin{bmatrix} \dfrac{g_1}{g_3} = x \\ \dfrac{g_2}{g_3} = x \\ g_3 = c \end{bmatrix},$$

$$\therefore \; c^{(-)} = \left(\frac{\partial f_i}{\partial y_j} \right) = \begin{bmatrix} \dfrac{1}{y_3} & 0 & -\dfrac{y_1}{y_3^2} \\ 0 & \dfrac{1}{y_3} & -\dfrac{y_2}{y_3^2} \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & -1.5 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \end{bmatrix} \tag{19}$$

The covariance matrix and the design matrix must be transformed in a covariant way;

$$V_{y'}^{(-)} = c^{(-)} V_y (c^{(-)})^t = \begin{bmatrix} 0.1125 & 0.06 & -0.06 \\ 0.06 & 0.05 & -0.04 \\ -0.06 & -0.04 & 0.04 \end{bmatrix}, \quad a' = c^{(-)} \cdot a = \begin{bmatrix} c & x-1.5 \\ c & x-1 \\ 0 & 1 \end{bmatrix} \tag{20}$$

Putting these quantities into Eq. (9), the answer is, of course, equal to the result obtained in example 3-1. Although the covariance matrix used here was criticized to be incorrect[2], we can still have the correct result if the design matrix is transformed in a covariant manner.

Example 3-3 (Criteria-2)

In Example 3-2, let us adopt $c^{(+)}$ instead of $c^{(-)}$;

$$c^{(+)} = \left(\frac{\partial f_i}{\partial g_j}\right) = \begin{bmatrix} \frac{1}{c} & 0 & -\frac{x}{c} \\ 0 & \frac{1}{c} & -\frac{x}{c} \\ 0 & 0 & 1 \end{bmatrix} \tag{21}$$

This matrix must be evaluated by using an appropriate initial guess p_0 and successively improved by new guesses. Then, the covariance matrix and the design matrix must be transformed in a covariant way;

$$V_{y'} = c^{(+)} V_y \, (c^{(+)})^t, \quad a' = c^{(+)} a = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{22}$$

The answer is again equal to that of Example 3-1. This method of solution is equivalent with Zhao's proposal[2].

Example 3-4 (Improper combination of $c^{(+)}$ and $c^{(-)}$)

Let us take the design matrix a' as $c^{(+)}a$, but covariance matrix $V_{y'}^{(-)}$. These quantities are given in Eqs. (22) and (20), respectively. The LSS becomes

$$p' = \begin{bmatrix} 0.882 \\ 1.235 \end{bmatrix}, \quad V_p = \begin{bmatrix} 0.048 & -0.035 \\ -0.035 & 0.031 \end{bmatrix} \tag{23}$$

This is the answer known as Peelle's Pertinent Puzzle[2,3,4]. The reason of obtaining such a fallacy result is obvious: the covariance matrix and design matrix were not transformed in a covariant way. Indeed, this solution is written down as;

$$p' = p_0 + [a^t c^{(+)t} (c^{(-)t})^{-1} V_y^{-1} (c^{(-)})^{-1} c^{(+)} a]^{-1} a^t c^{(+)t} (c^{(-)t})^{-1} V_y^{-1} (c^{(-)})^{-1} [y' - f(g(p_0))] \neq p \tag{24}$$

If the data y was reasonably close to the estimate g(p), difference of $c^{(+)}$ and $c^{(-)}$ became reasonably small, and then such strange results should have vanished.

When the data vector y is transformed into another, the design matrix "a" and data covariance matrix must be transformed in a covariant manner. If this is not done, it is likely that the results of the least-squares method is not equivalent with the correct answer obtained before the transformation. Then, which one (criteria-1, -2 or -3) should we adopt? Because the model g is not known from the outset to the experimentalist, it will be impossible for him to employ criteria-2 and -3 in data processing. Moreover, the "model" may change if different theory is used, and the "averaged quantity" in Zhao's method[2] may also change if different database is used in data fitting. Therefore, the data processor should adopt criteria-1, and the data covariance matrix is transformed into $V_{y'}^{(-)}$. If this has been done, he should also provide the matrix $c^{(-)}$ to the evaluators. If this information is available, the evaluators

can apply the least-squares method according to the criteria-1. Even the criteria-2 is applicable after $V_{y'}^{(+)}$ is calculated according to Eq. (15). Then, he will get the same answer as derived from the original data in both ways. Because $V_{y'}^{(-)}$ depends only on data while $V_{y'}^{(+)}$ depends also on the model, the former quantity must be regarded to be a more fundamental property associated with the data y'. In this sense, it is more reasonable for the experimentalist to report y', $V_{y'}^{(-)}$ and $c^{(-)}$ than y', $V_{y'}^{(+)}$ and $c^{(+)}$.

4. Impacts of the Truncation of Data Spaces on the Least-Squares Solutions

If the transformation f does not conserve dimensionality, i.e., if dimension (m) of y' is less than the dimension (n) of y, the transformation is called in this paper to be a truncation of the data space. The simplest of such transformations is the one that just deletes the k-th element of y, that is, $y'_i = y_j$, where (i=1,...,n-1), (j=1,..,k-1,k+1,...n). It can be easily shown that even the LSS p' in this most simply truncated space (y') is not equal to the solution p in the parent space (y). This fact also causes a problem in applying the LSM in actual data analyses, especially when the number of truncated dimensions are not negligible, i.e, if (n-m) ~ n. Therefore if n is a small number, impact of the truncation is sometimes serious. This is another reason of PPP.

By defining operators α_k and β_k that delete the k-th raw and column of a matrix, respectively, the truncation is schematically written as;

$$y' = \alpha_k y, \quad V_{y'} = \alpha_k \beta_k V_y, \quad a' = \alpha_k a, \quad g'(p) = \alpha_k g(p) \tag{25}$$

The least-squares solution p' is obtained by putting these quantities into Eq. (9). Usually, p' is not equal to p obtained by Eq. (3) before the truncation. This fact is illustrated below by numerical examples.

4.1 Example - LSS before the Truncation

Let us suppose that we have a data vector y of 4-dimension, and associated covariance matrix V_y,

$$y = \begin{bmatrix} a_1 \\ a_2 \\ c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} 2.5 \\ 2.0 \\ 1.0 \\ 1.0 \end{bmatrix}, \quad V_y = \begin{bmatrix} 0.15^2 & 0 & 0 & 0 \\ 0 & 0.09^2 & 0 & 0 \\ 0 & 0 & 0.3^2 & 0 \\ 0 & 0 & 0 & 0.134^2 \end{bmatrix} \tag{26}$$

and a parameter vector p = (x,c)' and linear design matrix g (=a) defined as;

$$y = \begin{bmatrix} a_1 \\ a_2 \\ c_1 \\ c_2 \end{bmatrix} \sim \begin{bmatrix} 1 & 1 \\ 1 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} x \\ c \end{bmatrix} = g \cdot p \tag{27}$$

Obviously, the design matrix g given above is equivalent with a model $a_i = x + c$ and $c_i = c$ where i=1,2. By putting these quantities in Eq. (3) and setting p_0 be a zero vector, the least

squares solution is obtained to be

$$p = \begin{bmatrix} x \\ c \end{bmatrix} = \begin{bmatrix} 1.132 \\ 1 \end{bmatrix}, \quad V_p = \begin{bmatrix} 0.021 & -0.015 \\ -0.015 & 0.015 \end{bmatrix} \tag{28}$$

Let us now transform the data vector y in an isomorphic way by using a linear transformation matrix F defined as follows;

$$F = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & -\frac{1}{3} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{29}$$

Then the transformed vector y', covariance matrix $V_{y'}$ and design matrix a' is calculated to be

$$y' = F \cdot y = \begin{bmatrix} 2.5 \\ \frac{5}{3} \\ 1 \\ 1 \end{bmatrix} \equiv \begin{bmatrix} a_1 \\ b_1 \\ c_1 \\ c_2 \end{bmatrix}, \quad V_{y'} = F \cdot V_y F^t = \begin{bmatrix} 0.0225 & 0 & 0 & 0 \\ 0 & 0.01 & 0 & -0.006 \\ 0 & 0 & 0.09 & 0 \\ 0 & -0.006 & 0 & 0.018 \end{bmatrix},$$

$$a' = g' = F \cdot g = \begin{bmatrix} 1 & 1 \\ 1 & \frac{2}{3} \\ 0 & 1 \\ 0 & 1 \end{bmatrix} \tag{30}$$

In this equation, a data corresponding to a physical quantity b is defined as $b_1 = a_2 - 1/3 \cdot c_2$ which has an implicit meaning of $x+2/3 \cdot c$. By putting these quantities in Eq. (3), we obtain the same result as shown in Eq. (28). Because this transformation is linear, the result is always equivalent with the original answer, as discussed at the last paragraph of section 2.

Now, let us truncate this (transformed) data space into the following four 3-dimensional sub-spaces.

4.2 Sub-space $\alpha_1 y'$

In this sub-space, the data vector y, its covariance matrix V_y and design matrix g is obtained according to Eq. (25).

$$y = \alpha_1 y' = \begin{bmatrix} \frac{5}{3} \\ 1 \\ 1 \end{bmatrix}, \quad V_y = \alpha_1 \beta_1 V_{y'} = \begin{bmatrix} 0.010 & 0 & -0.006 \\ 0 & 0.009 & 0 \\ -0.006 & 0 & 0.018 \end{bmatrix}, \quad g = a = \alpha_1 g' = \begin{bmatrix} 1 & \frac{2}{3} \\ 0 & 1 \\ 0 & 1 \end{bmatrix} \tag{31}$$

The least-squares solution in this sub-space is obtained as

$$p = \begin{bmatrix} x \\ c \end{bmatrix} = \begin{bmatrix} 1.0 \\ 1.0 \end{bmatrix}, \quad V_p = \begin{bmatrix} 0.014 & -0.006 \\ -0.006 & 0.006 \end{bmatrix} \tag{32}$$

4.3 Sub-space $\alpha_2 y'$

The quantities in this sub-space is obtained by replacing subscripts 1 in Eq. (30) by 2. The least-squares solutions is obtained as

$$p = \begin{bmatrix} x \\ c \end{bmatrix} = \begin{bmatrix} 1.5 \\ 1.0 \end{bmatrix}, \quad V_p = \begin{bmatrix} 0.037 & -0.015 \\ -0.015 & 0.037 \end{bmatrix} \tag{33}$$

4.4 Sub-space $\alpha_3 y'$

In the same way, the least-squares solution in this sub-space is obtained as

$$p = \begin{bmatrix} x \\ c \end{bmatrix} = \begin{bmatrix} 1.132 \\ 1.0 \end{bmatrix}, \quad V_p = \begin{bmatrix} 0.024 & -0.018 \\ -0.018 & 0.018 \end{bmatrix} \tag{34}$$

4.5 Sub-space $\alpha_4 y'$

By replacing the subscripts by 4, the quantities in this sub-space is obtained;

$$y = \alpha_4 y' = \begin{bmatrix} a_1 \\ b_1 \\ c_1 \end{bmatrix} = \begin{bmatrix} 2.5 \\ \frac{5}{3} \\ 1.0 \end{bmatrix}, \quad V_y = \begin{bmatrix} 0.0225 & 0 & 0 \\ 0 & 0.01 & 0 \\ 0 & 0 & 0.09 \end{bmatrix} = \begin{bmatrix} 0.15^2 & 0 & 0 \\ 0 & 0.1^2 & 0 \\ 0 & 0 & 0.3^2 \end{bmatrix}, \quad a = g = \begin{bmatrix} 1 & 1 \\ 1 & \frac{2}{3} \\ 0 & 1 \end{bmatrix} \tag{35}$$

By putting these quantities into Eq. (3), the least-squares solution is obtained as

$$p = \begin{bmatrix} x \\ c \end{bmatrix} = \begin{bmatrix} 0.882 \\ 1.353 \end{bmatrix}, \quad V_p = \begin{bmatrix} 0.0477 & -0.0529 \\ -0.0529 & 0.0688 \end{bmatrix} \tag{36}$$

The results obtained from this exercise are summarized in Table 1;

Table 1 Comparison of the least-squares solutions obtained in various sub-spaces

Least-Squares Solution in the parent 4-dimensional space (x, c) = (1.132, 1.0)			
Least-Squares Solutions in the truncated 3-dimensional sub-spaces			
Sub-space $\alpha_1 y'$ $y = (b_1, c_1, c_2)$	Sub-space $\alpha_2 y'$ $y = (a_1, c_1, c_2)$	Sub-space $\alpha_3 y'$ $y = (a_1, b_1, c_2)$	Sub-space $\alpha_4 y'$ $y = (a_1, b_1, c_1)$
(x, c) = (1.0, 1.0)	(x, c) = (1.5, 1.0)	(x, c)=(1.132, 1.0)	(x,c)=(0.882,1.353)

Apparently, the LSS in truncated data spaces yielded four different answers, indicating serious impacts of the data truncation on the LSS. The LSS obtained after truncating a part of the data space is therefore proved to be invalid. The truncation of the data space thus destroys the "causality" of the LSSs completely. This situation resembles a well-known fact that a

solution of the Dirac Equation in a finite sub-space has, after Lorentz transformation, improper normalization.

By the way, the data vector, covariance matrix and design matrix given in sub-space $\alpha_4 y'$ are exactly the same as those given in example 5.1 in Zhao's report[2]. Because physical quantity b has an implicit meaning of $b = a - 1/3 \cdot c$, it is quite natural to think that b_1 was derived by using two data a_2 and c_2 where a_1, a_2, c_1 and c_2 are independent of each other. Then, the complete data space of this problem has dimension of 4. Therefore, if Zhao's example is identified as a least-squares solution in a truncated space, it will not be reasonable to claim that the answer of $x = 0.882$ to be well established. At least, it was understood that the truncation causes the same type of anomaly of least-squares solutions as PPP.

The same argument is applicable to PPP, because it was first proposed as a problem in a two dimensional space[3,4] which is equivalent with $y = \alpha_3 y'$, $V_y = \alpha_3 \beta_3 V_{y'}$ where y' and $V_{y'}$ are given in Eqs. (19) and (20), respectively. Because the truncated (2×2) covariance matrix V_y has a non-zero off-diagonal term, it implies an existence of the third data which introduced correlation between the two data in the truncated space (y_1 and y_2). Therefore, minimum dimension of this problem must be recognized to be three. Once this is recognized, we then have the correct answer as given in Examples 3-1 to 3-3. Therefore, the PPP as it was originally proposed contains two problems; a problem arising from truncation, and a problem arising from neglect of the invariance criterion.

5. Conclusions

Relations of the least-squares solutions before and after two kinds of transformation of data spaces are investigated. The invariance criterion of the LSS under isomorphic transformations were derived. On the contrary, it was shown by numerical examples that the LSS is not invariant under truncations of data spaces. The consequence of the latter is important, because th least-squares method itself is a truncation of the data space into a parameter space having fewer dimensions. When the LSM yields a strange result, i.e., outside the range of the data, it will be extremely important to examine the problem of dimension and the history how the data are transformed. Then, those odd results as appeared in PPP will turn out to be incorrect in most cases.

If we are in an appropriate data space which has the correct dimensionality, the LSM will yield a correct answer. Then, if the data vector is transformed in an isomorphic way which conserves dimension, the LSM also produces the same answer as before the transformation provided that the design matrix and covariance matrix are transformed in a covariant manner. Then, the ultimate question is: How can we know that we have the correct dimensionality? The general answer is not known to the author, but it will be an interesting future subject. Furthermore, if the LSS can be written down in an invariant form under truncations, it will be extremely useful, and we do not have to worry about the problem of dimension any more. If not, some approximations must be involved, an example of which is given in Ref. 3.

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Appendix : Derivation of Eq. (10)

Let the data vector $y=(y_1,...,y_n)$ be sampled from a set of random variables $Y=(Y_1,...,Y_n)$. In this part, Einstein's summation rule is adopted which is defined that the occurrence of repeated subscripts implies a summation over the label. The (i,j) element of the covariance matrix of transformed data is defined as

$$(V_{y'})_{i,j} \equiv \langle (f_i(Y) - \langle f_i(Y)\rangle)\cdot(f_j(Y) - \langle f_j(Y)\rangle)\rangle \tag{37}$$

where <...> denote the statistical average with respect to Y. Let a certain set of fixed values be $v=(v_1,..,v_n)$. The following equation holds in the first order.

$$\begin{aligned} f_i(Y) - \langle f_i(Y)\rangle &= f_i[v+(Y-v)] - \langle f_i[v+(Y-v)]\rangle \\ &= f_i(v)+\frac{\partial f_i}{\partial v_k}(Y_k-v_k) - \langle f_i(v)+\frac{\partial f_i}{\partial v_k}(Y_k-v_k)\rangle \\ &= \frac{\partial f_i}{\partial v_k}\cdot[(Y_k-v_k)-\langle(Y_k-v_k)\rangle] \\ &= \frac{\partial f_i}{\partial v_k}\cdot(Y_k - \langle Y_k\rangle) \end{aligned} \tag{38}$$

where the equalities <v> = v, <f(v)> = f(v), etc., were used. Therefore, Eq. (37) is modified to be

$$\begin{aligned} (V_{y'})_{i,j} &\equiv \langle (f_i(Y) - \langle f_i(Y)\rangle)\cdot(f_j(Y) - \langle f_j(Y)\rangle)\rangle \\ &= \left(\frac{\partial f_i}{\partial v_k}\right)\langle(Y_k-\langle Y_k\rangle)\cdot(Y_m-\langle Y_m\rangle)\rangle\left(\frac{\partial f_j}{\partial v_m}\right) \\ &= (c\cdot V_y\cdot c^{\dagger})_{i,j} \end{aligned} \tag{39}$$

By replacing v with y, g or 1/2·(y+g), Eq.(10) is obtained with $c=c^{(-)}$, $c^{(+)}$, or $c^{(1/2)}$, respectively.

CROSS-SECTION FITTING AND COVARIANCE ANALYSIS WITH PADE-APPROXIMANTS

S.A.Badikov, E.V.Gai, N.S.Rabotnov
Institute of Physics and Power Engineering
249020 Obninsk, Russia

ABSTRACT

A convenient instrument is described to deal with the final stages of nuclear data evaluation process - producing the curve, its error band and covariance matrix of evaluated values - Pade-approximants generated by a discrete optimization. The method allowing to present the complete results of a cross section evaluation in explicit and coherent analytical form is illustrated by the example of $^{59}Co(n,2n)^{58}Co$ cross section evaluation.

Introduction.

Two large domains of activity may be singled out in evaluation process:

1. Collecting, selecting, compiling, expert studying of data with resulting possible modifications.

2. Employing this filtered and corrected information to generate the output - usually evaluated curve, its error band and covariance matrix of evaluated values. The first stage is not easy to formalize and reduce to algorithms but for the second stage it's achievable. What we consider a convenient instrument to deal with this subproblem is described and its basic properties illustrated below on an example making use of and allowing to compare the results with the material of /1/.

1. Analytical approximation in cross-section evaluation.

An evaluated cross section is a set of values for selected energies. Both to get and to use it one must be able to calculate the cross section for any value of the argument. The method of producing this continuous function of energy is an important feature of the evaluation process.

The general mathematical concept of analyticity includes the behavior of the function in the complex plane. Cross section $\sigma(E)$ is **not** formally analytical function. It is either squared module or real part of an analytical function - reaction's amplitude. But there always exists an analytical function coinciding with $\sigma(E)$ on the real axis.

The best known instruments of analitical approximation - polynomial and Fourier expansions - usually provide convergence inside an interval of real axis but not in the complex plane. Fitting is more general concept and algorithms used in the process may be complicated. Moving from "approximation" in the direction opposite to "fitting" we arrive at "analytical continuation". It must provide convergence not only in the real interval but in some domain of comlex plane. A lot of real computational problems arise from using approximants not providing analytical continuation. Rational functions having poles do provide it and are now widely used in computer codes to calculate various functions.

2. Pade-approximants.

The applications of well known methods of Pade-approximation /2,3/ in data processing was hindered so far by two obstacles. First is the difficulty of realisation. Rational approximants unlike polynomial ones lead to nonlinear systems of equations in the least squares method (LSM). Second is a special form of approximant

instability - real pole-zero pairs (noise doublets). We have proposed a method to circumvent both difficulties. The method is based on the recursive calculation of many approximants differing by the choice of interpolation knots. It is described in detail in a book /4/ (in Russian) and generally outlined in /5-6/.

A Pade-approximant of the second kind (Pade-II) of an order L=N+M+1 for a function f(z) is a rational function determined by equations

$$f_L(z)=P_N(z)/Q_M(z);$$
$$f(z_i)=f_L(z_i),\ i=1,2,\ldots L, \qquad (1)$$

where P and Q are polynomials of degrees N and M. Our method of discrete optimization includes choosing of L supporting points among N_{ex} experimental ones to get an interpolant. The approximant's polar expansion

$$f^L(z)= C + \sum_{i=1}^{l_1} \frac{a_i}{z-p_i} + \sum_{k=1}^{l_2} \frac{\alpha_k(z-\varepsilon_k)+\beta_k}{(z-\varepsilon)^2+\gamma^2}, \qquad (2)$$

may be called resonance expansion because ε and γ are energy and total half-width of a resonance level.

A prominent feature of rational approximants is appearance of real denominator zeros inside the approximation interval accompained by close real zeros of numerator "noise doublets" (NDs). It is the NDs that prevented wide use of Pade-approximants in data handling. But in our metod they are not only neutralized but become in a sense useful.

The NDs correspond to the terms with p_i inside the interval of approximation and relatively small a_i in the first sum of Eq(2). They are just cancelled from the sum and that regularization gives satisfactory results.

Normally NDs appear with encreasing L on final stages of approximation and indicate together with statistical criteria that analytical information is exhausted. Situation may be different if some points in the input data deviate abnormally from the general trend. In this case NDs appear at relatively low L near "bad points". smooth components. When the singularities are cancelled the resulting curve either "underrates" or practically ignores the "marked" bad points. That's a way to identify them automatically. We use $L'=L-2l_n$ where l_n is the number of NDs to notate final number of parameters.

A rational function $f(z) = P_N(z)/Q_M(z)$ may be parametrized in different ways besides (2). The parametrization by N+M+1 supporting ordinates $f(z) = f(z;f(z_1),f(z_2),..,f(z_{N+M+1}))$

is important. Unlike polynomial case no explicite expression like Lagrange formula is available for this parametrization, but simple linear recurrent relations exist allowing to generate rational function if supporting points (interpolation knots) are known.

The derivatives $\partial f(z)/\partial f_\nu$ depend on $f_\nu \equiv f(z_\nu)$. These derivatives are the coefficients of sensitivity of approximant's value in a point z to the values of supporting ordinates in the points z_ν. Explicit expression for sensitivity function of a rational approximant is

$$\frac{\partial f_L(z)}{\partial f_\mu} = \frac{Q_M^2(z_\mu)}{Q_M^2(z)} \prod_{\nu \neq \mu} \frac{(z-z_\nu)}{(z_\mu - z_\nu)} \quad (3)$$

The existence of the Eq (4) makes parametrization by supporting ordinates very useful in dealing with the statistical properties of the Pade-approximants.

3. Covariance and information matrices of experimental data

Practically most general expression for the functional to be minimized in the fitting process is LSM sum

$$S = \frac{1}{2} \sum_{i,k} \frac{\Delta f_i}{\sigma_i} a_{i,k} \frac{\Delta f_k}{\sigma_k} \quad (4)$$

where Δf_i is the difference between experimental and approximant's values, σ_i - experimental errors. Informational matrix of experimental values $a_{i,k}$ is inverse of the matrix of correlation coefficients $\rho_{i,k}$. We shall use Greek upperscripts to mark the points taken from different works: $\rho_{i,k}^{\alpha,\beta}$.

In the example considered below we know only the average correlation coefficients for all the points from given paper, so we shall use an assumption

$$\rho_{i,k}^{\alpha,\beta} = \delta_{\alpha\beta}[\delta_{ik}(1-\rho^\alpha)+\rho^\alpha] \quad (5)$$

i.e. that all the values from given work have the same correlation coefficients and interwork correlation is zero. Input correlation matrix has a square block structure in this case and is explicitly invertible

$$W_{ik} = \rho + (1-\rho)\delta_{ik}\ ; \quad (6)$$

$$W_{ik}^{-1} = \frac{1}{(1-\rho)} - \frac{\rho\delta_{ik}}{(1-\rho)(1-\rho+n\rho)}$$

where n is the order of the block.

4. Approximant's error-band and covariance matrix.

Information matrix of the parameters of approximant is

$$I_{\mu\nu} = \overline{\frac{\partial S}{\partial p_\mu} \times \frac{\partial S}{\partial p_\nu}}. \quad (7)$$

Putting (4) into (7) we get

$$I_{\mu\nu} = \sum_{i,k} \frac{\partial f_L(z_i)}{\partial p_\mu} \times \frac{\partial f_L(z_k)}{\partial p_\nu} a_{ik} / \sigma_i \sigma_k$$

The covariation coefficient for the approximant's values in two arbitrary points

$$\rho(x_i, x_k) = \langle \Delta f(x_i) \Delta f(x_k) \rangle =$$

$$= \sum_{\mu,\nu} (I^{-1})_{\mu\nu} \frac{\partial f_L(x_i)}{\partial p_\mu} \frac{\partial f_L(x_k)}{\partial p_\nu}$$

By proper choice of supporting abscissas (described elsewhere [4,5]) $I_{\mu\nu}$ may be made diagonal if input experimental values are uncorrelated.

In most practical applications the evaluated cross sections are used in the energy averaged form of group constants with their variances and covarinces. The ENDF-VI format permits including of these values directly (File 33) or the calculation of covariances by user on the basis of parameter sensitivities of the evaluated curve (File 30). Analytical approximation facilitates the formation of either File. In our case when $\sigma(E)$ is described by a rational function (2) all needed integrals are expressed explicitly but are too cumbersome so only numerical results will be presented. Now we consider a concrete example - $^{59}Co(n,2n)^{58}Co$ reaction cross section.

7. Different options.

We shall use a set of selected and corrected experimental values and their correlations (Tables 3.2.2 and 5.1 in /1/) as the input for our evaluation.

Our standard code "PADE2" did not take non-diagonal covariance was to handle all the $^{59}Co(n,2n)$ data as a single set of independent points. With more than twenty different sources it looks not unreasonable as far as the fitting stage is concerned. One just has to let χ^2-functional to become less than unity to allow for extra smoothness of correlated data. Then all the process is straightforward and we get optimum curve, evaluated error band and a covariance matrix of group cross sections. We call this oversimplified approach "zero option". Its results are compared with the results of /1/ in Fig.1-4 and Table 1.

The curve itself seems to agree with /1/, the only significant difference being upward deviation of a few per cent in 15-19 MeV region. It results from the effect described in section 3 which is illustrated by the Fig 3. The code uses noise poles to mark some points deviating down from what it determines as general trend and regularized curves go higher.

The differences in error band and correlation matrix

are drastic. The error band is considerably narrower than /1/ evaluation showing no "bulges" in the regions of conflicting experimental data. The reason is the same: the code "resolves the conflicts" and rejects suspicious points thus narrowing the band. This is further demonstrated by the Fig 4 where the error bands are drawn taking noise poles into account. They indicate the origine of "bulging".

The covariance matrix contains a lot of negative elements. This feature is **absolutely general for all mathematical models with more than two parameters**, i.e. for any model but linear interpolation and is, in this sense, quite natural. If input data are uncorrelated, a **model is the only source of output correlations and they are always oscillating and changing signs due to the general properties of supporting ordinates sensitivity functions mentioned above - each has L-1 zeroes.** Small negative correlations of more distant points are precisely as natural and inavoidable as strong positive correlations of close approximant's values. It does not lead to any contradictions being inherent property of any approximation. Input physical correlation of experimental values is usually positive and when taken into account overcomes this effect producing more positive output matrices. We first illustrate it on an "intermediate option".

This option means generating an approximant just like in zero option but taking input correlation into account on next stages - in calculating error band and correlation matrix of evaluated cross sections. Input correlation was described by constant positive coefficients equal to average values given in Table 5.1 of /1/ for all the values from the same experimental work, interwork correlations neglected.

The resulting error band is practically identical to that of zero option so it's not drawn.. The correlation matrix became essentially positive - negative elements are restricted to the last three rows, the largest module not exceeding 20 per cent, which is practically negligible. The resulting correlation is in general considerably stronger than in /1/. The matrix is very close to that of full option (see below), so only the latter is given in Table 1.

Atlast we have taken into account the input correlation on all the steps of evaluation process starting with curve fitting. The basic code was modified correspondingly. The method of discrete optimization allows to use **any functional** the only difference being in computing times. In the case of arbitrary input correlation

full matrix operations become too time consuming for PC but block-constant matrix corresponds to relatively simple functional so in fact only vector, not matrix, operations are used. The complete results are presented in the Figs 5-6 and Tab. 1-2. They are close to those of intermediate option. One common feature of all the options must be noted: optimum L'=12 curves (three "resonance" terms in Eq.(2)) differ from L'=8 curves (two such terms) by a small "resonance" near 13 MeV wich improves the functional significantly by some 5-10 per cent.

10. Conclusions.

Fig.6 confirms the consistency of /1/ evaluation - our curve is within the error band evaluated in /1/. The deviations go outside our much narrower band in 15 to 18 MeV region. That may be due to underestimating of error band in analytical model. But yet it's not impossible that the effect noted above is also real and the code is right in rejecting abnormally low points. Then both higher values and narrower band are qualitatively justified.

The covariance matrices of intermediate and full options correspond to stronger intergroup correlations than /1/ matrix - and it's partly due to the same effect and the truth again may be somewhere in between.

The final expression for $\sigma(E)$ provided by Eq(2) with the parameters given in Table 4 (energy, MeV, cross section, mb) is simple, convenient and accurate enough to be useful for many purposes.

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Table 1. Correlation matrices for group cross section.
L'=12, zero option (lower triangle) and /1/ (upper triangle)

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
1	*	50	50	31	29	10	8	0	0	0	7	0	0	0	0	0	0	0	0
2	38	*	50	31	29	10	8	0	0	0	7	0	0	0	0	0	0	0	0
3	-12	78	*	31	29	10	8	0	0	0	7	0	0	0	0	0	0	0	0
4	-11	26	67	*	35	16	11	18	26	0	14	23	21	22	21	0	0	0	0
5	2	-6	-2	26	*	17	13	35	28	5	10	41	37	27	36	31	0	0	0
6	-4	4	19	8	10	*	57	17	20	50	53	16	14	15	14	7	0	0	0
7	-2	8	-1	-13	1	-24	*	13	17	53	56	9	8	9	8	5	0	0	0
8	-1	0	11	7	-2	3	56	*	41	9	12	41	38	27	37	26	0	0	0
9	1	-8	6	15	-2	18	19	87	*	11	16	31	28	30	28	14	0	0	0
10	4	-10	-1	10	0	16	-4	54	86	*	52	4	4	4	4	5	0	0	0
11	2	-2	-6	-1	1	2	-12	10	46	84	*	7	7	7	7	0	0	0	0
12	-4	15	-1	-16	2	-19	0	-32	-17	24	70	*	46	38	46	31	0	0	0
13	-5	14	6	-10	0	-14	8	-23	-26	-6	26	76	*	35	42	28	0	0	0
14	2	-7	0	8	0	8	0	10	5	-4	-11	3	58	*	35	18	0	0	0
15	3	-6	-3	4	0	6	-3	8	10	4	-6	-19	-4	55	*	27	0	0	0
16	-3	9	3	-6	0	-7	3	-10	-9	-1	9	13	-6	-17	40	*	0	0	0
17	1	-4	0	4	0	4	0	5	2	-1	-4	1	11	-2	-17	52	*	0	0
18	5	-11	-3	8	0	10	-3	12	11	2	-9	-13	5	15	-14	3	72	*	0
19	-1	5	0	-4	0	-4	1	-4	-3	1	4	2	-6	-1	9	-9	-1	55	*

L'=12, full option (lower triangle)

1	*																		
2	52	*																	
3	1	85	*																
4	6	48	76	*															
5	13	13	12	34	*														
6	13	5	12	33	35	*													
7	8	22	20	16	34	36	*												
8	10	14	18	25	31	31	90	*											
9	12	10	14	26	34	38	82	97	*										
10	12	11	11	23	38	44	73	86	96	*									
11	11	15	11	18	41	46	63	71	84	95	*								
12	5	26	17	10	40	36	46	39	51	70	86	*							
13	6	26	23	17	37	27	39	29	33	44	57	83	*						
14	12	10	14	25	34	27	36	36	35	34	33	40	74	*					
15	7	10	8	14	31	26	30	30	33	36	36	29	29	62	*				
16	3	9	9	10	21	16	20	17	19	23	27	32	28	15	40	*			
17	7	-8	-2	10	5	6	6	10	7	1	-3	-1	18	13	18	57	*		
18	4	-7	-4	3	0	1	0	4	2	-1	-5	-9	1	9	-12	13	72	*	
19	-4	8	3	-6	0	-1	-1	-4	-2	1	4	2	-9	-5	9	-13	9	72	*

Table 2. Final parameters of the polar expansions, Eq(2).

L=24 L'=12 SUM=0.98732E+00 SUM1=0.10532E+01 (after regular.)

C= 0.00000E+00, no real poles

alfa	beta	eps	gamma
0.40337E+04	0.94412E+04	0.13075E+02	-0.42236E+01
0.38121E+03	0.18599E+04	0.19368E+02	-0.26225E+01
-0.35012E+01	0.71896E+01	0.12870E+02	0.32874E+00

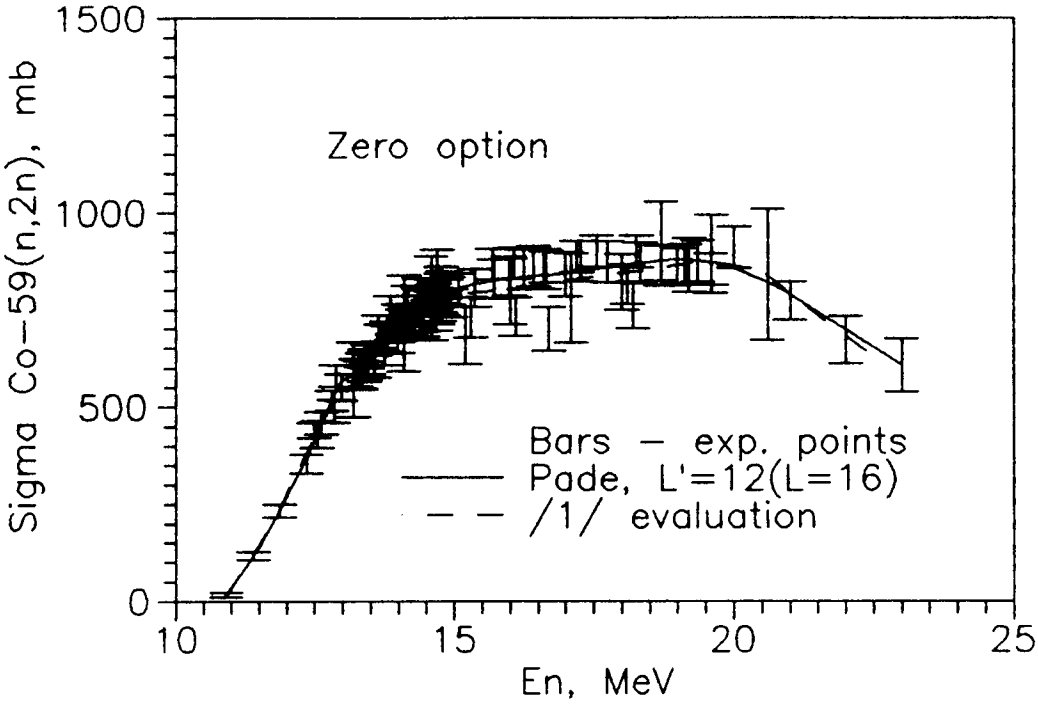

Fig.1. Pade-approximation of the /1/ set of corrected exp. data in zero option (correlation of input data neglected) compared with eval./1/.

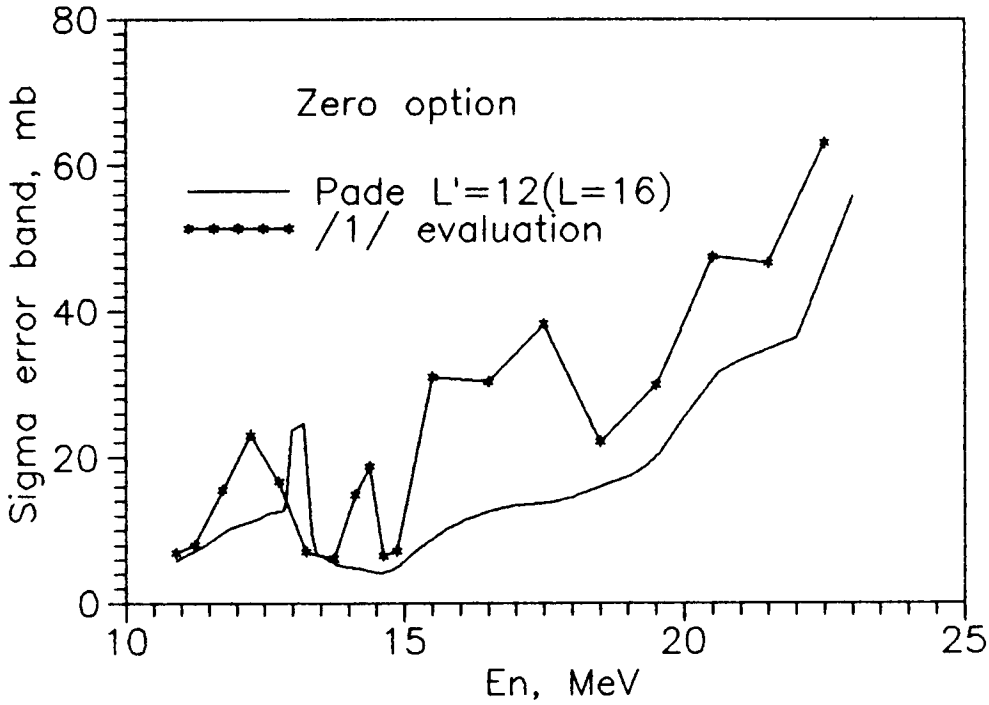

Fig.2. Pade error band of zero option compared with eval./1/ error band.

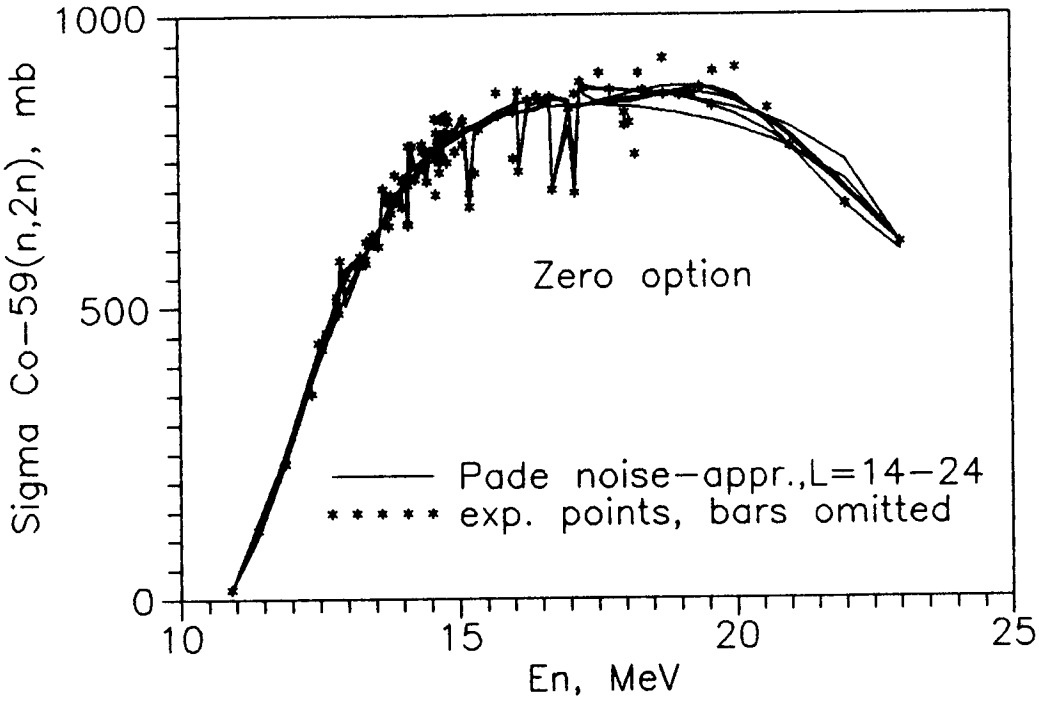

Fig.3. Successive Pade-approximants of zero option before regularization. Noise poles indicate bad points.

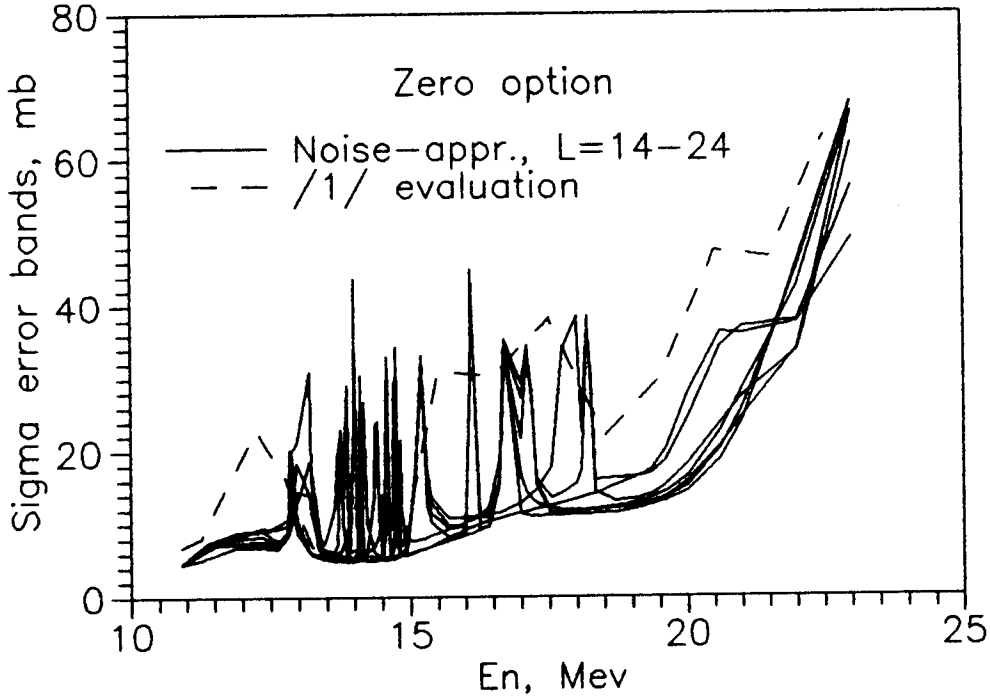

Fig4. Pade error bands for successive noise approximants.

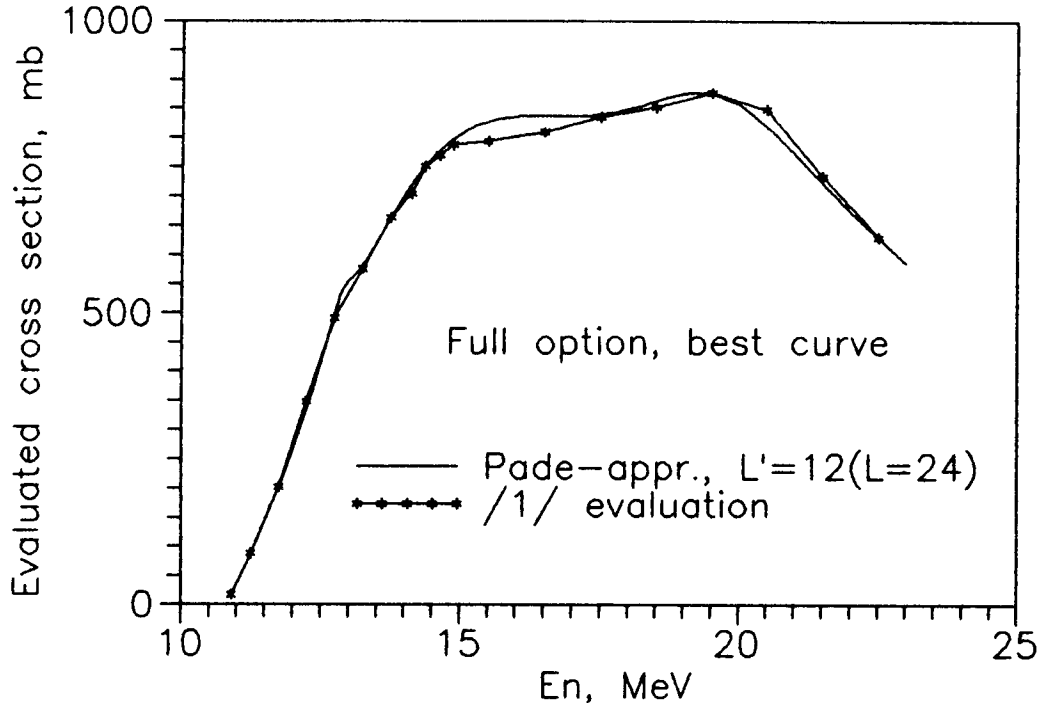

Fig.5. The best Pade approximant of full option (S=.99, S'=1.05).

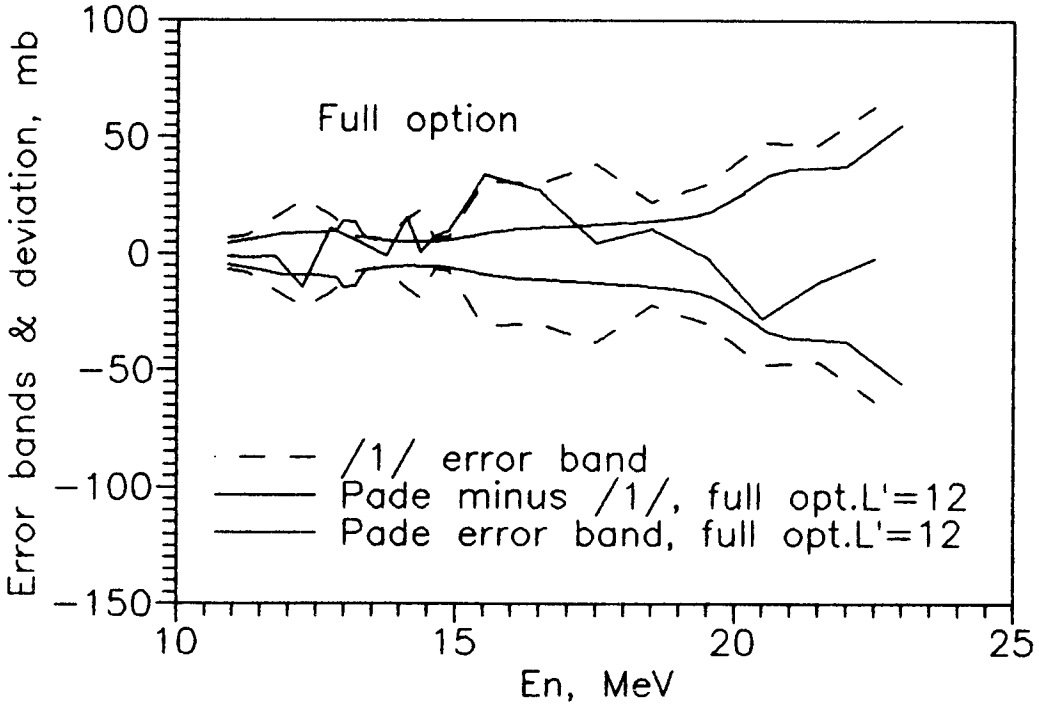

Fig.6. The deviation of Pade-approximant from /1/ and error bands of /1/ and of our full option.

"EVALUATION OF NEUTRON DOSIMETRY REACTIONS CROSS SECTIONS AND COVARIANCE ANALYSIS WITH RATIONAL FUNCTIONS"

S.A.Badikov, N.S.Rabotnov, K.I.Zolotarev

Institute of Physics and Power Engineering,
249020, Obninsk, Russia

ABSTRACT

Method for evaluation of the neutron dosimetry reactions cross sections is described. The method is based on the use of generalised least squares method and rational functions as model functions.Applicability of the method to nuclear data evaluation is demonstrated by the results of the $^{24}Mg(n,p)^{24}Na$ and $^{93}Nb(n,n')^{93m}Nb$ reaction cross section evaluations. The comparison of evaluations from present work and the IRDF-90 library is carried out.

INTRODUCTION

Basic properties of Pade-approximants as a tool of covariance analysis are outlined and illustrated on a relatively simple example in [1] where key references may also be found. In present paper all the working formulae of the method are given and applied to more complicated cases in the evaluation of neutron dosimetry reaction cross-sections with correlated input data.

1. STATISTICAL ANALYSIS OF CORRELATED DATA

Statistical analysis of correlated data (measured cross sections) is carried out within the framework of the regression model. In this model it is assumed that measured values are the sum of the hypothetical true dependence and experimental uncertainties:

$$\sigma^{k}_{i_k} = f(E^{k}_{i_k}, \theta_1, \ldots, \theta_L) + \varepsilon^{k}_{i_k} \quad (1)$$

$$k=1,..,M; i_k=1,..,n_k; n_1+..+n_M=n$$

In equation (1)

$$\vec{\sigma} = (\sigma^1_1, .., \sigma^1_{n_1}, \ldots, \sigma^M_1, \ldots, \sigma^M_{n_M})^T$$

- vector of cross sections from data base, superscript T denotes a transpose, $\vec{\theta} = (\theta_1, \ldots, \theta_L)$ - vector of the unknown parameters being estimated, M - the number of experiments, n_k - the number of cross section measurements in the k-th experiment, n - the number of cross section values in data base, $f(E^{k}_{i_k}, \theta_1, \ldots, \theta_L)$ - rational function. A rational function may be represented in different problem-oriented ways: by continued fraction, ratio of two polynomials or by polar expansion:

$$f^{[N_1,N_2]}(E) = C_{N_1-N_2}(E) + \sum_{i=1}^{l_1} \frac{a_i}{E - r_i} + \sum_{k=1}^{l_2} \frac{\alpha_k (E-\varepsilon_k) + \beta_k}{(E-\varepsilon_k)^2 + \gamma_k^2} \quad (2)$$

(N_1 and N_2 - the degrees of numerator and denominator, $C_{N_1-N_2}(E)$ - polynomial of degree N_1-N_2). In generating of optimal approximant we use the first type of rational function's representation while the third type is preferable for physical analysis of curve's parameters.

The uncertainties $\varepsilon^{k}_{i_k}$ have a zero mathematical expectation ($E\varepsilon^{k}_{i_k} = 0$). Covariation matrix of cross section uncertainties V is

known within accuracy factor Δ :

$$V^{kl}_{i_k j_l} = \Delta \cdot P^{kl}_{i_k j_l} \cdot e^{k}_{i_k} \cdot e^{l}_{j_l} \quad (e^{k}_{i_k} -$$

standard deviation of uncertainty $\varepsilon^{k}_{i_k}$, $P = (P^{kl}_{i_k j_l})$ - correlation matrix of cross section uncertainties, superscripts indicate the experiment's number).

In the most general form the minimized functional can be written

$$s(\vec{\theta}) = (\vec{\sigma} - \vec{f})^{T} V^{-1} (\vec{\sigma} - \vec{f}) \qquad (3)$$

Technical aspects of the minimization process based on the use of discrete optimization method and the Newton-Gauss algorithm are described in detail in Ref.[2]. Representing the covariation matrix of cross section uncertainties in the form

$$V = DPD$$

(D - diagonal matrix,

$d^{kl}_{i_k j_l} = \delta_{i_k j_l} \cdot \delta_{kl} \cdot e^{k}_{i_k}$), equation (3) can be transformed

$$s = \sum_{k}^{M} \sum_{l}^{M} \sum_{i_k}^{n_k} \sum_{j_l}^{n_l} \left\{ \frac{\sigma^{k}_{i_k} - f(E^{k}_{i_k}, \vec{\theta})}{e^{k}_{i_k}} \times \right.$$

$$\left. \times (P^{-1})^{kl}_{i_k j_l} \frac{\sigma^{l}_{j_l} - f(E^{l}_{j_l}, \vec{\theta})}{e^{l}_{j_l}} \right\} \qquad (4)$$

As follows from equation (4) the number of arithmetical operations necessary to minimize $\vec{s}(\vec{\theta})$ depends on n quadratically. With large n straightforward solution of minimization problem is impossible due to computer time and core memory restrictions. For simplification of calculational scheme two assumptions are used:

1) cross-sections measured in different experiments don't correlate with each other;

2) correlation coefficients of any two cross-sections measured in one experiment are equal to the same value - average correlation coefficient.

In formalized form the element of approximate correlation matrix can be written as

$$P^{kl}_{i_k j_l} = \delta_{kl} \{ \delta_{i_k j_l} (1 - \bar{P}^{k}) + \bar{P}^{k} \} \qquad (5)$$

($\bar{P}^{k}$ - average correlation coefficient of the k-th experiment). The approximate correlation matrix P has a block structure: the $(n_k \times n_k)$ square matrices P^{k} are arranged on the diagonal of P, while the other elements of P equal to 0. Every square matrix

P^k can be expanded in a linear sum of the unit matrix and the matrix with constant elements

$$P^k = \bar{P}^k \cdot A + (1-\bar{P}^k) \cdot E \quad (6),$$

where $A_{i_k j_k} = 1$, $E_{i_k j_k} = \delta_{i_k j_k}$.

Expansion (6) permits to invert the matrix P^k explicitly [5]:

$$(P^k)^{-1} = \alpha^k \cdot A + \gamma^k \cdot E \quad (7)$$

where $\alpha^k = 1/(1-\bar{P}^k)$,

$\gamma^k = -\bar{P}^k/(1-\bar{P}^k)/(1-\bar{P}^k+n_k\bar{P}^k)$. Thus the inversion of the $(n \times n)$ matrix P is equivalent to inversion of M $(n_k \times n_k)$ matrices of smaller dimensions.

Substitution of the equation (7) to (4) yields

$$\vec{s(\theta)} = \sum_{k=1}^{M} \{\alpha^k \Phi^k + \gamma^k F^k\},$$

where

$$\Phi^k = \left(\sum_{i_k=1}^{n_k} \frac{\sigma^k_{i_k} - f(E^k_{i_k}, \vec{\theta})}{e^k_{i_k}} \right)^2,$$

$$F^k = \sum_{i_k=1}^{n_k} \left(\frac{\sigma^k_{i_k} - f(E^k_{i_k}, \vec{\theta})}{e^k_{i_k}} \right)^2.$$

As a result a number of arithmecal operations necessary to minimize $\vec{s(\theta)}$ depends on $n/\sqrt{M}$ quadratically.

Finally let's list the formulae for calculation of covariance matrix of the estimated parameters $\hat{\vec{W}}(\theta)$ and for calculation of the error band of the evaluated curve $\Delta f(E^k_{i_k}, \hat{\vec{\theta}})$:

$$\hat{\vec{W}}(\theta) = \frac{s}{n-L}(X^T V^{-1} X)^{-1} = \frac{s}{n-L} C^{-1},$$

$$\Delta f(E^k_{i_k}, \hat{\vec{\theta}}) = \sum_{m=1}^{L} \sum_{j=1}^{L} X^k_{i_k m} X^k_{i_k j} W_{mj},$$

$$C_{rm} = \sum_{k=1}^{M} \{\alpha^k T^k_r T^k_m + \gamma^k Q^k_{rm}\} \quad (7),$$

where

$$T^k_r = \sum_{i_k=1}^{n_k} \frac{1}{e^k_{i_k}} X^k_{i_k r},$$

$$Q^k_{rm} = \sum_{i_k=1}^{n_k} \frac{1}{(e^k_{i_k})^2} X^k_{i_k r} X^k_{i_k m}.$$

X is a (n × L) matrix of the sensitivity coefficients of the rational function to a variation of parameters $\left(X^{k}_{i_k m} = \frac{\partial f(E^{k}_{i_k}, \hat{\vec{\theta}})}{\partial \theta_m} \right)$.

2. RESULTS OF CALCULATIONS

The method described in section 1 was used for approximation of correlated data with different degree of complexity - the $^{24}Mg(n,p)^{24}Na$ reaction cross section with complicated structure and relatively simple energy dependence of the $^{93}Nb(n,n')^{93m}Nb$ reaction cross section. In Fig.1 and Fig.2 the evaluated excitation functions of these reactions are compared with the IRDF-90 evaluation [3] and with the experimental data taken from 28 and 4 works respectively (for detailed references see [4,5]). It should be noted that besides experimental information the data base formed for the $^{93}Nb(n,n')^{93m}Nb$ reaction cross section evaluation includes the results of statistical model calculations (see Ref.[6]). As follows from Fig.1 and Fig.2 there is a good agreement between both evaluations. Our resulting curve for the $^{24}Mg(n,p)^{24}Na$ reaction cross section has 45 parameters (see Table 1). Its polar expansion includes constant background, one wide "resonance" with half-width of 4.6 MeV and 10 narrow "resonances" with half-widths from 18 KeV to 960 KeV. The parameters of the evaluated curve for the $^{93}Nb(n,n')^{93m}Nb$ reaction cross section are given in Table 2.It's expanded in three "resonances" and smooth background. The functional $\sqrt{s(\vec{\theta})/(n-L)}$ is 1.44 for the first curve and 1.31 for the second one. The errors of the evaluated cross sections are shown in Fig.3 and Fig.4.

In Table 3 evaluated cross sections averaged with the ^{252}Cf spontaneous fission neutron spectrum [7] are compared with experimental data. The data from the Table 3 demonstrate a good agreement between calculated and measured values for the $^{93}Nb(n,n')^{93m}Nb$ reaction. The large difference between calculated and recommended data for the $^{24}Mg(n,p)^{24}Na$ reaction is in our opinion due to some structures (unresolved hitherto experimentally) in the energy dependence of cross section in the range from 6.6 MeV to 12.1 MeV where about 90% of the reaction response function is concentrated.

The average cross-section $\bar{\sigma}$ from the Table 3 and its variance

$V(\bar{\sigma})$ can be written as:

$$V(\bar{\sigma}) = (\partial\bar{\sigma}/\partial\vec{\theta})^T \, W(\vec{\theta}) \, (\partial\bar{\sigma}/\partial\vec{\theta}) + \\ + (\partial\bar{\sigma}/\partial\vec{\mu})^T \, W(\vec{\mu}) \, (\partial\bar{\sigma}/\partial\vec{\mu}) \quad (8)$$

$$\bar{\sigma} = \int \sigma(E,\vec{\theta})\varphi(E,\vec{\mu})dE$$

The computation of $\bar{\sigma}$ and $V(\bar{\sigma})$ is reduced to the computation of the integrals of rational functions if cross section $\sigma(E,\vec{\theta})$ is approximated by rational function and spectrum $\varphi(E,\vec{\mu})$ is given in group representation [7].

The use of integral data in a variety of ways is a necessary step of evaluation procedure. Inclusion of integral data as an additional independent information in simultaneous fitting of differential and integral data decreases (in comparison with fitting of differential data only) the error of evaluated curve. On the other hand the fitting of differential data and comparison of evaluated curve averaged over the ^{235}U and ^{252}Cf fission neutron spectra carried out successively enable to detect inconsistency between differential and integral data. The second way of taking integral data into account is naturally entered as proposed in Ref.[2] algorithm of the search of optimal rational approximant. This algorithm permits to generate a few statistically equivalent curves (the values of functional $\sqrt{s(\vec{\theta})/(n-L)}$ varying in the third digit) with different polar structures. The optimal curve from this set is selected after comparison with integral data.

3. PREPARATION OF COVARIANCE DATA IN THE ENDF/B-VI FORMAT

The evaluated data must be represented in the ENDF/B format for the use in different applications. The ENDF/B-VI format enlarges (in comparison with the ENDF/B-V format) the possibilities for preparation of covariance evaluated data essentially. The new format ensures the representation of this information both as the group cross-section covariances and as arbitrary parameters covariances and sensitivities of the evaluated curve with respect to the parameters. In the case of reaction cross section approximation by rational function both possibilities are easily available. For example the computation of group cross-section covariances is reduced to computation of the integrals of rational functions.

Formula for group cross-section covariances and equation (8) for variance of average cross-section are obtained within the framework of sensitivity theory on the basis of the uncertainties of rational approximant's parameters. In this connection it is necessary to note following. Approximation of the correlation matrix of cross-sections measured in one experiment by the correlation matrix with the constant positive off-diagonal element (see equation (5)) has another aim besides simplification of calculational scheme - to ensure the positive definiteness of the correlation matrix of experimental data. The approximate correlation matrix is positive definite while the input one, generally speaking, is not. This property of approximate correlation matrix provides the positive semi-definiteness of informational matrix C (see equation (7)). In calculations the informational matrix is positive definite as a rule. Consequently the covariance matrix of rational function's parameters is positive definite too. This fact in its turn guarantees the positivity of variance for any value if the variance is calculated in terms of sensitivity theory from the uncertainties of rational approximant's parameters.

4. SUMMARY

In present work the method for rational approximation of correlated experimental dependences is proposed and the results of its application for the evaluation of neutron dosimetry reaction cross sections are described. The most important features of the method are of:

1. Due to flexible polar structure the rational functions are more efficient than other known classes of functions for approximation of both complicated energy dependences of reaction cross sections (the $^{24}Mg(n,p)^{24}Na$ reaction) and relatively simple ones (the $^{93}Nb(n,n')^{93m}Nb$ reaction).

2. The informational matrix calculated within the framework of this method is positive semi-definite. Moreover in calculational practice the informational matrix is positive definite as a rule. This fact guarantees the positivity of variance of any integral value (for example the variance of different functionals of cross-section) produced from rational approximant.

3. The proposed method simplyfies the representation of the evaluated data in the ENDF/B-VI format essentially - all the data needed for formation of the File 30 and File 33 are calcu-

lated analytically. The preparation of the File 33 is possible in any group representation.

The noted features of the method make it promising for the evaluation of neutron dosimetry reaction cross-sections.

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Table 1. Parameters of evaluated cross section for the $^{24}Mg(n,p)^{24}Na$ reaction in representation (2) ($N_1=N_2=22$, $l_1=0$, $l_2=11$, cross section in barns, energy in MeV, energy range - 5.31-20 MeV).

k	α	β	ε	γ
1	0.40110E-3	0.65636E-3	0.66655E+1	0.13687E+0
2	0.73651E-1	0.32841E-4	0.72198E+1	0.95753E+0
3	0.55413E-6	-0.39954E-3	0.74585E+1	0.11294E+0
4	0.74530E-3	-0.93307E-5	0.79939E+1	0.18201E-1
5	-0.45411E-4	-0.25635E-2	0.95729E+1	0.43074E+0
6	0.33014E+0	0.31970E+1	0.11330E+2	0.45703E+1
7	0.18147E-4	0.94807E-4	0.11644E+2	0.59361E-1
8	0.38163E-2	0.67030E-3	0.12403E+2	0.14371E+0
9	0.33846E-1	0.12277E-1	0.13145E+2	0.57549E+0
10	-0.20118E-3	-0.70623E-3	0.13182E+2	0.13659E+0
11	-0.55992E-6	-0.16098E-2	0.13755E+2	0.23661E+0
C = 0.14717E-1				

Table 2. Parameters of evaluated cross section for the $^{93}Nb(n,n')^{93m}Nb$ reaction in representation (2) ($N_1=6$, $N_2=7$, $l_1=1$, $l_2=3$, cross section in millibarns, energy in MeV, energy range - 0.17-20 MeV).

k	α	β	ε	γ
1	0.57616E+3	0.18716E+4	0.23927E+1	0.32473E+1
2	-0.24895E+3	0.47188E+3	0.96081E+1	0.24442E+1
3	0.49002E+2	-0.51003E+2	0.88204E+0	0.89371E+0
a = -0.10179E+2 r = 0.29285E+2				

Table 3. The average reaction cross sections in the ^{252}Cf spontaneous fission neutron field.

reaction	average cross section, mb	
	calculation	experiment
$^{24}Mg(n,p)^{24}Na$	2.151±0.044 (this work) 2.171±0.059 (IRDF-90)	2.005±0.048 [7]
$^{93}Nb(n,n')^{93m}Nb$	147.4±4.9 (this work) 142.7±4.2 (IRDF-90)	150.6±3.6 [8] 144.0±5.0 [9]

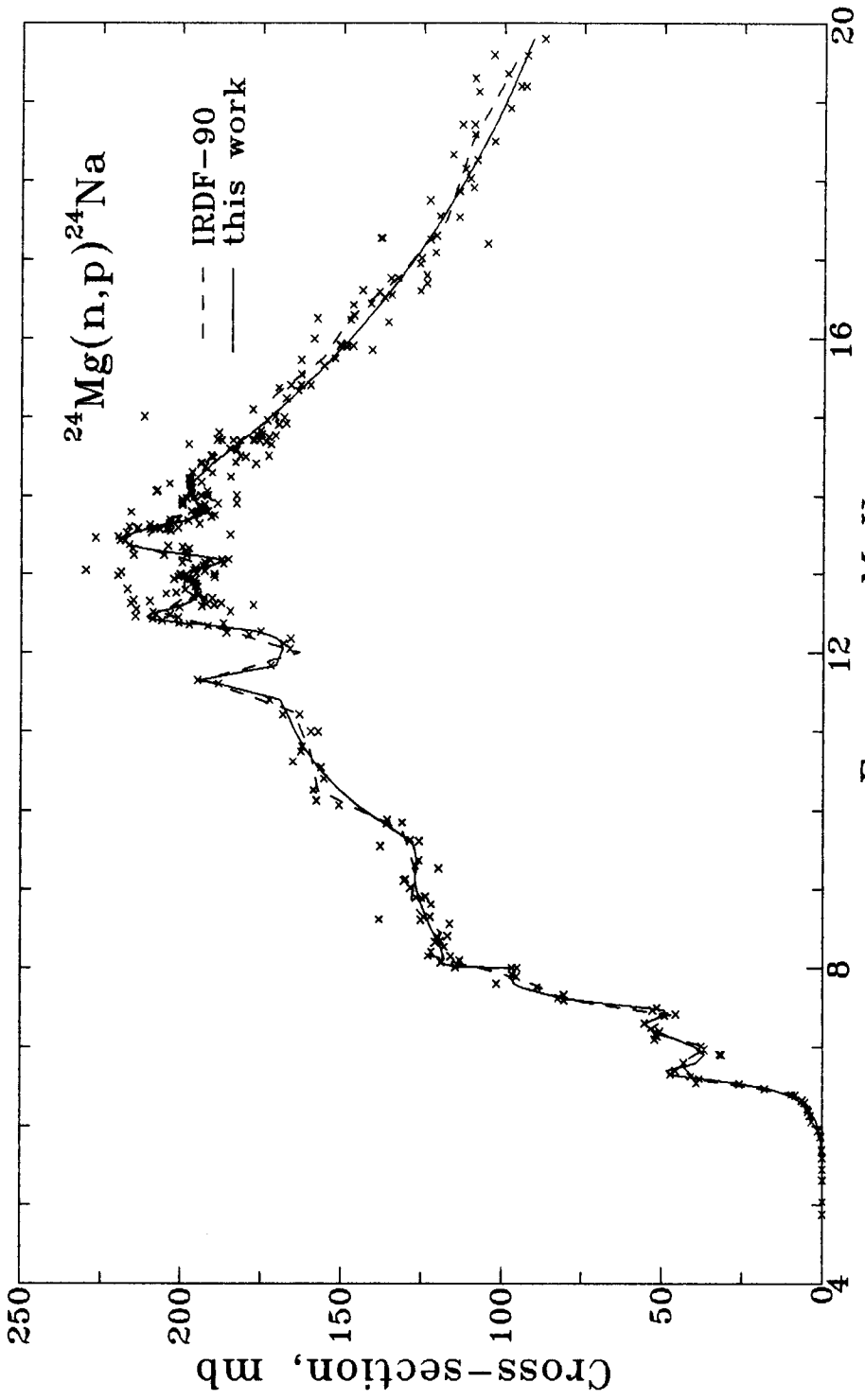

Fig.1 The evaluated reaction cross-section in comparison with experimental data and the IRDF-90 evaluation.

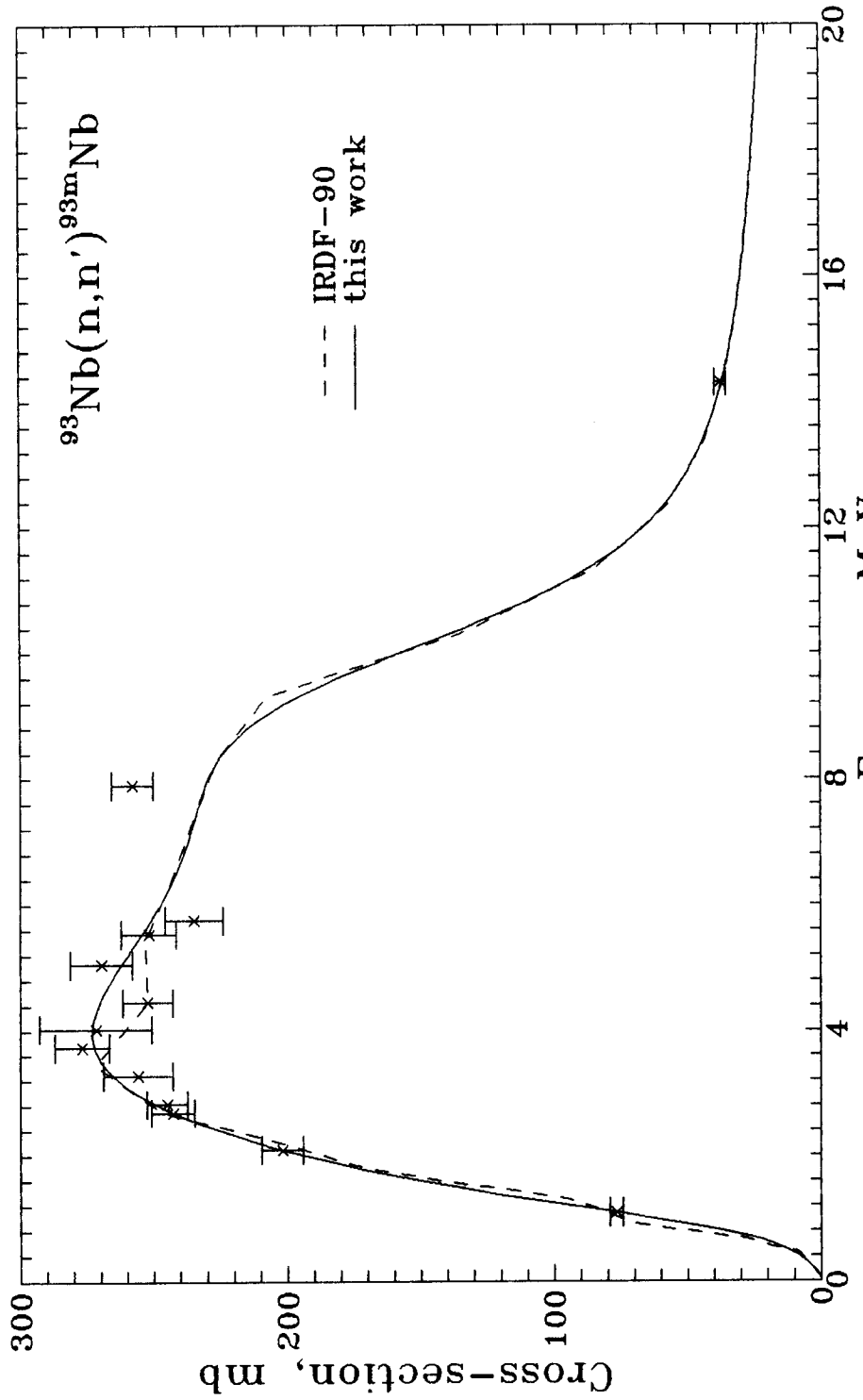

Fig.2 The evaluated reaction cross-section in comparison with the experimental data and the IRDF-90 evaluation.

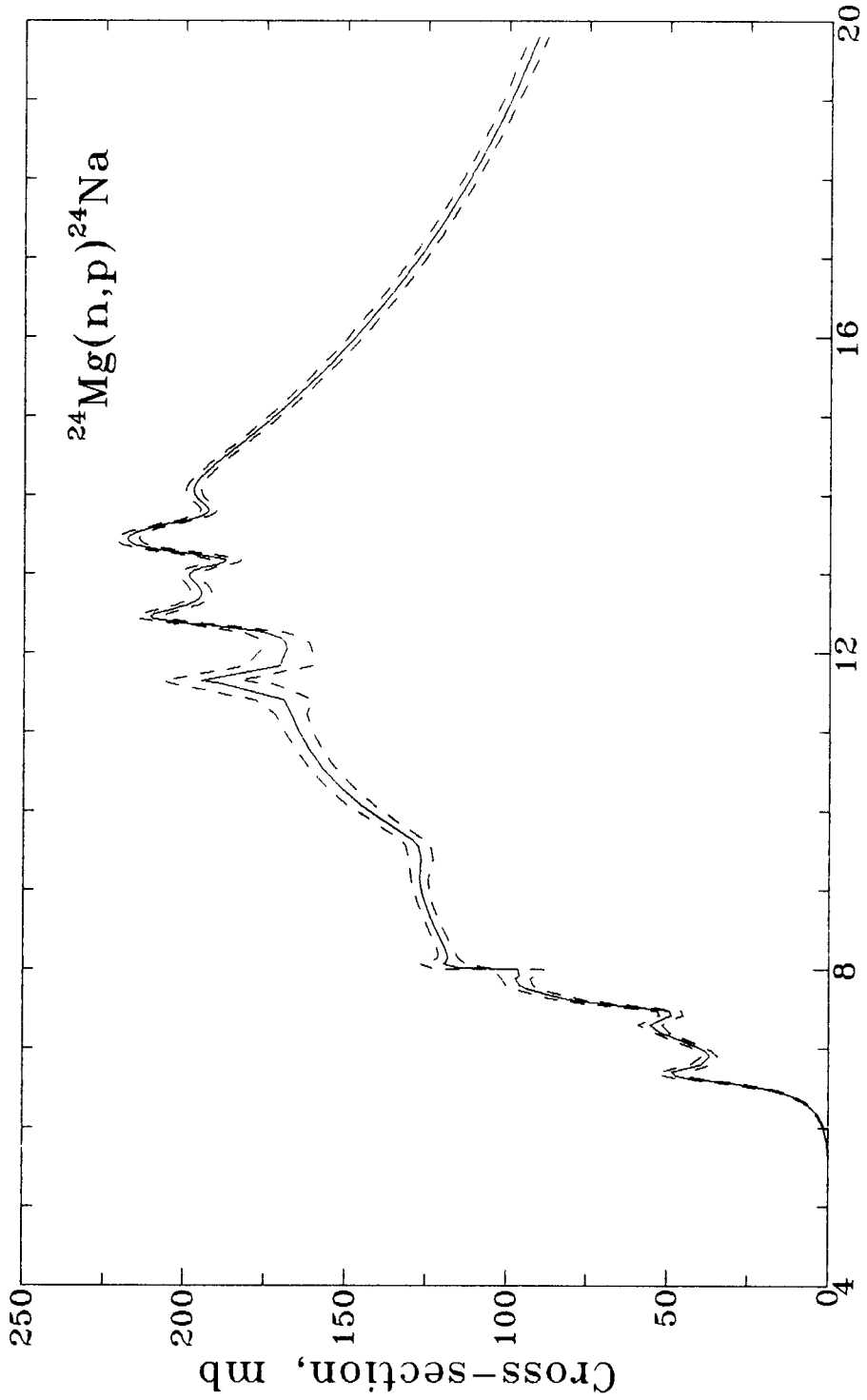

Fig.3 The results of reaction cross-section evaluation from this work. (Dashed lines display 1σ error of evaluation).

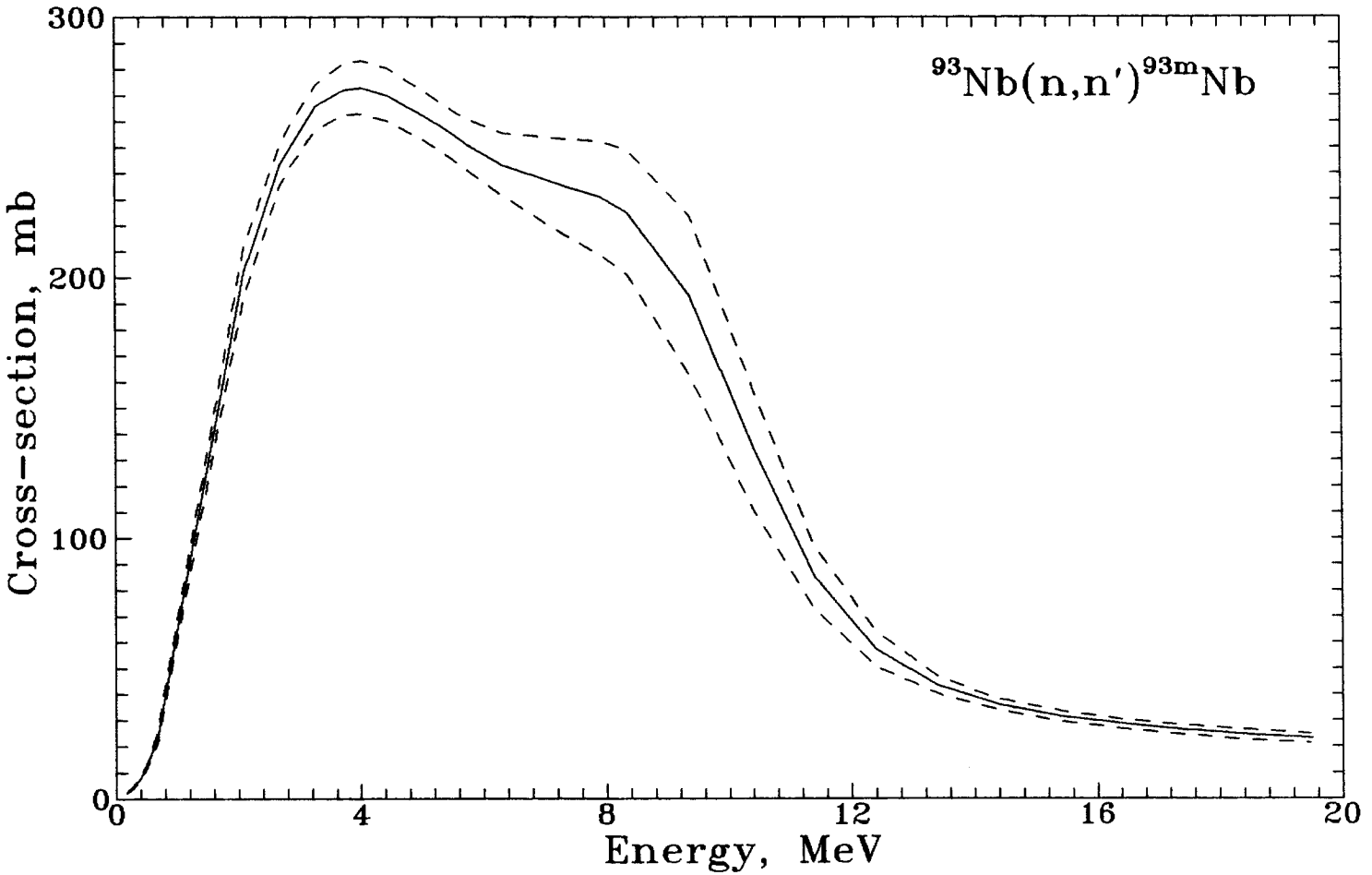

Fig.4 The results of reaction cross-section evaluation from this work. (Dashed lines display 1σ error of evaluation).

GENERATION OF COVARIANCE DATA FROM COMBINED EXPERIMENTAL AND THEORETICAL DATA

Y. KANDA
Department of Energy Conversion Engineering,
Kyushu University,
Kasuga, Fukuoka, 816, Japan

Abstract

Covariances for evaluated nuclear data can be usefully estimated by combining experimental and theoretical information. In this report, the covariances generated on various assumptions are compared to search their significance by using neutron-induced reactions of ^{56}Fe and ^{54}Fe as examples. The theoretical information used to calculate their cross sections is the Hauser-Feshbach formulae and the parameters required in it. Only level density parameters are considered as the sources of the theoretical uncertainty and the other parameters used in the cross section calculation such as optical model parameters are fixed.

The reference correlation (a covariance matrix is factored to a correlation matrix and a standard deviation vector) is defined as the resultant one calculated with prior level density parameters which originate in Gilbert-Cameron. The prior level density parameters are adjusted to make the calculated cross sections fitting to the experimental encounters as possible, and then the new covariance estimated with the adjusted level density parameters is obtained, called the posterior covariance. Comparing the posterior with the prior, the effect of the experimental information to the resultant covariance can be estimated. This makes it clear that the posterior correlation is finely changed as that correlation at the further distance is smaller than the prior (the reference). It is reasonably understood that short range correlation is strengthen through the experimental data. In addition, the effects of the correlation between level density parameters and between experimental points in the identical set are studied. They are small. On the basis of these works, the useful method of the covariances estimation from combined experimental and theoretical data can be developed.

1. Introduction

The covariance matrix for evaluated nuclear data represents the quantitative uncertainty which is estimated by evaluators inclusively taking account of whole possible error sources. The cross sections are a kind of physical constant and they must be equal in every data file. According to this point of view, their covariance matrices are also to be same values irrespective of evaluators. The latter, however at present, seems to be not expected or be resigned itself while the former is being established in the recently-revised versions of major files in the world. In the early stage of the nuclear data evaluation, there were considerable difference in the values of the cross section among the files. This main reason is that individual evaluators adopted their data base with their own standards of the judgment that some experiments were more reliable and accurate than others in the experimental evaluation or some nuclear reaction models with some parameters were fitting to their problem. As the results that the number of measured data increases and their uncertainty decreases, the data base the evaluators adopt in their works are focusing to the same so that the current evaluated data result in the consistent values. The problem about the discrepancy of the covariances has not been solved at the same time with the case of cross sections because the former does not originate in data bases themselves but in procedures of them and the latter strongly depends on the adopted data base.

2. Formulae

The experimental data vector $\mathbf{y}$ is assumed to be approximated as

$$\mathbf{y} \cong \phi(\mathbf{p}_0) + \Phi(\mathbf{p}-\mathbf{p}_0) \tag{1}$$

where $\phi(\mathbf{p}_0)$ is a model function vector of a parameter vector $\mathbf{p}$ which has a proper form depending on the model of the cross section curve and will be concretely given following discussions, $\mathbf{p}$ a parameter vector in the function ϕ, $\mathbf{p}_0$ the prior parameter vector given initially for $\mathbf{p}$, and Φ is called a design matrix or sensitivity matrix whose practical inclusions will be shown below. The posterior parameter vector $\hat{\mathbf{p}}$ estimated by the generalized least squares method which are used to discuss the covariance can be expressed as various forms in spite of mathematical equality the following formulae will be suitable to gain an insight into meaning of the generated covariance.

$$\hat{\mathbf{p}} = \left(\Phi^t\mathbf{V}^{-1}\Phi + \mathbf{M}_0^{-1}\right)^{-1}\left(\Phi^t\mathbf{V}^{-1}\mathbf{y} + \mathbf{M}_0^{-1}\mathbf{p}_0\right) \tag{2}$$

$$\mathbf{M} = \left(\Phi^t\mathbf{V}^{-1}\Phi + \mathbf{M}_0^{-1}\right)^{-1} \tag{3}$$

In these equations, $\mathbf{V}$ and $\mathbf{M}_0$ are the covariance matrix of $\mathbf{y}$ and the prior

matrix of $\mathbf{p}_0$, respectively, and $\mathbf{M}$ the posterior matrix for $\hat{\mathbf{P}}$. The covariance matrix of the nuclear data $\mathbf{C}$ can be generated by the equation

$$\mathbf{C} = \Phi \mathbf{M} \Phi^t . \qquad (4)$$

Nuclear data evaluation can be classified into the three : First, available experiments are sufficient to evaluate a curve only by themselves. Secondly, existing experimental data are too scarce to draw a curve by interpolating them but parameters in appropriate model formulae can be estimated from them and then they can use to draw the curve fitting to the experiments with the model calculation. Thirdly, there are no available measurements but parameters in applicable theoretical formulae can be obtained from systematics for the parameters. In every case, the above equations can be used to generate the covariance for the curve.

The equation (2) implies that the estimated parameter $\hat{\mathbf{P}}$ is the weighted average of the experimental data $\mathbf{y}$ and is the prior parameter $\mathbf{p}_0$ with the weight of the inverse of the uncertainty associated with $\mathbf{y}$ and $\mathbf{p}_0$, respectively. To supplement this description, simple examples are presented in Appendix.

3. Covariances generated with theoretical formulae

3.1 Procedures of Covariance Generation

The covariances used in this study as examples are the ones which are estimated for the neutron-induced reaction cross sections of ^{54}Fe and ^{56}Fe merging experimental and theoretical information. In the procedure to generate these covariances the formulae presented in the preceding section are applied on the various assumptions to make the significance of the deduced covariance clear.

The theoretical formulae used to calculate the reaction cross sections is based on Hauser-Feshbach model. As the level density parameters for the respective residual nuclides of the ^{54}Fe and ^{56}Fe reactions, which are 5 isotopes of Fe and 4 ones of Mn and Cr respectively, are leading in the model calculation, the parameter vector $\mathbf{p}$ is consist of them and the sensitivity matrix Φ is the differential coefficients of the calculated cross section with respective to the prior parameter vector $\mathbf{p}_0$. The prior level density parameters are taken from Gilbert and Cameron [1]. Their uncertainties are assumed to be 5% equally for all. The transmission coefficients of neutrons for relating nuclides in the cross section calculation are estimated from the optical model with the parameters which are deduced from available experimental data in our laboratory. They are not presented here because they are common to the present calculations and have no effect on the following discussion. The transmission coefficient of protons and α-particles are obtained from Perey [2] and Lemos [3].

The experimental data base are measurements for ^{54}Fe(n,p), (n,α) and (n,2n) and ^{56}Fe(n,p) and (n,2n). The correlation in experimental data is not considered except in 3.2.2. and 3.3.3. The posterior level density parameters can be estimated using the data base and the given prior level density parameters with eq.(2) and then the associated correlation matrices are computed through eqs.(3) and (4). These procedures have been presented in the previous reports [4].

In order to make it easy to discuss the generated covariance matrix it is separated into the two parts, the correlation matrix and a array of the standard deviation at the given energy points through the conventional manner. The former is expressed by multiplying correlation factors by 10^3 and the latter in %.

3.2 Covariances calculated with prior level density parameters

The correlation matrices in this sub-section are computed with the prior level density parameters, namely, the values of Gilbert and Cameron themselves.

3.2.1 Without correlation between prior level density parameters

It is assumed that the prior level density parameters do not correlate with the others so that the $\mathbf{M}_0$ is a diagonal matrix. In this case, experimental data is not used and the covariance is computed with eq. (4) passing eqs. (2) and (3). The resulted correlation matrix and standard deviations are presented in Tables 1(a) and 2(a) for ^{56}Fe and ^{54}Fe, respectively. They are reduced matrices to show a whole correlation matrix because a size of an original matrix is 64×64 and it can not be presented here. The full matrices of (n,p) for ^{56}Fe and ^{54}Fe, are shown in Tables 3 and 4, respectively. The individual values of the matrix components and of the standard deviations are rather large comparing with the others shown below : Namely, the excitation-function computed with the prior level density parameters is rather flexible in value, but fixed in shape. These results involve the inherent correlation in the Hauser-Feshbach calculation with the given conditions. Therefore, they must be designated in this work as the reference of a correlation matrix and standard deviations respectively against the following calculation with different assumptions.

3.2.2 With correlation between prior level density parameters for isotopes

The correlation of the prior level density parameters for isotopes is assumed to be 50% and then some off-diagonal elements in $\mathbf{M}_0$ are defined. This is the condition differing from that 3.2.1 : The experimental data are not used. In Table 5,the computed result for only ^{56}Fe(n,p) is presented because the others show similar features. These are identical with the reference correlation matrix(Table 3) and standard deviations so that the 50% correlation in the prior level density parameter has no effect on the result.

3.3. Covariances calculated with posterior level density parameters

Alternatively, we present here the correlation matrices calculated with the posterior level density parameters estimated from combined the experimental data and Hauser-Feshbach calculation comparing with the references mentioned in the previous sub-section.

3.3.1 Without correlation between prior level density parameters

This corresponds to the calculation in 3.2.1. The results in Tables 6 and 1(b) for ^{56}Fe(n,p) and Table 2(b) for ^{54}Fe(n,p) show large difference from the references (Tables 3 and 1(a) and 2(a)), respectively : The correlation matrices obtained here present sudden changes from a component to a component in contrast to a gradual change in the reference. The resulted standard deviations are smaller than the references by the magnitude of one order. These are the effect of the experimental data taken into account. In the energy region near 14MeV in which available experiments are numerous, the difference described above is markedly found.

3.3.2 With correlation for individual experimental sets

The different conditions of this calculation from the preceding 3.3.1. is the assumption that individual experimental sets have 50% correlation in their own data. The difference of this result shown in Table 7 from the preceding (Table 6) is not so large. The correlation matrix in this case express strong correlation and the standard deviations are equivalent. The values of Tables 7 and 6 are almost same. Therefore, the difference between table 7 and 3 is the experimental data base effect. This claims that the correlation of experimental data has almost no effects but it may depend on detailed experimental data base and then this problem should be further studied with appropriate examples.

3.3.3 With correlation between prior level density parameters for isotopes

The 50% correlation is given to the prior level density parameters for isotopes. This corresponds to the case in 3.2.2. except the level density parameters and also should be compared with one in 3.3.1. The result is presented in Table 8 for ^{56}Fe(n,p) as Table 5 in 3.2.2. It is almost identical to the result of Table 6 in 3.3.1. and the difference from the one (Table 5) in 3.2.2. shows the effect of the experiments. The effects of the experimental data base are considerably larger than the effects of the 50% isotope correlation. These are valuable results for us to use our method in the covariance generation.

3.3.4 Inclusion of neighbouring nuclides

The correlation matrix for ^{56}Fe(n,p) is deduced in the simultaneous estimation of the level density parameters taking account of the neutron-induced reactions with isotopes of Ni, Co and Fe. The result is presented in Table 9 and should be compared with Table 6 in 3.3.1. The correlation is slightly reduced when the neighbouring nuclides are taken into account.

3.4. Covariances of level density parameters

The correlation matrix of the posterior level density parameters estimated in the procedure in Fig.6 is shown in Table 10. In Fif.9, the similar matrix to this table is also available but in a larger size matrix because of including more nuclides, which is not presented here. Both matrices are same.

Simply considering, the correlation in the competing reactions like neutron-emission reaction, (n,p) and (n,α) should be negative. As you find in some tables presented above, however, there are positive correlations. This can be in the case in which the level density parameters relating to the competing reactions correlate positively and strongly. The main reactions for ^{54}Fe and ^{56}Fe are in this conditions and actually positive correlation is found in tables presented in this report.

4. Covariances from Curve Fitting

The covariances generated in the preceding section are based on the theoretical model and the parameters which are not freely adjustable but are physically limited in the some ranges determined from other information. A mathematical curve having no physical base, on the other hand, can be fitted to experimental data and reproduced it rather accurately than theoretical curve. The author has discussed on this issue[5] but will briefly do again because of comparing both curve fittings.

Spline functions used in the nuclear data evaluation by the author's group are never physical but purely mathematical. The correlation matrix generated by fitting the spline function expresses the characteristics of the function itself as shown in Table 11 (a) where a first-order spline function is used and does not give possibility to extract physical property from it. This can be seen also in Table.11 (b) where the correlation matrix for fitting of second-order spline function is shown. Both results show the correlation between the regions defined by the individual splines which are a component of the spline function used in fitting. The application of polynomials to curve fitting result oppositely in too strong long-range correlation.

The author has also compared the correlation matrices deduced by fitting optical model formula and Legendre functions to the angular distribution of the neutron elastic scattering[5]. It does not present the distinguished difference to discuss on the significance of correlations matrices. It has been experienced in our laboratory, however, that the giant resonance property at a minimum and maximum in a total cross section can be found in the correlation matrix generated by simultaneously applying the optical model formalism to the experimental data analysis of the total and differential elastic cross sections for Fe.

5. Discussion and Conclusion

The covariances calculated on various conditions are compared in order to search the significance of the covariance generated by merging experimental and theoretical data. This is necessary not only to understand the covariance

itself for nuclear data but to establish a reliable method for generating the covariance matrix valid for applications. Though the discussion in this study is performed on the examples for Fe isotopes using the Hauser-Feshbach formalism it can be extended to others and generalized to reach a goal.

It has been made clear in the present work that the covariance matrix definitely involves the effects propagated from the uncertainties contained in both experimental and theoretical data and they can be identified. It has been impossible, however, that both contributions are quantitatively separated. If the separation is possible the understanding of the covariances can be deepen and it is expected to develop the method to generate the ones agreeable for every evaluator and user of nuclear data. In spite of this, the presented procedure is practically applicable, to the some extent, since they are used as a covariance matrix and their separation is not needed. As an evaluator, however, it is a quite problem rather than this that the present method does not take account of the uncertainty of the used theoretical formula. The problem is left in future.

The presented method and discussion are devoted to the evaluation using theoretical data in part or wholly and do not to the one which is possible with only experimental data. The covariances generated from both procedures are reasonably compatible because they must be produced with the manners matching to the evaluation methods themselves.

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Appendix

A. Simplest Example

The simplest case is that the experimental data is $y=y$, the prior parameter $p_0=p_0$ and the design matrix $\Phi = 1$. Therefore,

$$\hat{p} = \left(\frac{1}{\sigma^2} + \frac{1}{\Delta^2}\right)^{-1}\left(\frac{y}{\sigma^2} + \frac{p_0}{\Delta^2}\right) \qquad \text{(A-1)}$$

$$M = \left(\frac{1}{\sigma^2} + \frac{1}{\Delta^2}\right)^{-1} \qquad \text{(A-2)}$$

and

$$C = \left(\frac{1}{\sigma^2} + \frac{1}{\Delta^2}\right)^{-1} . \qquad \text{(A-3)}$$

The equation (A-1) shows that the posterior parameter is estimated as the average of y and p_0 with the weight of the inverse of the uncertainty, respectively.

B. Two Data

As the next example, the following vectors and matrices are assumed.

$$\mathbf{y} = (y_1 , y_2)^t , \quad \mathbf{V} = \begin{pmatrix} \sigma_1^2 & 0 \\ 0 & \Delta_2^2 \end{pmatrix}$$

$$\mathbf{p}_0 = (p_{01} , p_{02})^t , \quad \mathbf{M}_0 = \begin{pmatrix} \Delta_1^2 & 0 \\ 0 & \Delta_2^2 \end{pmatrix}$$

$$\Phi = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} .$$

The results are

$$\begin{pmatrix} \hat{p}_1 \\ \hat{p}_2 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sigma_1^2} + \frac{1}{\Delta_1^2} & 0 \\ 0 & \frac{1}{\sigma_2^2} + \frac{1}{\Delta_2^2} \end{pmatrix}^{-1} \begin{pmatrix} \frac{y_1}{\sigma_1^2} + \frac{p_{01}}{\Delta_1^2} \\ \frac{y_2}{\sigma_2^2} + \frac{p_{02}}{\Delta_2^2} \end{pmatrix} ,$$

and

$$\mathbf{M} = \mathbf{C} = \begin{pmatrix} \frac{1}{\sigma_1^2} + \frac{1}{\Delta^2} & 0 \\ 0 & \frac{1}{\sigma_2^2} + \frac{1}{\Delta_2^2} \end{pmatrix}^{-1} .$$

These can be understood similar to the simplest example.

If we take accounts of the off-diagonal components of the matrices the results are too complicated to consider their physical meaning.

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Table 1 Reduced covariance matrix for ^{56}Fe
(a)With prior level density parameters(The original ones form Gilbert-Cameron).
(b)With posterior level density parameters(Adjusted ones through the experimental data).

(a)	ENERGY [MeV]	ERROR [%]	CORRELATION [x1000]												
$^{56}Fe(n,n)$	6.0	0.0521	1000												
	10.0	1.13	525	1000											
	14.0	1.95	283	771	1000										
	18.0	1.38	241	728	996	1000									
$^{56}Fe(n,p)$	6.0	1.91	-478	-939	-517	-465	1000								
	10.0	1.37	-426	-985	-850	-813	883	1000							
	14.0	21.9	-376	-943	-923	-894	786	983	1000						
	18.0	11.0	-389	-955	-902	-869	812	990	998	1000					
$^{56}Fe(n,\alpha)$	6.0	2.05	-476	-888	-404	-351	991	816	700	731	1000				
	10.0	11.9	-485	-864	-375	-327	978	783	659	689	993	1000			
	14.0	22.5	-390	-677	-312	-300	783	590	473	487	804	865	1000		
	18.0	28.2	-311	-518	-222	-225	623	432	322	329	650	732	974	1000	
$^{56}Fe(n,2n)$	6.0	0.00	0	0	0	0	0	0	0	0	0	0	0	0	1000
	10.0	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0 1000
	14.0	6.90	492	995	730	688	-961	-973	-917	-932	-920	-902	-735	-582	0 0 1000
	18.0	7.27	422	963	903	878	-830	-984	-982	-980	-754	-734	-619	-489	0 0 950 1000

(b)	ENERGY [MeV]	ERROR [%]	CORRELATION [x1000]												
$^{56}Fe(n,n)$	6.0	0.0449	1000												
	10.0	0.111	782	1000											
	14.0	0.351	233	128	1000										
	18.0	0.308	98	56	988	1000									
$^{56}Fe(n,p)$	6.0	0.241	108	-470	525	471	1000								
	10.0	0.497	0	-611	173	127	906	1000							
	14.0	0.290	8	-15	-388	-378	-191	150	1000						
	18.0	0.275	-10	-31	797	832	361	206	184	1000					
$^{56}Fe(n,\alpha)$	6.0	0.301	93	-474	543	493	999	895	-214	373	1000				
	10.0	1.95	2	-612	19	-39	858	940	-64	-99	847	1000			
	14.0	11.0	33	-330	-719	-779	173	462	199	-731	149	644	1000		
	18.0	17.3	37	-286	-766	-825	95	394	218	-767	71	581	996	1000	
$^{56}Fe(n,2n)$	6.0	0.00	0	0	0	0	0	0	0	0	0	0	0	0	1000
	10.0	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0 1000
	14.0	0.663	262	780	238	261	-684	-871	-69	224	-672	-941	-746	-696	0 0 1000
	18.0	1.02	146	380	834	855	8	-330	-307	730	30	-490	-943	-952	0 0 667 1000

Table 2 Reduced covariance matrix for ^{54}Fe

(a)With prior level density parameters(The original ones form Gilbert-Cameron).

(b)With posterior level density parameters(Adjusted ones through the experimental data).

(a)	ENERGY [MeV]	ERROR [%]	CORRELATION [x1000]														
$^{54}Fe(n,n)$	6.0	0.766	1000														
	10.0	5.84	994	1000													
	14.0	4.96	995	995	1000												
	18.0	1.74	967	986	972	1000											
$^{54}Fe(n,p)$	6.0	1.83	-992	-993	-997	-964	1000										
	10.0	10.0	-995	-994	-997	-964	999	1000									
	14.0	11.2	-990	-997	-989	-978	992	993	1000								
	18.0	4.54	-962	-977	-954	-968	961	964	987	1000							
$^{54}Fe(n,\alpha)$	6.0	1.36	-159	-240	-155	-379	144	146	244	356	1000						
	10.0	9.12	72	-7	64	-169	-91	-91	-8	82	936	1000					
	14.0	18.5	134	67	102	-94	-149	-154	-112	-87	702	891	1000				
	18.0	23.9	154	96	116	-56	-167	-174	-150	-149	577	803	985	1000			
$^{54}Fe(n,2n)$	6.0	0.00	0	0	0	0	0	0	0	0	0	0	0	0	1000		
	10.0	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0	1000	
	14.0	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1000
	18.0	14.6	965	983	970	996	-962	-962	-975	-964	-370	-161	-89	-52	0	0	0 1000

(b)	ENERGY [MeV]	ERROR [%]	CORRELATION [x1000]														
$^{54}Fe(n,n)$	6.0	0.0831	1000														
	10.0	0.293	836	1000													
	14.0	0.383	713	907	1000												
	18.0	0.0703	729	907	667	1000											
$^{54}Fe(n,p)$	6.0	0.131	-129	-589	-778	-384	1000										
	10.0	0.610	-508	-849	-955	-635	918	1000									
	14.0	0.392	-369	-773	-592	-859	627	709	1000								
	18.0	0.308	255	170	533	-219	-400	-427	333	1000							
$^{54}Fe(n,\alpha)$	6.0	0.380	549	607	869	230	-671	-787	-145	872	1000						
	10.0	1.87	440	562	849	176	-747	-810	-174	857	987	1000					
	14.0	0.828	206	230	378	-75	-356	-391	-96	379	521	585	1000				
	18.0	1.50	-315	-447	-658	-269	571	605	117	-673	-693	-651	233	1000			
$^{54}Fe(n,2n)$	6.0	0.00	0	0	0	0	0	0	0	0	0	0	0	0	1000		
	10.0	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0	1000	
	14.0	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1000
	18.0	1.16	285	355	275	419	-166	-262	-324	-33	285	355	275	419	0	0	0 1000

Table 3 Covariance for $^{56}Fe(n,p)$ with the prior level density parameters. Expanded matrix of the partial matrix for (n,p) in Table 1(a).

ENERGY [MeV]	ERROR [%]	CORRELATION [x1000]															
5.0	0.0404	1000															
6.0	1.91	40	1000														
7.0	4.53	32	999	1000													
8.0	7.46	51	979	984	1000												
9.0	10.6	70	932	941	986	1000											
10.0	13.7	82	883	894	959	992	1000										
11.0	16.7	90	843	856	934	980	996	1000									
12.0	19.3	95	812	826	913	967	990	998	1000								
13.0	21.4	98	792	806	898	958	985	995	999	1000							
14.0	21.9	99	786	800	894	955	983	995	999	999	1000						
15.0	20.3	99	790	804	897	957	985	995	999	999	999	1000					
16.0	17.5	98	797	812	902	961	986	996	999	999	999	999	1000				
17.0	14.1	97	803	817	906	963	988	997	999	999	999	999	999	1000			
18.0	11.0	96	812	826	912	967	990	997	999	998	998	999	999	999	1000		
19.0	8.18	95	817	830	915	969	990	997	999	998	998	998	999	999	999	1000	
20.0	5.82	96	813	827	913	967	989	997	998	998	998	998	999	999	999	999	1000

Table 4 Covariance for $^{54}Fe(n,p)$ with the prior level density parameters. Expanded matrix of the partial matrix for (n,p) in Table 2(a).

ENERGY [MeV]	ERROR [%]	CORRELATION [x1000]															
5.0	0.345	1000															
6.0	1.83	776	1000														
7.0	4.02	758	999	1000													
8.0	6.26	763	999	999	1000												
9.0	8.31	770	999	999	999	1000											
10.0	10.0	769	999	999	999	999	1000										
11.0	11.4	771	999	999	999	999	999	1000									
12.0	12.4	760	998	999	999	999	999	999	1000								
13.0	12.2	736	997	998	998	997	998	998	999	1000							
14.0	11.2	703	992	995	994	993	993	993	995	998	1000						
15.0	9.55	668	984	988	987	985	986	986	989	994	998	1000					
16.0	7.75	637	975	980	978	976	977	977	981	988	995	998	1000				
17.0	6.01	615	967	972	970	968	969	969	974	982	990	996	999	1000			
18.0	4.54	608	961	967	965	963	964	965	970	978	987	994	997	999	1000		
19.0	3.38	621	962	967	965	963	964	965	970	978	987	993	996	998	999	1000	
20.0	2.56	658	967	971	970	969	970	971	975	982	988	992	993	994	996	998	1000

Table 5 Covariance for ^{56}Fe(n,p) with the prior level density parameters. Assumed 50% correlation in the individual isotopes.

ENERGY [MeV]	ERROR [%]	CORRELATION [x1000]														
5.0	0.0404	1000														
6.0	1.93	525	1000													
7.0	4.56	518	999	1000												
8.0	7.49	518	979	984	1000											
9.0	10.6	504	933	941	986	1000										
10.0	13.7	486	884	895	959	992	1000									
11.0	16.7	470	843	856	934	980	996	1000								
12.0	19.4	457	812	826	913	967	990	998	1000							
13.0	21.4	448	792	806	898	958	985	995	999	1000						
14.0	21.9	446	786	801	894	955	983	995	999	999	1000					
15.0	20.4	448	790	805	897	957	985	995	999	999	999	1000				
16.0	17.5	451	798	812	902	961	986	996	999	999	999	999	1000			
17.0	14.1	454	803	818	906	963	988	997	999	999	999	999	999	1000		
18.0	11.1	458	813	827	913	967	990	997	999	998	998	999	999	999	1000	
19.0	8.19	460	817	831	916	969	990	997	999	998	997	998	999	999	999	1000
20.0	5.83	459	814	828	913	967	989	997	998	998	997	998	999	999	999	999 1000

Table 6 Covariance for ^{56}Fe(n,p) with the posterior level density parameters. Expanded matrix of the partial matrix for (n,p) in Table 1(b).

ENERGY [MeV]	ERROR [%]	CORRELATION [x1000]														
5.0	0.0397	1000														
6.0	0.241	164	1000													
7.0	0.548	73	995	1000												
8.0	0.665	56	991	997	1000											
9.0	0.615	52	972	979	991	1000										
10.0	0.497	52	906	914	940	977	1000									
11.0	0.383	48	732	740	785	859	947	1000								
12.0	0.313	34	354	361	423	534	698	889	1000							
13.0	0.304	12	-70	-65	-2	118	315	594	894	1000						
14.0	0.290	0	-191	-187	-134	-28	150	429	771	962	1000					
15.0	0.256	-1	-52	-48	-13	55	178	381	647	817	925	1000				
16.0	0.251	1	168	170	178	193	225	298	406	499	658	894	1000			
17.0	0.262	4	270	272	259	234	199	174	170	212	394	712	951	1000		
18.0	0.275	8	361	362	336	285	206	111	17	4	184	541	860	975	1000	
19.0	0.256	7	359	359	326	262	162	38	-86	-107	77	448	800	946	993	1000
20.0	0.212	8	294	293	255	184	75	-55	-171	-167	31	406	765	924	978	993 1000

Table 7 Covariance for $^{56}Fe(n,p)$ with the posterior level density parameters. Assumed 50% correlation for the experimental points in an identical set.

ENERGY [MeV]	ERROR [%]	CORRELATION [x1000]														
5.0	0.0398	1000														
6.0	0.292	178	1000													
7.0	0.665	104	997	1000												
8.0	0.815	89	994	998	1000											
9.0	0.762	85	982	987	994	1000										
10.0	0.619	84	940	946	963	985	1000									
11.0	0.472	78	822	828	857	905	963	1000								
12.0	0.370	56	519	525	569	647	763	907	1000							
13.0	0.353	21	108	113	162	252	400	624	893	1000						
14.0	0.360	6	-10	-6	35	115	252	478	784	968	1000					
15.0	0.352	10	110	113	144	202	305	482	729	884	956	1000				
16.0	0.354	18	266	269	285	315	372	479	629	720	821	951	1000			
17.0	0.348	23	335	337	342	350	371	425	504	556	677	862	976	1000		
18.0	0.344	29	411	413	408	399	390	397	408	412	538	759	922	984	1000	
19.0	0.305	28	408	409	399	380	355	339	324	320	455	694	882	963	994	1000
20.0	0.245	27	342	342	328	304	271	249	240	262	415	661	855	945	981	994 1000

Table 8 Covariance for $^{56}Fe(n,p)$ with the posterior level density parameters. Assumed 50% correlation in the individual isotopes. The encounter of Fig 5.

ENERGY [MeV]	ERROR [%]	CORRELATION [x1000]														
5.0	0.0326	1000														
6.0	0.240	187	1000													
7.0	0.545	113	997	1000												
8.0	0.662	98	993	997	1000											
9.0	0.612	92	976	981	992	1000										
10.0	0.493	87	915	922	945	979	1000									
11.0	0.376	73	749	756	798	866	949	1000								
12.0	0.304	39	370	377	435	541	698	886	1000							
13.0	0.298	0	-65	-60	0	115	305	582	890	1000						
14.0	0.288	-13	-188	-184	-132	-30	144	421	773	965	1000					
15.0	0.256	-2	-52	-49	-12	58	185	397	676	844	936	1000				
16.0	0.246	17	166	168	181	206	254	347	476	565	700	905	1000			
17.0	0.249	29	275	275	269	256	241	241	256	292	450	734	952	1000		
18.0	0.259	40	375	374	354	316	256	184	103	79	237	561	859	973	1000	
19.0	0.238	41	377	375	348	296	214	110	-4	-37	125	464	795	941	992	1000
20.0	0.197	39	311	308	277	217	125	13	-94	-102	76	420	758	918	977	993 1000

Table 9 Covariance for $^{56}Fe(n,p)$ with the posterior level density parameters estimated in a simultaneous evaluation for isotopes of Ni,Co and Fe.

ENERGY [MeV]	ERROR [%]	CORRELATION [x1000]												
5.0	0.0397	1000												
6.0	0.204	196	1000											
7.0	0.518	81	993	1000										
8.0	0.720	58	985	995	1000									
9.0	0.775	53	958	970	987	1000								
10.0	0.744	51	874	887	924	972	1000							
11.0	0.694	46	694	706	764	854	951	1000						
12.0	0.672	33	379	390	465	593	760	922	1000					
13.0	0.703	15	48	55	133	273	476	716	928	1000				
14.0	0.674	3	-65	-59	7	130	318	563	817	962	1000			
15.0	0.558	0	15	19	62	142	269	452	662	816	931	1000		
16.0	0.475	0	143	147	156	174	210	286	401	525	700	912	1000	
17.0	0.417	1	194	195	179	150	118	113	156	255	460	751	955	1000
18.0	0.381	4	250	250	218	158	77	11	-8	56	265	597	873	977
19.0	0.317	3	238	237	196	119	16	-75	-118	-59	155	503	812	947
20.0	0.245	4	176	173	126	42	-68	-165	-203	-128	96	451	772	922

Table 10 Covariance for $^{56}Fe(n,p)$ with the posterior level density parameters. Adjusted to the experimental data for Fe.

NUCLEUS	PARAMETER [/MeV]	ERROR [%]	CORRELATION [x1000]											
FE-57	7.2410	4.74	1000											
FE-56	7.9347	0.578	1	1000										
FE-55	5.9526	4.91	0	0	1000									
FE-54	5.5079	0.990	0	0	-70	1000								
FE-53	5.8184	5.03	0	0	5	3	1000							
MN-56	8.6537	0.634	44	979	0	0	0	1000						
MN-55	6.7054	4.97	0	-1	0	0	0	-1	1000					
MN-54	5.8632	1.18	0	0	-3	969	6	0	0	1000				
MN-53	6.3101	3.94	0	0	-64	-16	58	0	0	-51	1000			
CR-53	8.9639	3.05	-32	127	0	0	0	279	-2	0	0	1000		
CR-52	6.1538	5.00	0	0	0	0	0	0	0	0	0	0	1000	
CR-51	7.2459	1.33	0	0	-1	967	6	0	0	978	-44	0	0	1000
CR-50	6.5453	5.00	0	0	0	0	0	0	0	0	0	0	0	0 1000

Table 11 Covariance for spline function fitted to $^{56}Fe(n,p)$ experiments.
(a)First order spline function.
(b)Second order spline function.

(a)

ENERGY [MeV]	PARAMETER [mb]	ERROR [%]	CORRELATION [x1000]								
5.0	0.446	9.50	1000								
6.0	10.5	1.22	-472	1000							
8.0	47.9	0.893	78	-165	1000						
10.0	72.5	1.23	-15	33	-200	1000					
12.0	107	1.22	4	-9	55	-278	1000				
14.0	113	0.660	-1	3	-19	96	-348	1000			
15.0	104	0.714	0	-1	7	-35	125	-361	1000		
16.0	84.7	0.994	0	0	-1	5	-17	51	-142	1000	
18.0	60.6	1.13	0	0	0	-1	6	-17	49	-347	1000
20.0	45.1	2.85	0	0	0	0	-2	6	-16	117	-338	1000

(b)

ENERGY [MeV]	PARAMETER [mb]	ERROR [%]	CORRELATION [x1000]								
5.0	0.260	15.6	1000								
6.0	11.5	0.923	-385	1000							
8.0	45.0	0.794	-10	17	1000						
10.0	76.0	0.778	44	-93	258	1000					
12.0	101	0.710	-30	63	-201	461	1000				
14.0	112	0.433	4	-10	32	-87	153	1000			
15.0	103	0.505	-1	3	-10	28	-76	117	1000		
16.0	86.3	0.790	2	-5	16	-46	132	-329	657	1000	
18.0	60.1	0.890	0	0	-2	6	-17	43	-89	-58	1000
20.0	46.6	4.17	0	0	-2	6	-18	46	-95	5	-376	1000

UPDATING OF A THEORETICAL EVALUATION BY EXPERIMENTAL DATA IN THE CASE OF ^{56}Fe

V. PRONYAEV*), S. TAGESEN, H. VONACH and M. WAGNER

Institut für Radiumforschung und Kernphysik
University of Vienna, Boltzmanngasse 3, A-1090 Vienna, Austria

ABSTRACT

The neutron total and partial reaction cross sections and their pertinent covariance matrices for the ^{56}Fe nucleus from the EFF-2 evaluated data file were updated by using experimental data available from the EXFOR data base. To this aim an extended version of the GLUCS code, based on the Bayesian method, was developed and applied. Attention was paid to the construction of a realistic covariance matrix for each individual experimental data set. 40 groups were used for the presentation of the cross sections and matrices in the energy range between 0.85 MeV and 20 MeV. The procedure we applied has shown its ability to improve the quality of the evaluated data files.

*)Permanent address: Institute of Physics and Power Engineering, 249020 Obninsk, Russian Federation.

1. INTRODUCTION

For application purposes evaluated data files containing not only the central values or central values supplemented by variances but a more complete information which also includes correlation matrices, are indispensable. Though these requirements were formulated more than 30 years ago /1-3/ up to now only a few special purpose files for Standard or Reactor Dosimetry Reactions provide these data with satisfactory quality. Two main reasons complicate the work in this direction. The first one is purely technical: for an array of n elements of central values we have to create $n(n+1)/2$ elements of the triangle covariance matrix. The second one is of a more basic nature: In most cases the complete experimental information needed to create such a matrix is not available. Therefore we have to rely on some supplementary information which can be provided by theoretical models of different levels of generality.

The Bayesian method as applied by the authors of the GLUCS code /4/ offers a convenient way to update cross sections evaluated in model calculations by using experimental data for the reactions in question. Such an approach was chosen for a re-evaluation of the high-energy (0.85 MeV < E < 20 MeV) neutron cross sections for the ^{56}Fe nucleus, starting in most cases from the EFF-2 evaluated data file /5/ and employing the GLUCS code in order to insert experimental data available from the EXFOR data base or from very recent measurements. The Bayesian method states /6, 7/ that if we have the central values vector T and the covariance matrix M as prior data, vector R and matrix V presenting new experimental data, we may get, for $M = M^+$, the updated estimate or posterior data T' and M' as

$$T' = T + M\,G^+\,(G\,M\,G^+ + V)^{-1}\,(R - R_T) \qquad (1)$$

$$M' = M - M\,G^+\,(G\,M\,G^+ + V)^{-1}\,G\,M \qquad (2)$$

where R_T presents the prior value interpolated at the point where R is given, G is the sensitivity matrix of the new experimental data relative to the prior data with the matrix elements $g_{ij} = dR_i/dT_j$, and the upscript (+) means transpose and (-1) - inverse operation. One of the most important conditions for obtaining these formulae is an absence of correlations between the data vectors T and R.

Due to the different completeness of the data for different reaction cross sections a different choice of the priors was used ranging from purely experimental data and covariances to the results of theoretical model calculations for central values and expert evaluation of their covariance matrix. To some extent, this is equivalent to "objective" and "rather subjective" choices of prior values. In most cases the initial prior values were taken from the EFF-2 cross section files, which are based on theoretical calculations using the optical and statistical models /5/, and from an expert evaluation of the covariances /8/ obtained by intercomparison of the data from four major evaluated data libraries (ENDF/B-VI, JENDL-3, EFF-2 and BROND-2) and by assigning the uncertainties corresponding to the level of data spread. We always tried to choose the best available prior data which still were explicitly not correlated with experimental data. For the non-diagonal elements of the corresponding correlation matrix an energy dependence was assumed which can be described by a Gaussian function with a width Γ being either constant over the entire energy range or variable with energy according to the characteristic features of the considered reactions.

The general principle of this evaluation is shown schematically in Figure 1. As a

first step the cross sections and covariances for individual reactions are evaluated independently from each other. From this procedure (depicted at the left side of Fig. 1) we get a set of improved cross sections with much reduced uncertainties compared to the prior EFF-2 values. Cross sections for which no experimental data exist (e.g. $\sigma_{n,np}$, $\sigma_{n,ncont}$) remain unchanged at this step. Due to the independent adjustment of the individual cross sections the internal consistency (e.g. between σ_{non} and the sum of partial cross sections) gets lost to some degree. Therefore, in a final step (see right side of Fig. 1) this consistency - that is the physical relation between the different cross sections - is restored by a least - squares adjustment. For this purpose a set of independent cross sections is selected as the new prior, whereas the remaining redundant cross sections, such as for proton production, for nonelastic processes, for elastic and inelastic scattering, which can be expressed as linear functions of the basic cross sections are used as "data" for application of the equations 1 and 2. A more detailed description of the evaluation procedure is given below.

2. THE EVALUATION PROCEDURE

2.1 Construction of covariance matrices of the experimental data.

We used the experimental data compiled in EXFOR /9/ and supplemented them by very recent ones as a base for our evaluation. Usually, beside the measured values, the authors supply information on some partial variances. In those cases where sufficient information on the total uncertainties and their correlated properties was lacking, the following procedure was adopted in order to construct a complete covariance matrix of uncertainties for any separate experimental data set:

We assumed that the covariance matrix of total uncertainties can be split into three matrices of partial uncertainties:

i) a covariance matrix of partial uncertainties describing short-energy-range (SER) correlation properties such as statistical uncertainties due to a finite number of counts per channel;

ii) a covariance matrix of partial uncertainties connected with properties that give rise to medium-energy-range (MER) correlations, such as uncertainties due to the correction for the dead time and to the determination of the detector efficiency, the effect/background separation, multiple scattering and scattering at the collimator, the spectrometer resolution function and neutron source properties;

iii) a covariance matrix of partial uncertainties connected with properties which induce large-energy-range (LER) correlations, such as systematical errors due to any normalization of the cross sections in order to get absolute values, to the determination of the number of nuclei in a sample, to geometrical sizes and distances and to sample self-absorption properties for the non-resonance energy region.

These three matrices are combined as described below in order to get the final covariance matrix. For these matrices an energy - group structure was introduced to arrive at a reasonable number of elements. The correlations existing between different experimental data sets due to the common experimental conditions or to the cross section normalization procedure were not accounted for except for the data for the (n,2n), (n,p) and (n,α) reactions.

2.2 Evaluation of the total cross section.

We started with the evaluation of the total cross section for which the number of data points is maximal. Because most of the high energy neutron data were obtained for natural iron containing 91.7% of ^{56}Fe and since the isotopical dependence of the total cross section for the non-resonance region is rather weak, we used the data for natural iron for the evaluation of the ^{56}Fe total cross section.

All high-resolution data for the total cross section from the EXFOR data base were averaged with a constant averaging function in a 40 - group structure for the energy region 0.85 MeV < E < 20 MeV. We chose the following energy grid: the first group extended from 0.85 to 1.0 MeV, up to 3.0 MeV 0.2 MeV wide steps were taken, between 3.0 and 15.0 MeV the group width was 0.5 MeV and, finally, 1.0 MeV in the neutron energy range from 15.0 to 20.0 MeV. Data were intercompared and evidently discrepant data were discarded as well as in some cases those in the first and the last group for a given data set. Very often the authors specify only the statistical component of the uncertainty. The elements of the SER vector of the correlation matrix will be just 1 along the main diagonal and 0 for non-diagonal elements.

The LER correlation matrix of uncertainties is also simple as each element of this matrix is equal to 1. Some of the authors state the contribution of the systematical error for high resolution total cross-section measurements to amount to about 1%; we used this value practically for all data sets.

MER variances and covariances were obtained in the following manner: An arithmetical average $<<tot(k)>>$ for 16 averaged data sets $<tot(j,k)>$ (where k is a group number and j is a data set number) was calculated. The absolute deviations for each data set then were obtained as

$$\varepsilon^{k,j}_{MER} = |<<tot(k)>>-<tot(j,k)>|/<<tot(k)>> \qquad (3)$$

and squares of these values averaged over 2 MeV intervals were treated as the diagonal elements for a MER correlation matrix. In order to determine the non-diagonal elements of this matrix, we used the hypothesis /8/ that the propagation of these correlations has a Gaussian shape and calculated correlation coefficients (normalized to 1) as:

$$<\varepsilon^{k,j}_{MER}\,\varepsilon^{l,j}_{MER}>/(<\varepsilon^{k,j}_{MER}><\varepsilon^{l,j}_{MER}>) = \exp(-((E_k - E_l)/\Gamma_j)*\ln(2)) = f(E_k, E_l) \quad (4)$$

Γ_j = 2 MeV was usually taken because the scale for major changes in the shape of LER data was similar. Then a MER covariance matrix may be obtained in a simple way. The complete covariance matrix is constructed from the partial SER, MER and LER matrices by summing the corresponding elements.

At the next step the GLUCS code was used to obtain the evaluated average cross sections and their covariances. The averaged cross sections from the experiment by Cierjacks et al. /10/ with the covariances assigned to them were chosen as an initial prior data set as it covers the entire energy range considered in this evaluation, and then step by step 23 experimental data sets (comprising cross sections and covariances) were added applying the Bayesian method by means of GLUCS. The correlations between different experimental data sets were considered to be negligible. Beside the high-resolution data, also the data from measurements at a single energy were used. The reason why we have

not used the EFF-2 evaluation of the total cross section as a prior data set is a big (up to 30%) well-known discrepancy between the optical model predictions of the total cross section (taken as EFF-2 evaluated cross section) for energies below 4 MeV and the existing experimental data.

The overall χ^2 value per degree of freedom, considering all experimental data sets, was about 1.7. This result indicated that we had to go to the next step in the iteration procedure: namely to increase the assigned LER and MER components of the covariances for those experimental data sets which have a χ^2 value higher than 1 and repeat the Bayesian procedure. In order to avoid this we increased the standard deviation values by a factor 1.5. The obtained low uncertainty of the group-averaged evaluated data (standard deviations up to 0.5% for some energy groups) reflects a rather high accuracy of the experimental data base for the iron neutron total cross section.

2.3. Evaluation of partial cross sections.

A similar procedure was applied in general for the evaluation of the central values and the covariances for the following measured partial cross sections: for the nonelastic process, inelastic scattering with excitation of partial levels and groups of levels, and the (n,2n), (n,p) and (n,α) reactions.

The following features of ^{56}Fe cross sections for energies between 0.85 MeV and 20 MeV were taken into account during the evaluation procedure:

i) The nonelastic cross section:

- As the capture cross section is less than a few mb in this energy region and the effective thresholds of the (n,p) and (n,α) reactions are higher than 5 MeV, the total inelastic cross section for 0.85 < E < 5 MeV is with a high accuracy (< 0.1%) equal to the nonelastic one;

- due to the specific nuclear structure properties of the ^{56}Fe nucleus observed in many experiments with γ-ray transition measurements, the production of the 0.847 MeV γ-rays (transition between the first excited 2^+ level and the ground state) is equal to 0.93 - 1.00 times the total inelastic scattering cross section with an energy dependence of this correction factor that can be evaluated from known decay schemes and experimental data on partial γ-ray production;

- most of the high - energy nonelastic cross sections obtained in sphere transmission measurements and presented in the EXFOR data base as total nonelastic cross sections are in reality the partial nonelastic cross sections without inclusion of the inelastic scattering cross section for the first (2^+) excited level.

As a result 46 data sets were chosen for the evaluation of the nonelastic cross section and its covariances. Again, the Bayesian method employed in the GLUCS code was used in order to obtain the evaluated nonelastic cross section and the respective covariance matrix. The prior values were taken from the EFF-2 cross section files and the corresponding covariances.

The overall χ^2 was equal to 1.1 and was obtained in a second run after some adjustment of the correlation matrix for a few shape-type experimental data which were inconsistent with the prior data (usually χ^2 for these data is much higher than 1 due to a different shape as compared with the prior data).

The evaluated central values and covariances for the nonelastic cross section were considered as redundant and included in the further evaluation process as pseudo-experimental data when consistency conditions between total and partial cross sections were imposed.

ii) The cross sections for inelastic scattering

The existing experimental information on the excitation functions for the separate levels and groups of levels gives a chance to improve the cross sections and related covariances if the Bayesian procedure is applied to the following levels and groups of levels (with MT reaction numbers from EFF-2 file):

1. MT = 51, E_{lev} = 0.847 MeV
2. MT = 52, E_{lev} = 2.085 MeV
3. MT = 53, E_{lev} = 2.658 MeV
4. MT = 54 - 58, E_{lev} = 2.942 - 3.123 MeV
5. MT = 59 - 65, E_{lev} = 3.370 - 3.607 MeV
6. MT = 66 - 83, E_{lev} = 3.748 - 4.510 MeV
7. MT = 91, E_{lev} = 4.52 MeV, continuum of levels.

MT = 54 - 58 group does not include the 3.070 MeV level (MT = 56 in EFF-2) because it was not observed in any measurement of γ-transitions; its presence and competition in statistical model calculations, however, leads to a substantial decrease of the inelastic scattering cross section for other levels.

In order to preclude a double counting of the data which were accounted for as total nonelastic cross section, only the experimental data for neutron energies higher than 2.08 MeV were taken into account when the excitation function for inelastic scattering to the first excited level was evaluated. The χ^2 values per degree of freedom obtained were equal to 0.35 for the MT = 51 level, 1.3 for the MT = 52 level, 0.95 for the MT = 53 level, 0.65 for the group of MT = 54 - 58 levels, and 0.73 for the group of MT = 59 - 65 levels.

The cross section data for total inelastic scattering were considered as redundant and included in the evaluation process at the last stage when consistency conditions between total and partial cross sections were imposed.

iii) The (n,2n), (n,p) and (n,α) reaction cross sections

A more detailed analysis of experimental data was carried out for these reactions. This concerns especially the (n,p) reaction which is used as a dosimetry reaction. The literature data were carefully reviewed in order to discard obsolete or obviously wrong results. The published experimental values were renormalized to the most recent reference cross sections.

A complete experimental data base comprises the results for ^{56}Fe and ^{nat}Fe; a correction for the contribution from minor isotopes was carried out where necessary. The experimental correlation matrices included the parts which present the correlations

between different experimental data sets in those cases where these correlations are important.

The high long-energy-range correlations given for the ^{56}Fe file in the EFF-2 library and taken as prior data, however, conflicted with the relatively high correlations present in a number of experiments which, too, covered a large energy region. This was especially true for the more accurate (n,p) reaction measurements, as soon as a slight deviation of the shape of both the respective prior excitation function and the new experimental data set occurred. In order to amend this situation a "white-sheet-prior" was taken where the off-diagonal elements of the covariance matrix were practically set to zero.

The general χ^2 per degree of freedom was 1.06 for the (n,2n) reaction, 1.47 for the (n,p) and 0.90 for the (n,α) reactions, indicating an only moderate consistency of the experimental data.

2.4. "Redundant" cross sections and consistency conditions.

The following consistency conditions between the cross sections for different reactions were introduced at the last stage of the evaluation:

$$\sigma_{\text{p-prod}} = \sigma_{\text{n,p}} + \sigma_{\text{n,np}} \tag{5}$$

$$\sigma_{\text{inel}} = \sigma_{\text{n,n1}} + \sigma_{\text{n,n2}} + \sigma_{\text{n,n3}} + \sigma_{\text{n,n4-n7}} + \sigma_{\text{n,n8-n14}} + \sigma_{\text{n,n15-n32}} + \sigma_{\text{n,ncont}} \tag{6}$$

$$\sigma^*_{\text{non}} = \sigma_{\text{n,2n}} + \sigma_{\text{n,}\alpha} + \sigma_{\text{n,p}} + \sigma_{\text{n,np}} + \sigma_{\text{n,n1}} + \sigma_{\text{n,n2}} + \sigma_{\text{n,n3}} + \sigma_{\text{n,n4-n7}} + \sigma_{\text{n,n8-n14}} + \sigma_{\text{n,n15-n32}} + \sigma_{\text{n,ncont}} \tag{7}$$

$$\sigma_{\text{el}} = \sigma^*_{\text{tot}} - \sigma_{\text{n,2n}} - \sigma_{\text{n,}\alpha} - \sigma_{\text{n,p}} - \sigma_{\text{n,np}} - \sigma_{\text{n,n1}} - \sigma_{\text{n,n2}} - \sigma_{\text{n,n3}} - \sigma_{\text{n,n4-n7}} - \sigma_{\text{n,n8-n14}} - \sigma_{\text{n,n15-n32}} - \sigma_{\text{n,ncont}} \tag{8}$$

where the right side presents the data evaluated as described above, which are considered now as new prior data, and the left side presents new experimental or pseudo-experimental data as, e.g., for the nonelastic cross section. σ^*_{tot} and σ^*_{non} are the total and nonelastic cross sections evaluated above, from which a part representing the sum of so-called minor cross sections for the energy range considered, such as the (n,γ), (n,d), (n,t), (n,^{3}He) and (n,nα) reaction cross sections, was subtracted. Since the EFF-2 file was incomplete with respect to some of these reaction cross sections, we took these data from the ENDF/B-VI file. Then all relevant data were processed by the GLUCS code in one run.

In order to cope with this task, the original GLUCS code was revised by one of us (S.T.) in two aspects: First of all, it is now possible to introduce new experimental data for the sum and the difference or for any linear combinations of prior reaction cross sections. Secondly, thanks to a new option, a much simpler format for the correlation matrix can by used in those cases where no correlations exist between two or more subsets of one data set.

Total proton production, inelastic, nonelastic and elastic scattering cross sections were used for imposing the consistency conditions. Only a few experimental data sets with rather low accuracy exist for the (n,np) reaction and correspondingly the final evaluated cross sections are insensitive to these data.

As most of the data on total inelastic scattering were already accounted for when evaluating the nonelastic cross section and the respective covariances, we considered inelastic scattering cross section data only for neutron energies above 12 MeV, where the difference between the nonelastic and the inelastic cross sections becomes substantial. An evaluation of experimental data in the 14-MeV energy region (13.5 - 14.8 MeV) performed previously at the IRK /8/ resulted in a cross section value of high accuracy, which can be included by means of the Bayesian method replacing all experimental data in that energy range. The remaining data are the 847 keV γ-ray production cross-section measurements which can be reduced to the total inelastic scattering cross section. By doing this we found that the experimental data are not consistent with the evaluated value at 14.0 MeV, being usually too low. The reason for this discrepancy is unclear, but probably it is partly a problem of background separation when the spectrometer resolution function is not explicitly known. To avoid further complications with accounting for these discrepant data we treated them as shape cross section measurements. The procedure for obtaining the pseudo-experimental nonelastic cross sections was described above.

In order to include the existing experimental information on elastic scattering cross sections and their covariances into the evaluation we proceeded as follows: As a first step the evaluation of the elastic scattering cross section and the covariances was performed independently from the data on the total and the nonelastic cross sections. For this purpose the elastic scattering cross section and its covariance matrix from the EFF-2 file including only elastic scattering cross section correlations between different energies were taken as a prior. They were obtained by a purely mathematical procedure of converting a NC-type into a NI-type subsection. Then the Bayesian method was used to account for all experimental cross-section data on elastic scattering existing in the EXFOR data base. The covariance matrices for these data were prepared as described in section 2.2 for the total cross section. Then, by intercomparison with the elastic scattering cross section and covariances obtained from the evaluated total and nonelastic data, we found a serious discrepancy between these two independent evaluations of the elastic scattering cross section in the energy region between 4 and 8 MeV. The apparent reason is an underestimation of the integral elastic scattering cross sections by 5 to 15% in practically all measurements for this energy region.

Although we mentioned to have taken the ^{56}Fe elastic scattering cross section from the EFF-2 library as a prior, this is true only for neutron energies above 4 MeV. For lower energies, due to the problems with an optical model description of the total and elastic scattering cross sections (this approach was used for the EFF-2 evaluation for ^{56}Fe) we chose as a prior a group-averaged cross section obtained as the difference between the new evaluated total and nonelastic cross sections in group structure with their respective covariance matrices as described above.

At the last stage of the evaluation process, the covariances for practically all experimental data on elastic scattering in the energy region between 4 and 8 MeV were revised by increasing the total errors up to 15% and decreasing the correlations between different energy points. As a result the χ^2 value for the 34 chosen data sets was close to 1.

Because of the consistency conditions expressed by the equations (5) - (8) and the consideration of all 12 non-redundant cross sections as one coupled set, the resulting correlation matrix now includes parts which describe correlations between different energy intervals of different cross sections.

3. RESULTS AND DISCUSSION

The main result of this evaluation is a complete, but non-redundant set of cross sections (σ_{tot}, $\sigma_{n,n1}$, $\sigma_{n,n2}$, $\sigma_{n,n3}$, $\sigma_{n,n4\text{-}n7}$, $\sigma_{n,n8\text{-}n14}$, $\sigma_{n,n15\text{-}n32}$, $\sigma_{n,ncont}$, $\sigma_{n,p}$, $\sigma_{n,np}$, $\sigma_{n,\alpha}$, $\sigma_{n,2n}$) and their covariances in the fast neutron energy range 0.85 - 20 MeV in a 40 - group structure. In addition, cross sections and covariances for σ_{el}, σ_{non} and σ_{inel}, were obtained by expressing these cross sections as linear functions of the basic cross sections (see equations 5 - 8). Examples of these results are given in Fig. 2 - 7. In addition Table 1 compares the cross sections and uncertainties obtained in this evaluation with the results of our starting point EFF-2 and with these of ENDF/B-VI.

From these figures and table we can immediately see the progress achieved in this evaluation.

1) The largest improvement in the evaluated cross sections was achieved in the energy range below 3 MeV. At these low energies the theoretical description of the cross sections by the optical model gets rather poor and thus the replacement of these calculated values by accurate experimental data resulted in rather large cross section changes. This weakness of the original EFF-2 file, however, has been recognized in mean time and corrected in the most recent EFF-2 version by using the total cross section from ENDF/B-VI instead of the original evaluation.

2) For all cross sections above 3 MeV our new evaluated cross sections are essentially in agreement with the prior (EFF-2) - evaluation within its uncertainty limits confirming the validity of the EFF-2 uncertainty estimates derived from the dispersion of recent evaluations.

3) The most important improvement of our new evaluation (see Table 1) is certainly the considerable reduction of the uncertainties for the cross sections in energy ranges where accurate measurements exist. For the most important cross sections σ_{tot} and σ_{non} the uncertainties are reduced by about a factor of three to six over the whole energy range up to 14 MeV. Essentially our evaluation procedure is an evaluation of experimental data in the energy regions where such data were measured with a high accuracy, joined smoothly to the theory-based EFF-2 evaluation in those regions where data are lacking.

One might question the rather small uncertainties resulting from our evaluation because of possible correlations between our prior and the added data sets. This objection, however, is not valid firstly because we only admitted experimental data sets which had not been used in the determination of the model parameters for EFF-2, and secondly because the statistical weight of the priors becomes negligible if the added data are of much higher accuracy than the prior, and just this situation exists in these parts of our evaluation with very low uncertainties.

Of course, as is the case with any evaluation of experimental data, the uncertainties of our results could be too small, because of unrealistically low uncertainty estimates given for the data or because of neglect of correlations between different data sets. As discussed in the text we accounted for such effects by increasing the uncertainty components as estimated by the authors in all cases which appeared doubtful to us. Correlations between different data sets were checked and found to be small. Finally our uncertainty estimates are confirmed by the fact that in all evaluations of individual cross sections and in the final joint evaluation chi-square values of about unity were obtained. This is also based on our previous experience with experimental evaluations /8/. We feel that our uncertainties are realistic effective standard deviations at the 1σ confidence level.

We have also compared our results to the recent ENDF/B-VI evaluation /11/. Examples of this comparison are shown in Fig. 8 and 9. In general both evaluations agree within their combined uncertainties. On the average it appears that the uncertainties in ENDF/B-VI have been estimated somewhat too pessimistic.

The energy group structure chosen for our evaluation is appropriate for covariances, but will be too coarse for handling the fine structure of the cross sections in the energy region below E = 3 MeV. Therefore, in constructing the final evaluation data file, the group cross sections are replaced by the results of high-resolution measurements normalized within each energy group to the respective evaluted group cross section. This is done for σ_{tot}, σ_{non} and $\sigma_{n,n1}$.

4. CONCLUSIONS

The results obtained in this paper show that the application of the Bayesian method for updating theoretically evaluated cross sections taken as prior data by experimental data can result in a much improved evaluation. Essentially in all energy regions where accurate data exist, the evaluations are dominated by these data with corresponding reduction of the uncertainties, while at the same time the basic advantages of theory-based evaluations, - completeness and consistency - remain fully conserved. In our case of ^{56}Fe a reduction of about a factor 2 - 6 has been obtained for the most important cross-section uncertainties over extended energy ranges. It is to be expected that similar improvements can be obtained for all materials for which accurate experimental data are available, which mostly are also materials of high importance for applications as other structural materials.

Furthermore our results have confirmed the validity of the recent evaluations EFF-2 and ENDF/B-VI within their stated uncertainties. Thus it appears that a rather qualitative and rough method for generating covariances as used in these evaluations seems to be quite reliable.

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Table 1: Comparison of the group-averaged total cross sections and their uncertainties (given in brackets) from the present evaluation with those from the EFF-2 and ENDF/B-VI libraries.

Group number	E_n (min) [MeV]	Cross Section (in barns) and Standard Deviation (in %) Present	EFF-2	ENDF/B-VI
1	0.85	2.29 (0.6)	3.08 (3.0)	2.30 (3.3)
2	1.00	2.43 (0.5)	3.30 (3.0)	2.48 (3.4)
3	1.20	2.79 (0.5)	3.30 (3.0)	2.88 (3.4)
4	1.40	2.93 (0.5)	3.32 (3.0)	3.00 (3.4)
5	1.60	2.81 (0.5)	3.34 (3.0)	2.85 (3.5)
6	1.80	2.90 (0.5)	3.36 (3.0)	3.01 (3.5)
7	2.00	3.18 (0.5)	3.38 (3.0)	3.23 (3.5)
8	2.20	3.10 (0.5)	3.40 (3.0)	3.07 (3.5)
9	2.40	3.63 (0.5)	3.42 (3.0)	3.64 (3.6)
10	2.60	3.32 (0.5)	3.44 (3.0)	3.33 (3.6)
11	2.80	3.28 (0.4)	3.46 (3.0)	3.28 (3.6)
12	3.00	3.40 (0.4)	3.48 (3.0)	3.46 (3.7)
13	3.50	3.47 (0.4)	3.53 (3.0)	3.49 (3.7)
14	4.00	3.61 (0.4)	3.57 (3.0)	3.67 (3.9)
15	4.50	3.64 (0.5)	3.60 (3.0)	3.72 (3.9)
16	5.00	3.64 (0.5)	3.61 (3.0)	3.69 (3.9)
17	5.50	3.63 (0.5)	3.60 (3.0)	3.67 (3.9)
18	6.00	3.58 (0.5)	3.57 (3.0)	3.64 (3.8)
19	6.50	3.53 (0.5)	3.53 (3.0)	3.62 (3.8)
20	7.00	3.47 (0.5)	3.48 (3.0)	3.55 (3.7)
21	7.50	3.41 (0.5)	3.42 (3.0)	3.49 (3.6)
22	8.00	3.32 (0.5)	3.35 (3.0)	3.40 (3.6)
23	8.50	3.22 (0.5)	3.29 (3.0)	3.27 (3.5)
24	9.00	3.16 (0.5)	3.22 (3.0)	3.24 (3.5)
25	9.50	3.09 (0.5)	3.16 (3.0)	3.16 (3.4)
26	10.0	3.02 (0.5)	3.09 (3.0)	3.09 (3.4)
27	10.5	2.95 (0.6)	3.03 (3.0)	3.02 (3.4)
28	11.0	2.89 (0.6)	2.96 (3.0)	2.95 (3.5)
29	11.5	2.82 (0.7)	2.90 (3.0)	2.87 (3.5)
30	12.0	2.75 (0.6)	2.85 (3.0)	2.78 (3.5)
31	12.5	2.68 (0.6)	2.79 (3.0)	2.72 (3.5)
32	13.0	2.60 (0.5)	2.74 (3.0)	2.68 (3.6)
33	13.5	2.58 (0.5)	2.69 (3.0)	2.62 (3.6)
34	14.0	2.53 (0.6)	2.65 (3.0)	2.57 (3.6)
35	14.5	2.47 (0.8)	2.61 (3.0)	2.52 (3.6)
36	15.0	2.41 (0.8)	2.53 (3.0)	2.45 (3.6)
37	16.0	2.25 (0.7)	2.46 (3.0)	2.37 (3.7)
38	17.0	2.24 (1.6)	2.40 (3.0)	2.31 (3.7)
39	18.0	2.19 (1.1)	2.36 (3.0)	2.28 (3.7)
40	19.0	2.16 (1.1)	2.33 (3.0)	2.25 (3.7)

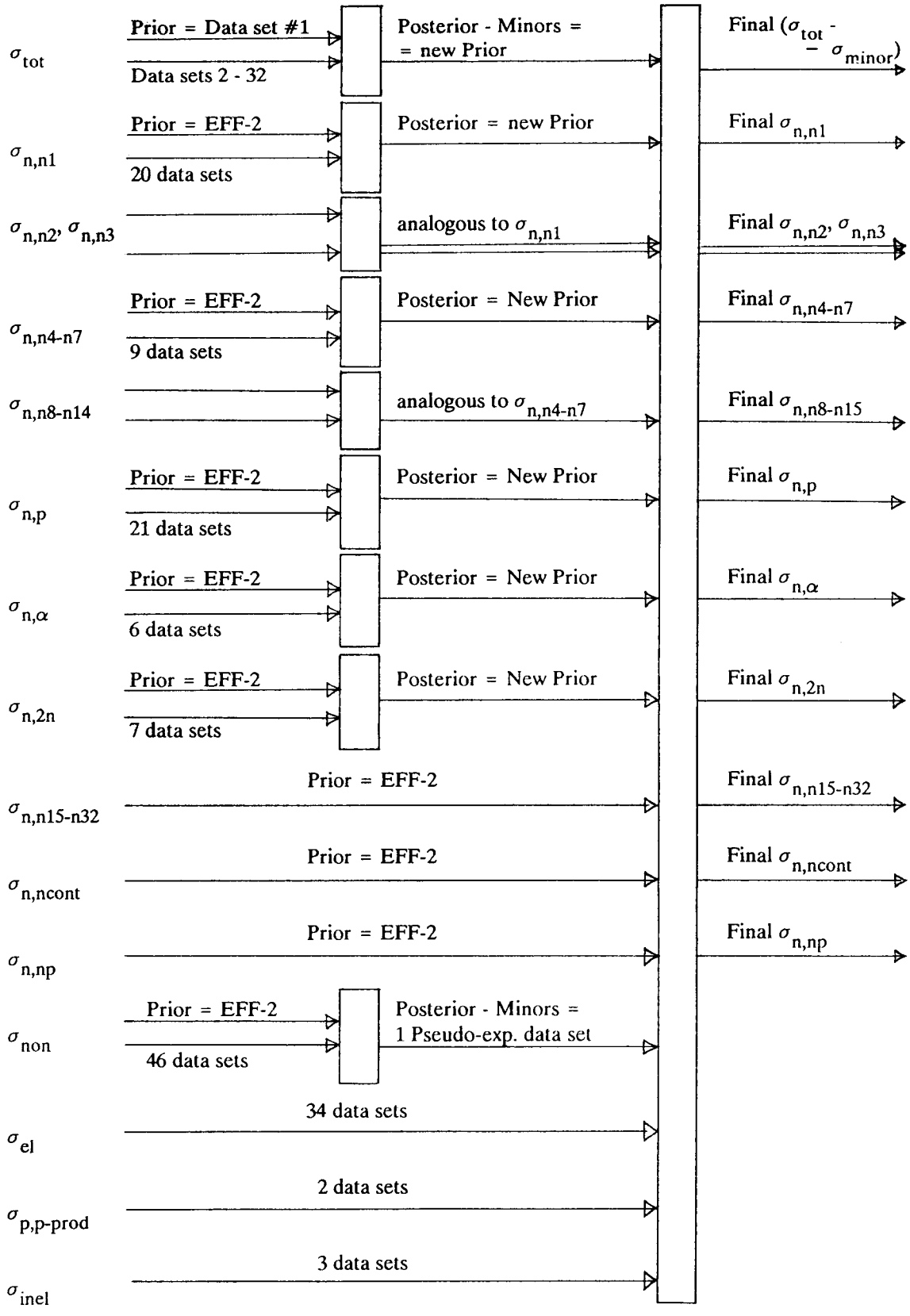
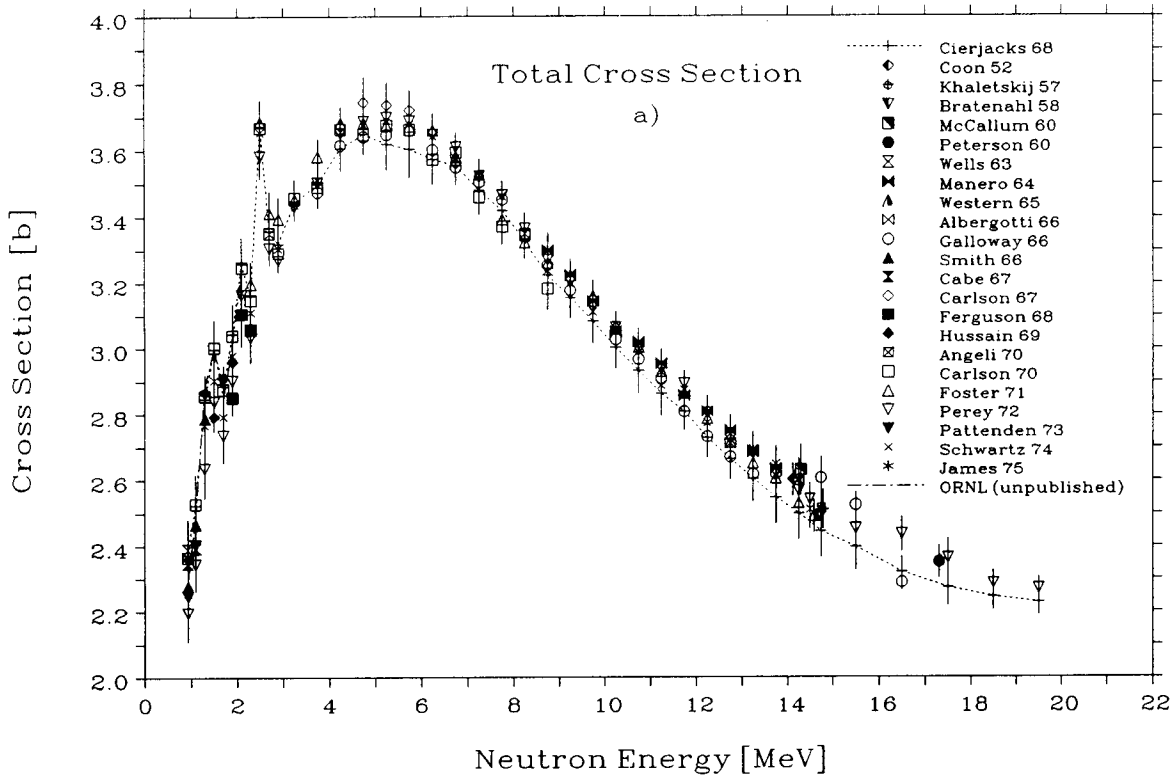


Fig.1: Data processing chart. GLUCS running is shown by the vertical boxes. As the final output we get 12 independent evaluated cross sections and a large covariance matrix including covariances between the basic reaction cross sections. The cross section for total proton production, the nonelastic, the total inelastic and the elastic scattering cross sections are considered as redundant. "Minors" represents the sum of the (n,γ) -, (n,d) -, (n,t) -, (n,^{3}He) - and (n,nα) - reaction cross sections.



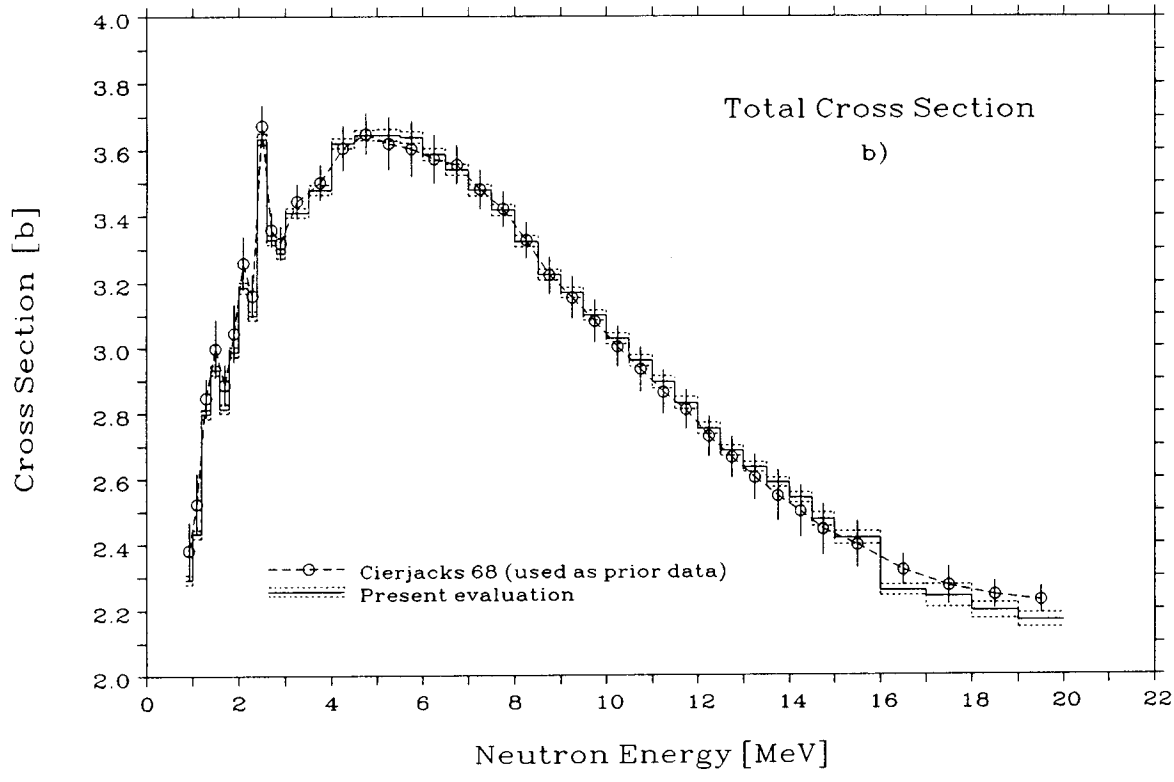


Figure 2: The total cross section of ^{56}Fe:

a) The experimental data base used for the present evaluation. The names of the first authors and the year in which the experimental data were published are given in the legend. The excitation function as measured by Cierjacks et al. /10/ was taken as the prior data set.

b) Comparison of the prior data with the group-averaged cross sections obtained as the final result of the present evaluation.

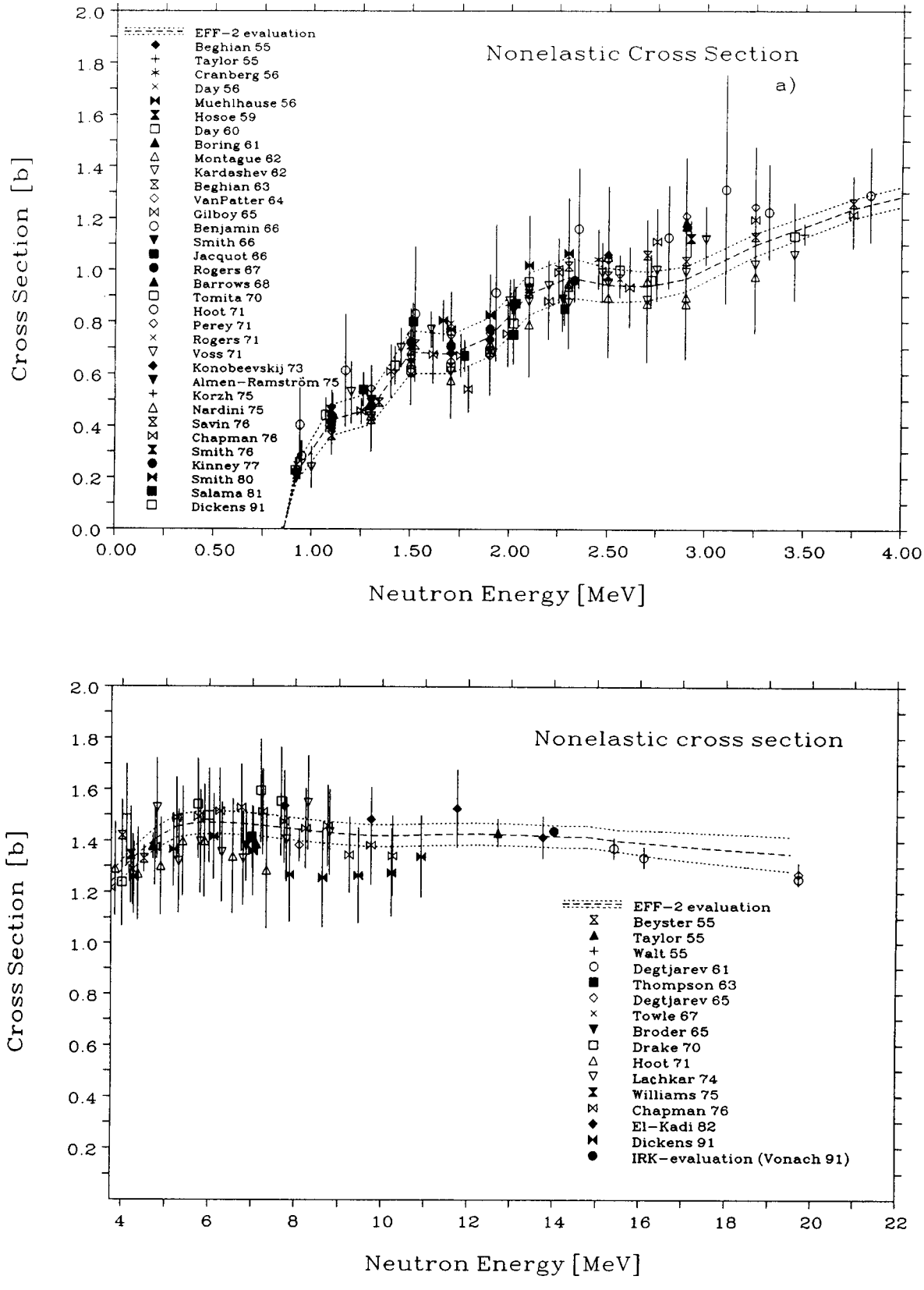


Figure 3 a: The nonelastic cross section of ^{56}Fe:
The experimental data base used for the present evaluation as compared with the excitation function recommended in the EFF-2 evaluation (prior data). For improved legibility the data are displayed separately for the 0 - 4 MeV and the 4 - 20 MeV energy regions.

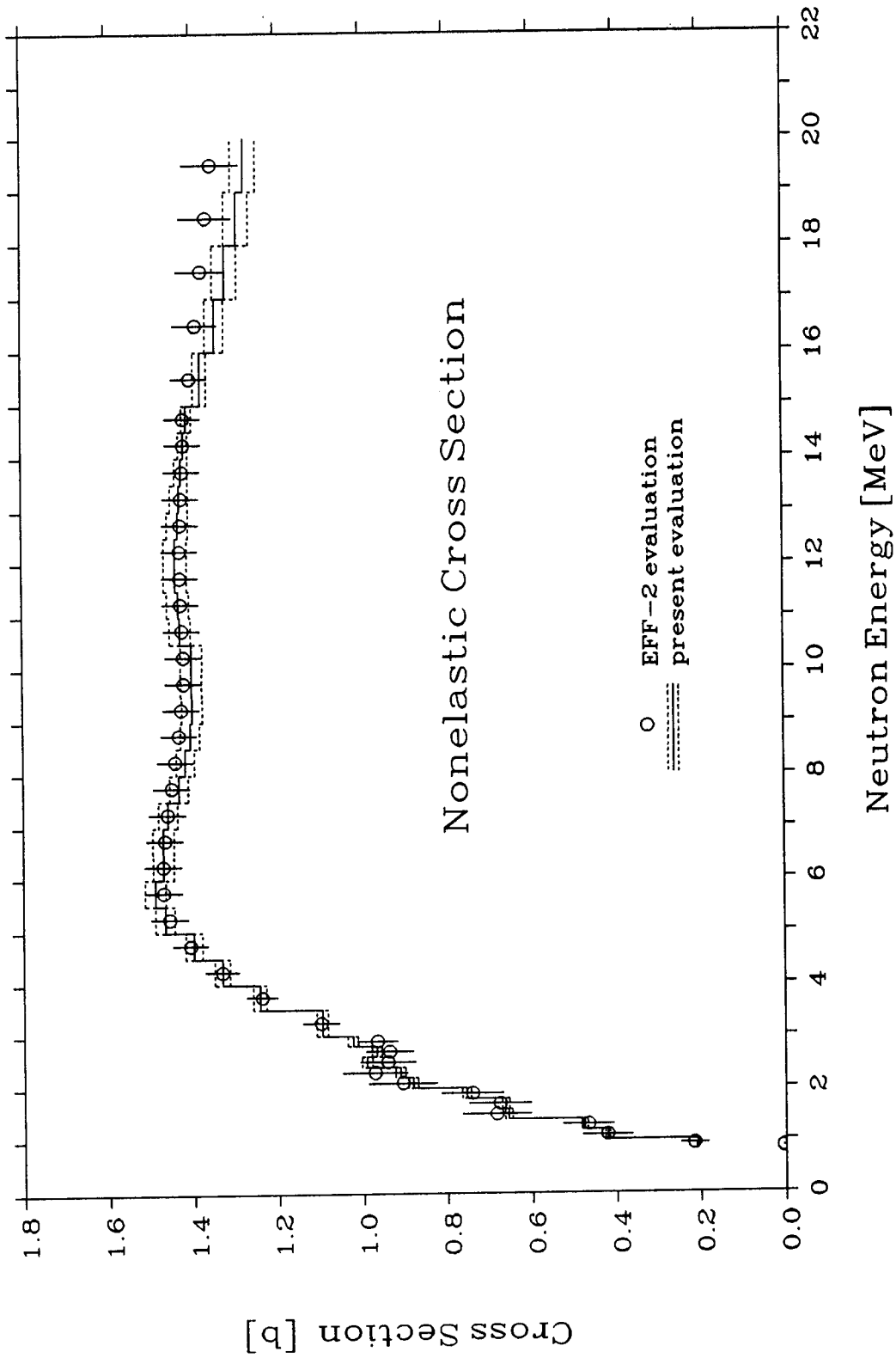


Figure 3 b: The nonelastic cross section of ^{56}Fe: Comparison of the EFF-2 evaluation (prior data) with the group-averaged cross sections obtained as the final result of the present evaluation.

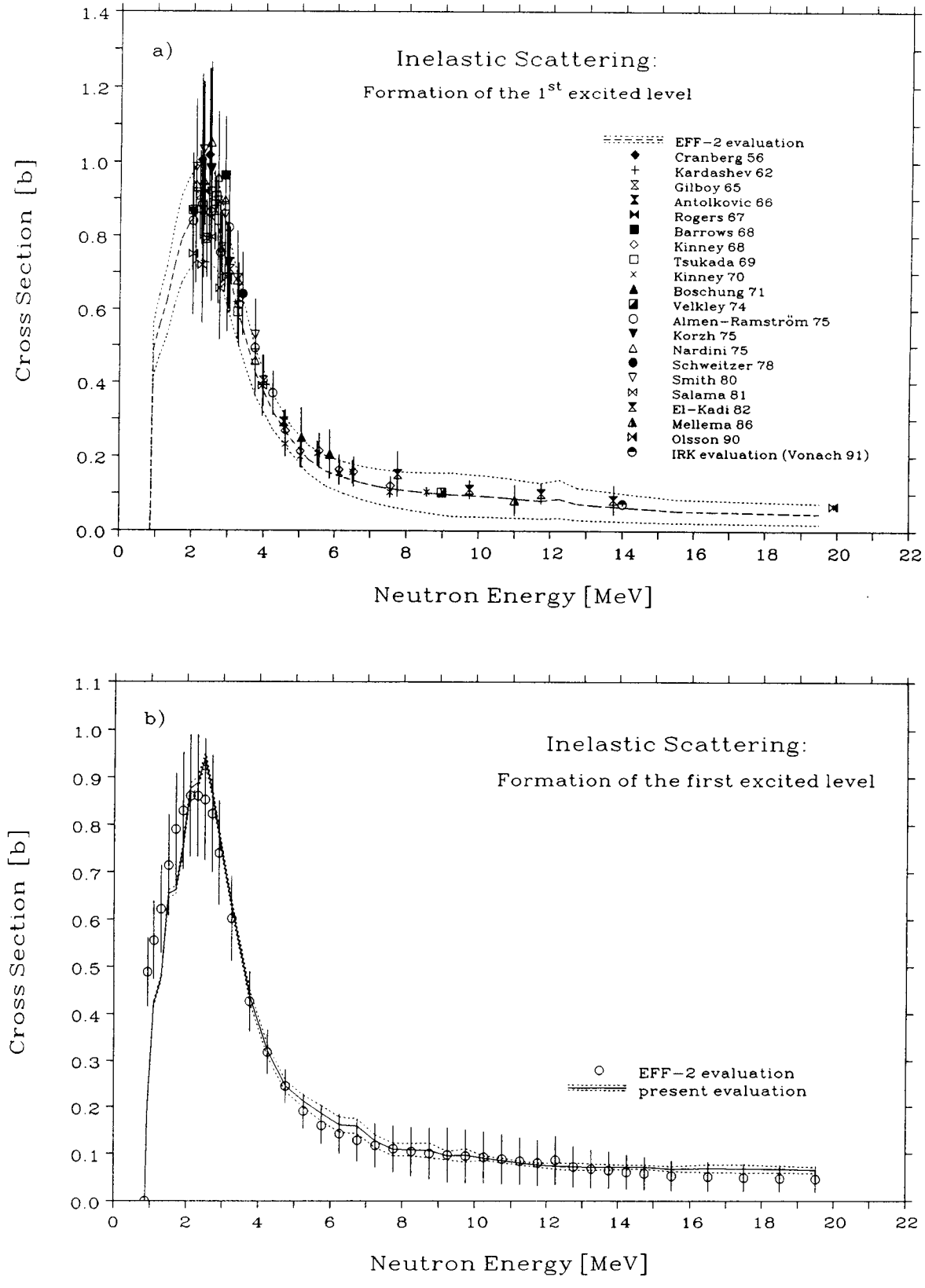


Figure 4: The cross section for the formation of the first excited ^{56}Fe level (E_{lev} = 0.847 MeV) by inelastic neutron scattering:

a) The evaluated cross section from EFF-2 used as prior data and experimental data providing additional information.

b) Comparison of the EFF-2 evaluation with the final results of the present evaluation.

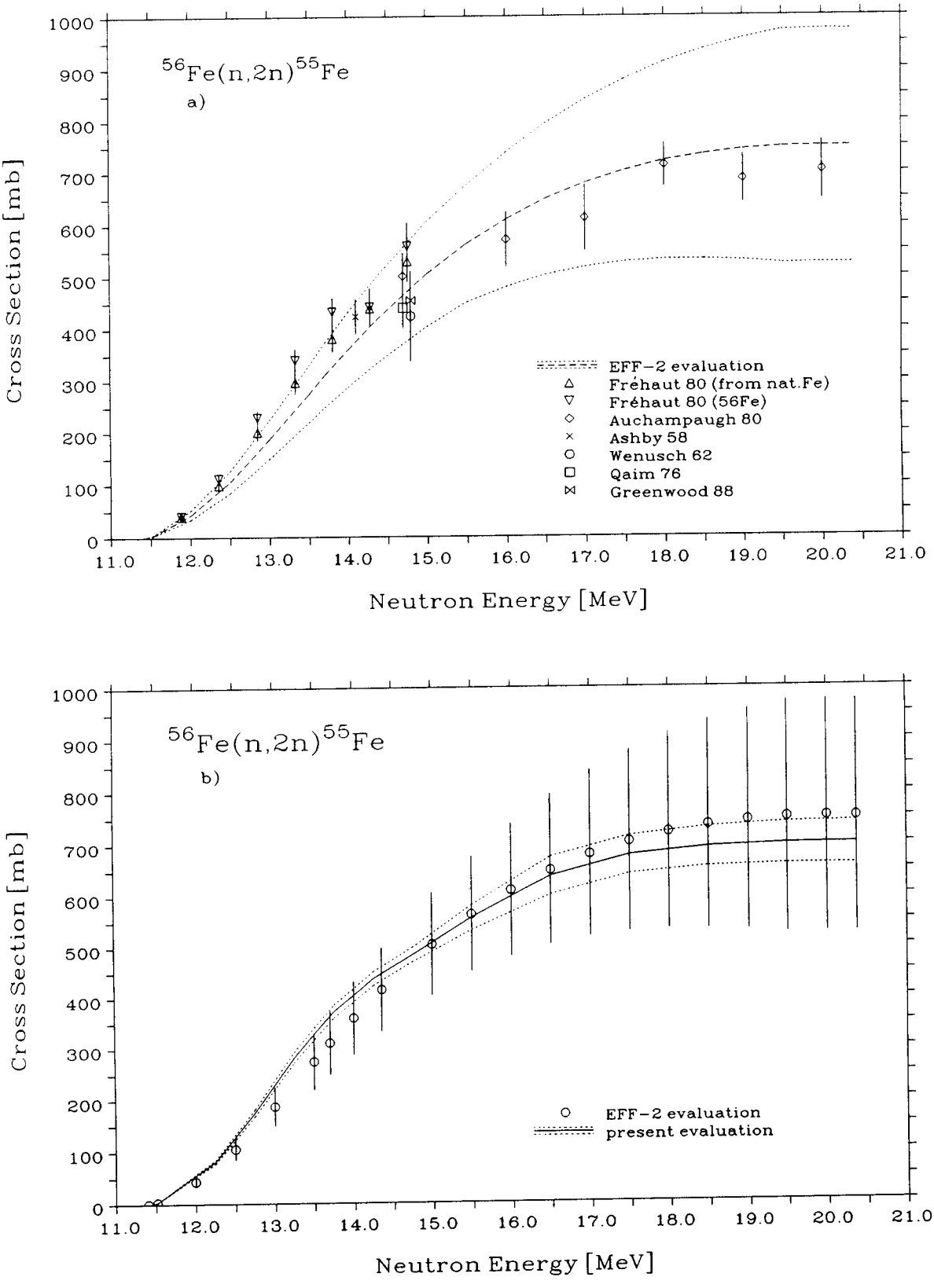


Figure 5: The excitation function for the ^{56}Fe(n,2n)^{55}Fe reaction:

a) The evaluated cross section from EFF-2 taken as prior data and the renormalized experimental data providing additional information.

b) Comparison of the EFF-2 evaluation with the final results of the present evaluation.

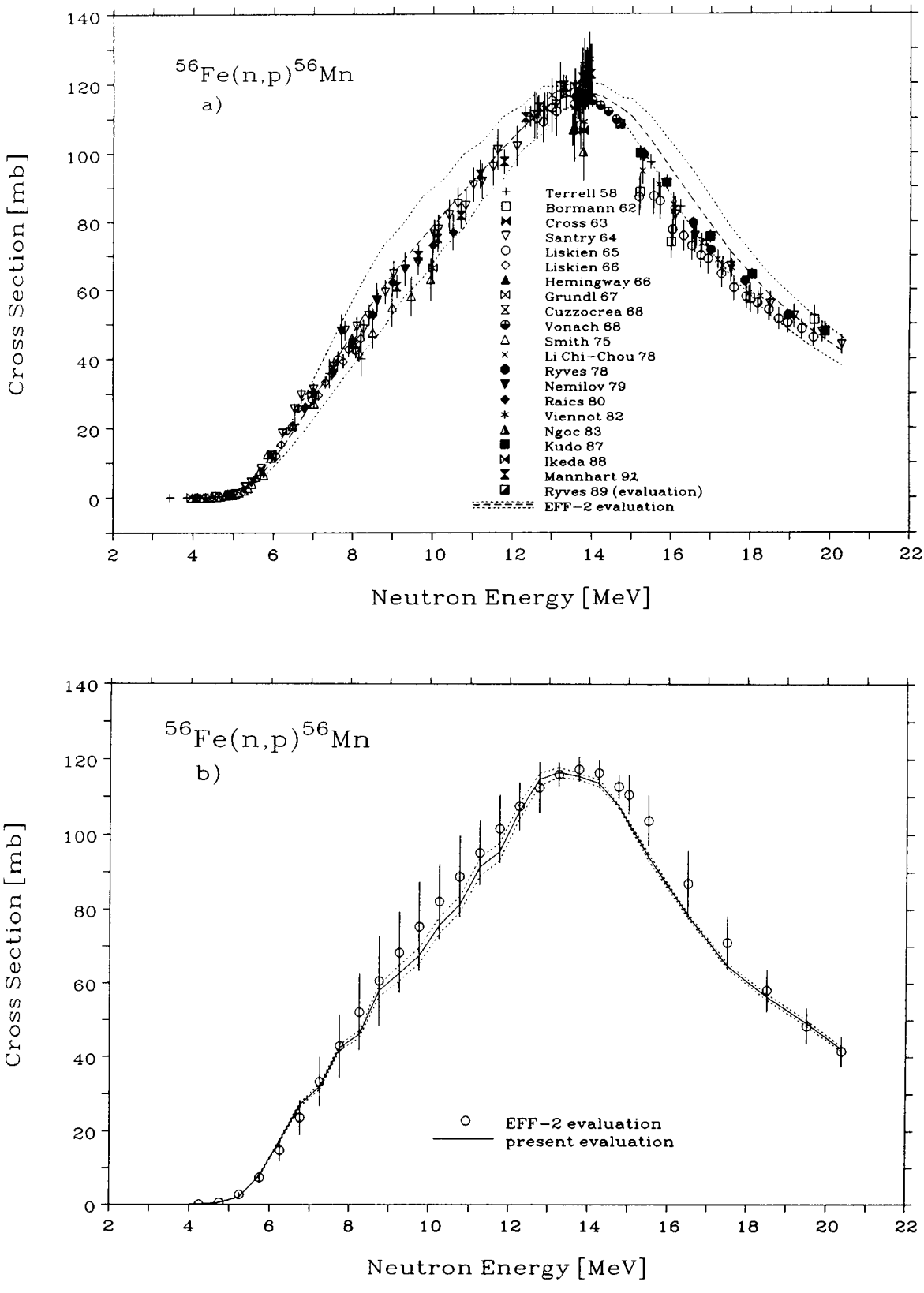


Figure 6: The excitation function for the ^{56}Fe(n,p)^{56}Mn reaction:

a) The evaluated cross section from EFF-2 taken as prior data and renormalized experimental data providing additional information.

b) Comparison of the EFF-2 evaluation with the final results of the present evaluation.

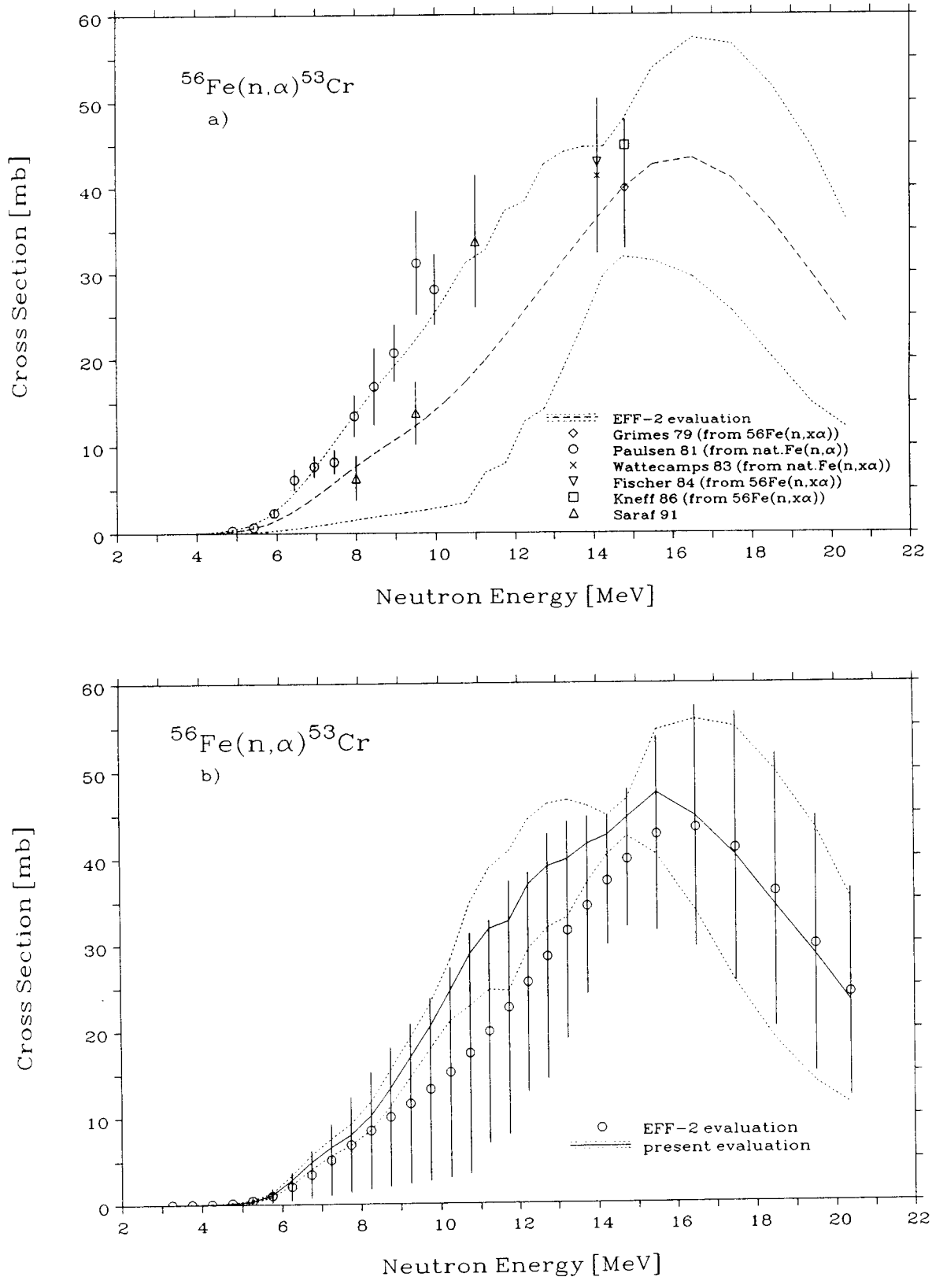


Figure 7: The excitation function for the $^{56}Fe(n,\alpha)^{53}Cr$ reaction:

a) The evaluated cross section from EFF-2 taken as prior data and experimental data providing additional information.

b) Comparison of the EFF-2 evaluation with the final results of the present evaluation.

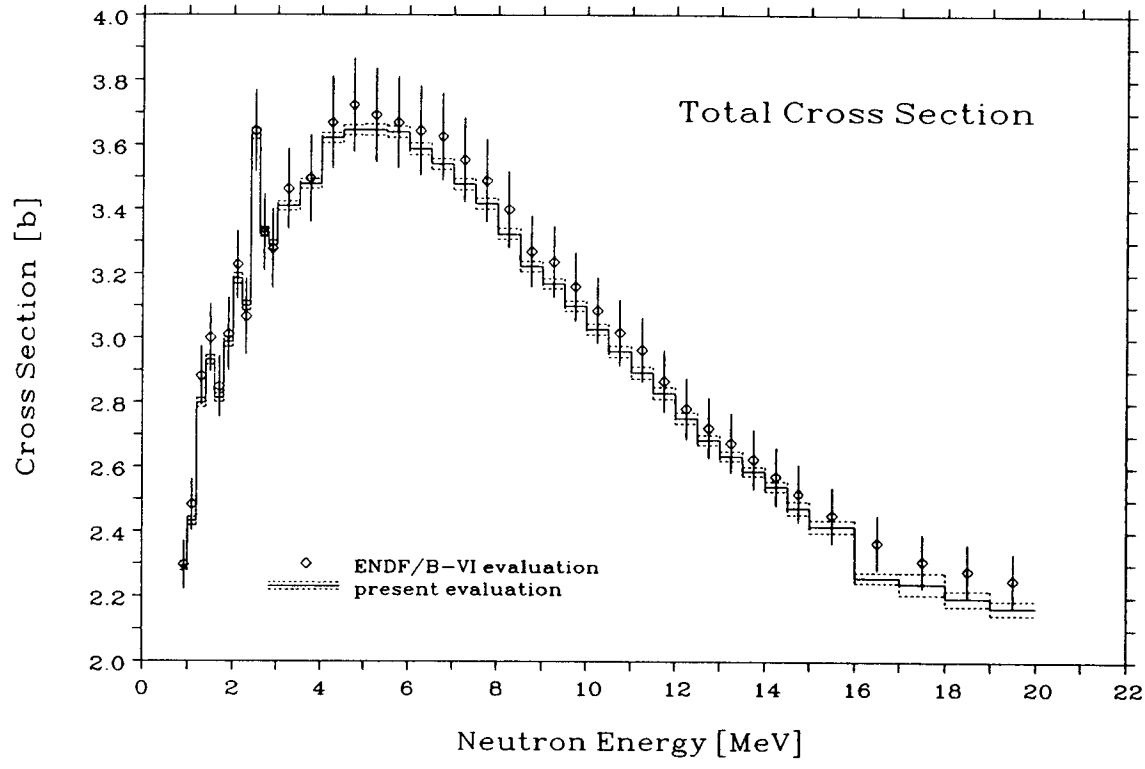


Figure 8: Comparison of the group-averaged total cross sections from the ENDF/B-VI evaluation and those obtained in the present evaluation. The uncertainties are shown by dashed lines and error bars.

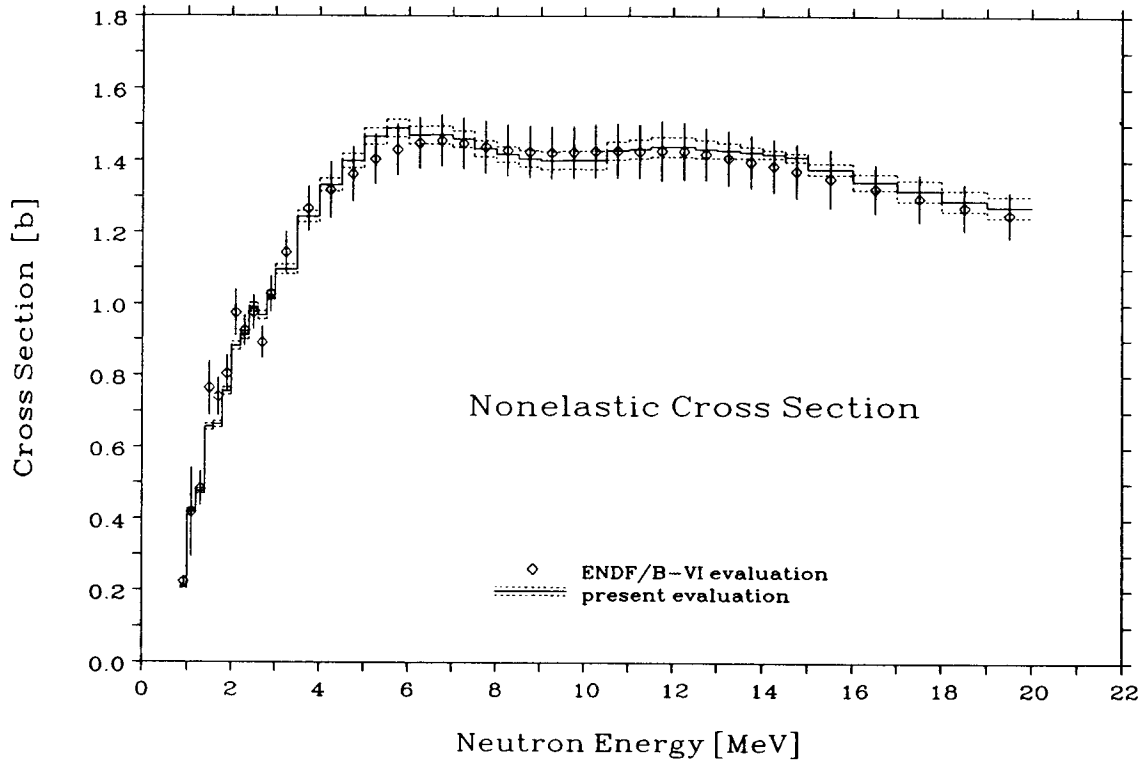


Figure 9: Comparison of the results of the present evaluation with the ENDF/B-VI evaluation for the nonelastic cross section in energy-group presentation.

GENERATION OF COVARIANCE DATA WHILE UPDATING EVALUATED DATA USING 'BAYESIAN' METHODS

W. Mannhart
Physikalisch-Technische Bundesanstalt
W-3300 Braunschweig, Federal Republic of Germany

Abstract:

The basic concept of updating existing evaluations is reviewed. The methodology is demonstrated with numerical examples of an evaluation of experimental data of spectrum-averaged cross sections measured in the neutron field of spontaneous fission of californium-252. The experimental data base comprises direct and ratio measurements, and the handling of both types of data is shown. Attention is given to the generation of covariance data of the individual experimental sets. Procedures for checking the internal consistency of the generated covariances are discussed. Finally, the successive steps of the evaluation procedure are shown and the fundamental limitations of the method and possible ways out of such difficulties are discussed.

1. Introduction

A fundamental point in the data evaluation process is the question of how to combine new data and prior information with statistical methods. This question is strongly linked with how the definition of probability is understood. In conventional statistics, probability has to do with the relative frequency of observed events, and therefore such statistics fail in all cases where there are no observables. To answer the question, a more general concept of the understanding of probability is needed. Such a concept is offered by Bayesian statistics, which understands probability as a numerical description of the state of incomplete knowledge. In this context, estimators can be assigned to all quantities involved in an evaluation process, i.e., Bayesian inference by inductive reasoning allows random variables with corresponding distributions to be assigned to non-random quantities. The estimate of a quantity is completely described by an expectation value and a variance as a measure of the width of the distribution. Many of the general aspects are reviewed in detail in the recent literature [1-4] and the references cited there.

The present work will concentrate upon the application of the Bayesian concept in the evaluation process. Each evaluation process needs a mathematical model which relates observables (data) to parameters. A well-known procedure with such a capacity is the least-squares method. A combination of the conventional least-squares with the Bayesian methodology results in a general least-squares procedure with a great flexibility potential for evaluation purposes.

2. Evaluation with the general least-squares method

We assume an experimental data set of the dimension n, represented by the column vector $\mathbf{D}^0$:

$$\mathbf{D}^0 = (d_1^0, d_2^0, \ldots . d_n^0)^T \qquad (1)$$

The associated uncertainties and correlations are expressed by a (n x n) covariance matrix **V**.

In addition, we assume the existence of a set of parameter estimates, described by the vector **P**,

$$\mathbf{P} = (p_1 , p_2 , \ldots . p_m)^T \qquad (2)$$

with a dimension m and a corresponding covariance matrix **M** of (m x m).

The model for the data fitting is given by:

$$\mathbf{D'} = \mathbf{D} + \mathbf{G} (\mathbf{P'} - \mathbf{P}) \qquad (3)$$

The vector **D** represents arbitrary functions

$$\mathbf{D} = f\ (\ \mathbf{P}\ ) \tag{4}$$

of the vector **P**, and the elements of the matrix **G** are:

$$g_{ij} = \frac{\partial d_i}{\partial p_j} \tag{5}$$

With the definitions of Eqs. (4) and (5), Eq. (3) is the well-known Taylor expansion of a linearization which remains valid only as long as

$$|\ \mathbf{P'} - \mathbf{P}\ | \ll \mathbf{P} \tag{6}$$

is valid. The solution of the fit procedure, a refined parameter vector **P'** , can be obtained by minimizing the expression:

$$\begin{aligned} \chi^2_{MIN} = \quad & (\mathbf{D}^0 - \mathbf{D'})^T\ \mathbf{V}^{-1}\ (\mathbf{D}^0 - \mathbf{D'}) + \\ & + (\mathbf{P} - \mathbf{P'})^T\ \mathbf{M}^{-1}\ (\mathbf{P} - \mathbf{P'}) \end{aligned} \tag{7}$$

The superscript (T) denotes the transpose of a vector (or matrix) and (-1) denotes the inverse of a matrix. The second term of Eq. (7) results from the introduction of the Bayesian concept into the least-squares equations.

The solution of **P'** and the associated covariance matrix **M'** is then given by:

$$\mathbf{P'} = \mathbf{P} + \mathbf{A}\ [\ \mathbf{N} + \mathbf{V}\ ]^{-1}\ (\ \mathbf{D}^0 - \mathbf{D}\ ) \tag{8}$$

and

$$\mathbf{M'} = \mathbf{M} - \mathbf{A}\ [\ \mathbf{N} + \mathbf{V}\ ]^{-1}\ \mathbf{A}^T \tag{9}$$

with the additional definitions of

$$\mathbf{A} = \mathbf{M}\ \mathbf{G}^T \qquad \text{and} \qquad \mathbf{N} = \mathbf{G}\ \mathbf{A} \tag{10}$$

After this short sketch of the general least-squares formalism, it seems worth discussing some aspects of the potential of this method. The essential point is the introduction of quantified prior information with the vector **P** and the matrix **M**. This prior information is treated as experimentally gained information and naturally influences the final result of Eqs. (8) and (9). Even in the case of a linear fitting model, the general form of Eq. (3) is quite useful because it allows the combination of new data with prior information, for example, given by previous evaluations or by other experiments.

In all cases, the condition of Eq. (6) must be fulfilled. This means that the data combination process cannot handle strongly discrepant data, a condition which generally hampers any evaluation success. The formalism shown avoids the classic distinction between data and parameters, regarding both as interchangeable quantities. Another aspect of the conventional least-squares method which requires that the number of parameters must be always smaller

than the number of data, also loses its importance in the general methodology. A small data set $\mathbf{D}^0$ can easily be added to the result of a previous evaluation **P** which strongly exceeds $\mathbf{D}^0$ in size. From Eqs. (8) and (9) it can also be seen that in such cases, the dimension of the matrix to be inverted is that of the additional set of data and not that of the large previous evaluation. To summarize, the general least-squares method allows the combination, in sequential steps, of new data sets $\mathbf{D}^0$ with the results of previous evaluations given by **P** and **M**. In such cases, a side condition must be fulfilled which can be better recognized when we re-write Eq. (7) as:

$$\chi^2_{MIN} = \begin{bmatrix} \mathbf{D}^0 - \mathbf{D}' \\ \mathbf{P} - \mathbf{P}' \end{bmatrix}^T \begin{bmatrix} \mathbf{V} & 0 \\ 0 & \mathbf{M} \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{D}^0 - \mathbf{D}' \\ \mathbf{P} - \mathbf{P}' \end{bmatrix} \qquad (11)$$

This means that Eqs. (8) and (9) are only valid without a correlation between the new data and the prior information. The minimum chi-square value of Eq. (11) does not really depend on the result of the vector **P'**. It can be shown that Eq. (11) is also equivalent to

$$\chi^2_{MIN} = (\mathbf{D}^0 - \mathbf{D})^T [\mathbf{N} + \mathbf{V}]^{-1} (\mathbf{D}^0 - \mathbf{D}), \qquad (12)$$

which means that the final chi-square value can be calculated before the least-squares method is applied to the data.

3. Numerical example

In order to demonstrate the application of the general least-squares method in the evaluation process, a relatively simple example of an evaluation has been chosen, based on the evaluation of experimental spectrum-averaged cross sections measured in the reference neutron field of spontaneous fission of californium-252. The experimental data can be compared with

$$\langle\sigma\rangle = \int_0^\infty \sigma(E)\ N(E)\ dE \qquad (13)$$

N(E) is the spectral distribution of the Cf-252 neutron spectrum and σ (E) is a specific reaction cross section. In a recent evaluation [5,6], knowledge of the Cf-252 neutron spectrum N(E) was established to a high degree of precision and thus the comparison of the experimental data with Eq. (13) is a valuable basis for proving the validity of differential cross section data. Various steps in the present evaluation example have already been published [7-9]. A direct comparison of the older results with the present ones is not possible due to the fact that the previous results reflected various incomplete stages of all the information available today . The present evaluation is performed sequentially and the various data sets are grouped together according to their specific similarities.

The whole evaluation comprises 35 different reaction cross sections, and the experimental data were either direct measurements or ratio measurements. The final result is a "best" set of experimental spectrum-averaged cross sections. With the abbreviation of σ_j for the spectrum-averaged cross section $<\sigma_j>$ of the nuclear reaction j, the parameter vector **P** of Eq. (2) is given by

$$\mathbf{P} = (p_j) = (\sigma_j) \quad j = 1 \ldots 35 \tag{14}$$

The elements of the corresponding data vector of Eq. (4) are:

$$d_i = p_j = \sigma_j \tag{15}$$

for a direct measurement and

$$d_i = p_j \; / \; p_k = \sigma_j \; / \; \sigma_k \tag{16}$$

for a ratio measurement.

The first data set, given in Table 1, comprises 14 data points taken from two similar experiments [10,11]. The number in the second column (NUM) of the table describes the type of nuclear reaction, also given in abbreviated form in the 6th column. These numbers are uniquely connected with those in the first column of Table 6, where the reaction channel is explicitly quoted. The third column (DEN) of Table 1 describes the number (denominator) of the second reaction channel in the case of a ratio measurement. For direct mesurements DEN = 0 is valid. Column 4 gives the experimental value which is either the spectrum-averaged cross section in mb or the measured cross section ratio. The corresponding relative standard deviation of the experimental quantity is given in column 5. The correlation matrix associated with the experimental data set is given in the lower part of each table.

Both of the experiments given in Table 1 were performed at the Physikalisch-Technische Bundesanstalt (PTB) and are direct measurements. The irradiations were done in a 4π geometry, i.e. with the sample material completely surrounding the neutron source. The experimental details are given in the original work and are also summarized elsewhere [7,9]. The high positive correlations of Table 1 are typical of direct measurements with small uncertainty components from counting statistics. The correlations are mainly from the common neutron source strength determination and from the calibration of the radioactivity counting detector. The cross section of the In-115(n,n')In-115m reaction was measured in each experiment and therefore Table 1 contains two values for this cross section. The data given in Table 1 formed the first data vector $\mathbf{D}^0$ (Eq. 1) and the data covariance matrix **V** for the present evaluation. The result of the first step of the evaluation according to Eqs. (8) and (9) is listed in Table 6. While this first step of the evaluation did not require any prior information on the parameter estimates of Eq. (2), such information is needed in the subsequent steps due to the nonlinear relationship of the measured cross section ratios. To keep the influence of the estimated priors on the evaluated result at a minimum, high uncertainties and no correlations were attributed to any artificially introduced priors.

Table 1: Experimental data set no. 1

No.	NUM	DEN	Value	RSD %	Reaction	Ref.
1	4	0	1.006E+0	2.14	AL27A	PTB [10,11]
2	6	0	1.380E+1	2.37	TI46P	
3	7	0	1.890E+1	2.29	TI47P	
4	8	0	4.200E-1	2.54	TI48P	
5	12	0	8.460E+1	2.36	FE54P	
6	13	0	1.450E+0	2.39	FE56P	
7	14	0	1.180E+2	2.35	NI58P	
8	23	0	3.940E+1	2.51	ZN64P	
9	25	0	1.600E+2	2.42	IN113N'	
10	26	0	1.241E+2	2.89	IN115G	
11	27	0	1.980E+2	2.53	IN115N'	
12	27	0	1.950E+2	2.46	IN115N'	
13	29	0	7.620E+1	2.37	AU197G	
14	30	0	5.500E+0	2.59	AU197N2	

Correlation matrix (*100)

I=	J= 1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	100													
2	74	100												
3	77	74	100											
4	69	77	69	100										
5	74	67	70	63	100									
6	74	66	69	62	71	100								
7	75	68	70	63	68	67	100							
8	70	63	66	59	64	63	64	100						
9	73	66	68	61	66	65	66	62	100					
10	61	55	57	51	55	55	55	52	77	100				
11	70	63	65	74	63	62	63	59	66	55	100			
12	71	65	67	60	65	64	65	61	90	75	67	100		
13	74	67	69	62	67	66	68	63	89	75	69	88	100	
14	68	61	64	57	62	61	62	58	82	68	63	80	87	100

For the second and all other steps of the evaluation, the vector **P** and the matrix **M** were equated with **P'** and **M'** of the previously performed step. The second set of data, given in Table 2, consists exclusively of ratio measurements. Such measurements avoid the cumbersome normalization to the absolute neutron fluence at the geometrical position of the sample. In addition, many of the common factors in absolute measurements have a tendency to be cancelled in ratio measurements. This can be clearly seen from the low-valued correlations and anti-correlations given in Table 2. The data of Refs. [8] and [9] were determined with the same experimental procedure and must therefore show correlations. The evaluation result obtained after the inclusion of the data set of Table 2 is again given in Table 6.

The generation of the covariance matrices of the individual experiments has been done with a careful analysis of the various components contributing to the overall uncertainty. These matrices reflect to a high degree the experimental procedure and are essential in any further processing of the data. Particularly in

Table 2: Experimental data set no. 2

No.	NUM	DEN	Value	RSD %	Reaction	Ref.
1	1	14	1.381E-4	3.64	F19N2/NI58P	PTB Antwerp
2	2	4	1.998E+0	2.40	MG24P/AL27A	[8]
3	3	27	2.459E-2	2.45	AL27P/IN115N'	
4	11	14	3.458E-3	2.00	MN55N2/NI58P	
5	16	14	1.424E-2	2.49	CO59P/NI58P	
6	17	14	1.877E-3	1.52	CO59A/NI58P	
7	18	14	3.441E-3	2.19	CO59N2/NI58P	
8	15	14	7.572E-5	3.64	NI58N2/NI58P	
9	19	27	5.328E-2	3.18	CU63G/IN115N'	
10	20	14	5.686E-3	3.00	CU63A/NI58P	
11	21	27	9.390E-4	3.98	CU63N2/IN115N'	
12	24	14	1.873E-3	2.68	ZR90N2/NI58P	
13	9	27	3.266E-3	1.54	V51P/IN115N'	PTB Geesthacht
14	10	14	3.285E-4	2.17	V51A/NI58P	[12]
15	22	14	5.636E-3	2.62	CU65N2/NI58P	
16	23	14	3.486E-1	2.13	ZN64P/NI58P	
17	28	14	1.757E-2	2.58	I127N2/NI58P	
18	31	27	1.511E+0	1.22	HG199N'/IN115N'	

Correlation matrix (*100)

I=	J= 1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	100																	
2	-1	100																
3	-23	0	100															
4	27	-1	4	100														
5	21	0	-12	13	100													
6	18	-1	21	42	27	100												
7	23	-1	0	45	5	27	100											
8	31	0	-23	25	28	16	21	100										
9	23	0	29	6	0	7	5	3	100									
10	23	0	-15	15	51	31	8	33	1	100								
11	27	-1	28	20	3	14	19	11	38	4	100							
12	25	0	-2	39	21	27	29	26	4	20	15	100						
13	3	1	32	5	15	39	4	3	4	18	13	4	100					
14	35	-1	-10	47	58	53	35	38	5	55	16	44	20	100				
15	66	-1	-32	40	29	30	33	40	31	34	36	31	5	53	100			
16	58	0	-40	4	31	6	0	29	33	32	27	10	0	28	81	100		
17	25	-1	-39	34	8	30	30	23	-16	18	-3	21	5	31	39	15	100	
18	-1	0	19	-2	0	4	-2	-1	12	1	10	-2	6	-2	-2	0	12	100

data evaluations, these matrices guarantee the most objective handling of the common components of a whole data set. For such purposes, however, the matrices must be valid and correct. A valid matrix is non-negative definite (either positive definite or semi-definite). This condition is fulfilled when

$$\mathbf{X}^T \mathbf{V} \mathbf{X} \geq 0 \qquad (17)$$

is valid for each possible vector **X**. Before including a covariance matrix **V** into an evaluation, a test of the validity of Eq. (17) is therefore mandatory. A quite useful algorithm for this test is given in Ref. [4], for example. Here the matrix is decomposed into an upper (**T**) and a lower ($\mathbf{T}^T$) triangular matrix with

$$\mathbf{V} = \mathbf{T}^T \mathbf{T} \qquad (18)$$

The elements of **T** can be recursively formed and if none of the diagonal elements of **T** is negative, the non-negative definiteness is confirmed. Each of the matrices given in the present work has successfully passed this test.

The third data set (Table 3) comprises various experiments [13-18], all of which are based on a primary or secondary neutron source strength calibration performed at the National Institute of Technology (formerly NBS). This explains the correlations given between the various experiments. The quoted uncertainties of Ref. [13] were given as double standard deviations. These values were reduced to single standard deviations, but due to strong inconsistencies with other data, they were enlarged again by a constant factor

Table 3: Experimental data set no. 3

No.	NUM	DEN	Value	RSD %	Reaction	Factor	Ref.
1	4	0	1.060E+0	7.36	AL27A	*2.0	NBS-VNC [13]
2	4	0	1.060E+0	7.14	AL27A	*2.0	
3	6	0	1.500E+1	6.54	TI46P	*2.0	
4	7	0	2.020E+1	6.16	TI47P	*2.0	
5	8	0	4.340E-1	8.28	TI48P	*2.0	
6	12	0	9.000E+1	5.76	FE54P	*2.0	
7	14	0	1.188E+2	4.56	NI58P	*2.0	
8	32	0	1.216E+3	1.62	U235F		NBS (revised)
9	34	32	2.681E-1	1.27	U238F/U235F		[14,15]
10	33	32	1.123E+0	1.47	NP237F/U235F		
11	35	32	1.502E+0	0.97	PU239F/U235F		
12	32	0	1.215E+3	1.79	U235F		Knoll [16]
13	35	0	1.790E+3	2.26	PU239F		
14	20	0	7.090E-1	2.40	CU63A		Winkler [17]
15	12	0	8.900E+1	1.83	FE54P		NBS Antwerp
16	14	0	1.210E+2	1.82	NI58P		[18]
17	27	0	1.960E+2	1.94	IN115N'		

Correlation matrix (*100)

I=	J= 1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	100																
2	95	100															
3	49	42	100														
4	52	45	79	100													
5	39	33	59	63	100												
6	46	48	52	55	41	100											
7	71	64	79	84	63	79	100										
8	10	11	12	12	9	13	17	100									
9	0	0	0	0	0	0	0	23	100								
10	0	0	0	0	0	0	0	-7	29	100							
11	0	0	0	0	0	0	0	-9	15	36	100						
12	2	2	2	3	2	3	3	9	0	0	0	100					
13	2	2	2	2	2	2	3	7	0	0	0	59	100				
14	12	13	14	15	11	16	20	31	0	0	0	6	5	100			
15	17	17	18	19	15	21	27	41	0	0	0	8	6	50	100		
16	17	17	18	19	15	21	27	41	0	0	0	8	6	51	91	100	
17	15	16	17	19	14	20	25	39	0	0	0	7	6	47	47	47	100

[9]. The actual value of this factor is shown in Table 3. The evaluated result obtained with the additional inclusion of the data of Table 3 is given in Table 6 as step no. 3.

The data set of Table 4 contains some pecularities. The fission cross section measurements of Refs. [13] and [19] are quoted as direct measurements. A comparison of these data with other experiments [14-16] showed strong discrepancies which exceeded the quoted uncertainties. As discussed in detail in Ref. [7], the original measurements were transformed into ratios to eliminate a suspected, but not fully understood, systematic error in the data. This procedure was only a partial success and in intermediate steps of the evaluation, the uncertainties of the derived ratios of both experimets were enlarged by constant factors. After a revision of the NBS fission cross section measurements [14,15], the previously used factor of 1.5 [9] became obsolete for the ratios of Ref. [19]. However, for the ratios of Ref. [13] the factor could not be eliminated. As shown in Table 3, a common factor of uncertainty enlargement was applied to the non-fission and the fission cross section measurements of Ref. [13] given in Table 4.

The last data set used in the successive evaluation process is given in Table 5. All the data are from a single experiment [21] and are ratio measurements. The uncertainty analysis of this experiment is documented in Ref. [21].

The final result of the evaluation is given in the last two columns of Table 6. The relative standard deviations (RSD) represent only the diagonal elements of the evaluated covariance matrix. The non-negligible off-diagonal elements are shown in the form of a correlation matrix in Table 7. The overall consistency of the evaluation is quite fair. With 70 data points and 35 parameters determined, the value of degrees of freedom is f = 35 and is comparable with the resulting value χ^2 of of 35.3. In previous versions of the evaluation [7-9], the value of

Table 4 Experimental data set no. 4

No.	NUM	DEN	Value	RSD %	Reaction	Factor	Ref.
1	34	32	2.741E-1	1.66	U238F/U235F	*1.0	Adamov [19]
2	33	32	1.139E+0	1.80	NP237F/U235F	*1.0	
3	33	32	1.035E+0	8.48	NP237F/U235F	*2.0	NBS-VNC [13]
4	34	32	2.491E-1	5.22	U238F/U235F	*2.0	
5	14	12	1.326E+0	2.26	NI58P/FE54P		Spiegel [20]

Correlation matrix (*100)

I=	1	2	3	4	5
1	100				
2	39	100			
3	0	0	100		
4	0	0	33	100	
5	0	0	0	0	100

J= 1 2 3 4 5

Table 5: Experimental data set no. 5

No.	NUM	DEN	Value	RSD %	Reaction	Ref.
1	2	27	9.651E-3	4.24	MG24P/IN115N'	Kobayashi
2	3	4	4.797E+0	3.73	AL27P/AL27A	[21]
3	3	4	4.892E+0	4.68	AL27P/AL27A	
4	3	4	4.936E+0	5.58	AL27P/AL27A	
5	5	4	7.296E+1	3.75	S32P/AL27A	
6	5	4	7.098E+1	5.06	S32P/AL27A	
7	9	4	7.058E-1	8.13	V51P/AL27A	
8	12	27	4.361E-1	4.16	FE54P/IN115N'	
9	13	27	7.166E-3	4.02	FE56P/IN115N'	
10	14	4	1.183E+2	2.77	NI58P/AL27A	
11	17	4	2.157E-1	6.17	CO59A/AL27A	
12	23	4	4.145E+1	3.66	ZN64P/AL27A	
13	25	4	1.668E+2	5.56	IN113N'/AL27A	
14	25	27	8.511E-1	4.90	IN113N'/IN115N'	
15	27	4	1.989E+2	4.39	IN115N'/AL27A	
16	30	4	5.219E+0	3.80	AU197N2/AL27A	

Correlation matrix (*100)

I=	J= 1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	100															
2	-7	100														
3	-6	23	100													
4	-5	19	15	100												
5	2	8	19	5	100											
6	2	6	5	45	41	100										
7	-8	15	6	5	2	2	100									
8	26	-4	-3	-2	3	2	-5	100								
9	27	-4	-3	-3	3	2	-5	31	100							
10	-10	16	30	11	32	8	10	-5	-6	100						
11	-4	18	5	5	6	4	10	-2	-1	9	100					
12	-2	28	8	6	9	7	13	0	0	13	17	100				
13	-10	10	8	44	3	44	8	-6	-6	14	6	6	100			
14	21	0	0	0	0	0	-1	16	16	-1	0	0	10	100		
15	-31	13	11	56	4	55	10	-25	-26	18	8	8	62	-15	100	
16	-15	32	11	10	5	4	21	-9	-9	20	21	28	15	-1	21	100

χ^2/f exceeded unity and in consequence the final uncertainties of the whole evaluation were scaled up. In the present work, a scaling was only applied to the data of a single experiment [13], giving some controversial results.

4. Some final remarks

The χ^2 value of the evaluation is the sum of the individual components calculated according to Eq. (12) in the sequential steps. In each of the steps of Table 6, the number of data is less than the number of parameters and therefore the well-known relation for the calculation of the number of degrees of freedom of

$$f = (\text{number of data}) - (\text{number of parameters})$$

Table 6: Result of the sequential steps of the evaluation

ID	Reaction	Step no. 1 <Sigma> mb	Step no. 1 RSD %	Step no. 2 <Sigma> mb	Step no. 2 RSD %	Step no. 3 <Sigma> mb	Step no. 3 RSD %	Step no.4 <Sigma> mb	Step no.4 RSD %	Step no. 5 <Sigma> mb	Step no. 5 RSD %
1	F-19(n,2n)			1.580E-2	3.85	1.607E-2	3.45	1.606E-2	3.45	1.613E-2	3.40
2	Mg-24(n,p)			2.010E+0	3.14	2.043E+0	2.78	2.042E+0	2.78	1.998E+0	2.42
3	Al-27(n,p)			4.879E+0	3.21	4.875E+0	2.69	4.873E+0	2.69	4.885E+0	2.14
4	Al-27(n,a)	1.006E+0	2.12	1.006E+0	2.10	1.023E+0	1.52	1.023E+0	1.52	1.017E+0	1.47
5	S-32(n,p)									7.262E+1	3.50
6	Ti-46(n,p)	1.380E+1	2.35	1.380E+1	2.33	1.411E+1	1.76	1.410E+1	1.76	1.409E+1	1.76
7	Ti-47(n,p)	1.890E+1	2.27	1.891E+1	2.25	1.932E+1	1.66	1.932E+1	1.66	1.929E+1	1.66
8	Ti-48(n,p)	4.184E-1	2.48	4.185E-1	2.46	4.251E-1	1.89	4.250E-1	1.89	4.251E-1	1.89
9	V-51(n,p)			6.414E-1	2.69	6.463E-1	2.05	6.461E-1	2.05	6.493E-1	1.95
10	V-51(n,a)			3.821E-2	3.02	3.901E-2	2.23	3.899E-2	2.23	3.904E-2	2.22
11	Mn-55(n,2n)			4.045E-1	3.00	4.081E-1	2.35	4.078E-1	2.35	4.079E-1	2.34
12	Fe-54(n,p)	8.460E+1	2.34	8.463E+1	2.32	8.683E+1	1.36	8.692E+1	1.35	8.692E+1	1.34
13	Fe-56(n,p)	1.450E+0	2.37	1.451E+0	2.35	1.474E+0	1.84	1.474E+0	1.84	1.466E+0	1.77
14	Ni-58(n,p)	1.180E+2	2.33	1.171E+2	2.25	1.177E+2	1.31	1.176E+2	1.31	1.176E+2	1.30
15	Ni-58(n,2n)			8.766E-3	4.15	8.951E-3	3.62	8.947E-3	3.62	8.961E-3	3.59
16	Co-59(n,p)			1.653E+0	3.24	1.690E+0	2.50	1.689E+0	2.50	1.692E+0	2.49
17	Co-59(n,a)			2.196E-1	2.66	2.220E-1	1.92	2.219E-1	1.92	2.220E-1	1.86
18	Co-59(n,2n)			4.028E-1	3.14	4.058E-1	2.53	4.055E-1	2.53	4.055E-1	2.52
19	Cu-63(n,g)			1.035E+1	3.83	1.039E+1	3.39	1.039E+1	3.39	1.045E+1	3.24
20	Cu-63(n,a)			6.587E-1	3.69	6.886E-1	1.99	6.883E-1	1.99	6.893E-1	1.98
21	Cu-63(n,2n)			1.823E-1	4.51	1.834E-1	4.14	1.834E-1	4.14	1.845E-1	3.98
22	Cu-65(n,2n)			6.449E-1	2.84	6.561E-1	2.30	6.558E-1	2.30	6.587E-1	2.24
23	Zn-64(n,p)	3.940E+1	2.49	3.989E+1	2.30	4.047E+1	1.71	4.045E+1	1.72	4.063E+1	1.64
24	Zr-90(n,2n)			2.187E-1	3.47	2.213E-1	2.91	2.212E-1	2.91	2.212E-1	2.90
25	In-113(n,n')	1.608E+2	2.31	1.608E+2	2.29	1.620E+2	1.61	1.620E+2	1.61	1.622E+2	1.57
26	In-115(n,g)	1.247E+2	2.79	1.247E+2	2.77	1.257E+2	2.25	1.256E+2	2.25	1.257E+2	2.23
27	In-115(n,n')	1.963E+2	2.26	1.964E+2	2.23	1.972E+2	1.41	1.971E+2	1.41	1.976E+2	1.37
28	I-127(n,2n)			2.048E+0	3.38	2.072E+0	2.83	2.070E+0	2.83	2.071E+0	2.75
29	Au-197(n,g)	7.647E+1	2.30	7.648E+1	2.28	7.704E+1	1.62	7.702E+1	1.62	7.686E+1	1.59
30	Au-197(n,2n)	5.519E+0	2.52	5.521E+0	2.50	5.565E+0	1.92	5.564E+0	1.92	5.511E+0	1.83
31	Hg-199(n,n')			2.968E+2	2.53	2.980E+2	1.85	2.979E+2	1.85	2.986E+2	1.80
32	U-235(n,f)					1.209E+3	1.21	1.210E+3	1.20	1.210E+3	1.20
33	Np-237(n,f)					1.355E+3	1.81	1.361E+3	1.58	1.361E+3	1.58
34	U-238(n,f)					3.238E+2	1.86	3.256E+2	1.63	3.257E+2	1.63
35	Pu-239(n,f)					1.809E+3	1.39	1.812E+3	1.37	1.812E+3	1.37

Table 7: Correlation matrix of the last step of the evaluation

Correlation matrix (*100)

I=	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	100																	
2	17	100																
3	15	29	100															
4	30	56	46	100														
5	12	24	22	34	100													
6	24	34	35	58	23	100												
7	26	37	38	62	25	60	100											
8	22	31	35	52	21	66	54	100										
9	22	30	55	46	20	37	39	38	100									
10	39	24	28	41	18	34	37	31	38	100								
11	40	24	30	40	18	33	36	30	27	62	100							
12	31	42	46	69	30	57	61	52	45	48	48	100						
13	24	36	36	59	25	47	51	44	38	34	33	59	100					
14	33	44	49	73	32	61	66	56	47	52	54	88	60	100				
15	29	15	9	25	11	21	23	20	19	39	36	29	21	32	100			
16	21	22	24	37	16	30	33	28	32	60	31	42	30	46	28	100		
17	34	29	45	50	22	41	44	37	50	65	60	58	41	66	29	43	100	
18	37	22	25	37	16	31	33	28	26	53	59	45	30	50	33	25	50	100
19	24	20	48	31	14	24	26	24	27	18	19	27	25	27	11	10	21	19
20	24	27	30	44	19	36	39	34	40	53	35	51	37	54	31	48	48	31
21	29	15	42	25	11	19	21	20	28	24	28	22	20	22	17	10	22	28
22	59	26	23	45	19	37	40	34	34	63	63	46	37	49	40	31	55	57
23	48	36	29	60	25	49	53	45	40	43	37	62	49	66	30	40	46	33
24	33	19	23	32	14	27	29	24	22	54	51	38	26	42	32	32	44	43
25	26	39	48	62	25	49	52	49	54	36	34	60	50	62	23	33	42	32
26	18	27	33	43	17	34	37	35	38	26	24	42	36	44	16	23	30	22
27	28	42	57	66	27	53	57	56	67	41	38	66	55	69	26	37	46	35
28	31	19	3	33	13	28	30	26	29	44	50	40	28	44	28	20	51	46
29	26	37	47	61	24	49	52	47	52	36	34	59	49	62	23	32	42	32
30	23	33	42	54	21	42	47	41	46	32	31	53	44	55	20	29	38	28
31	21	32	51	50	21	40	43	42	52	29	27	50	42	52	20	27	36	25
32	11	16	19	25	11	21	22	20	21	18	17	31	21	31	11	16	21	16
33	9	12	14	19	8	16	17	15	16	14	13	23	16	24	8	12	16	12
34	8	10	13	17	7	14	15	14	14	12	12	20	14	21	8	11	14	11
35	10	13	16	22	9	18	19	17	18	16	15	26	18	27	10	14	18	14

(continued)

I=19	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35
19	100																
20	17	100															
21	39	15	100														
22	36	38	42	100													
23	41	45	34	73	100												
24	15	31	22	46	31	100											
25	33	41	27	39	52	28	100										
26	23	29	19	28	36	19	59	100									
27	41	48	32	43	57	31	78	55	100								
28	2	31	11	52	32	34	30	21	35	100							
29	33	41	26	39	51	28	76	55	76	30	100						
30	29	36	24	35	46	25	67	46	66	26	75	100					
31	36	37	29	32	44	22	59	41	75	36	57	50	100				
32	12	22	10	17	23	14	25	18	30	15	25	22	23	100			
33	9	16	7	13	17	10	19	13	23	11	19	16	17	71	100		
34	8	15	6	12	15	9	17	12	20	10	17	15	15	80	71	100	
35	10	19	8	15	20	12	22	15	26	13	22	19	20	79	67	69	100

fails. The valid value of f is obtained by replacing the expression "number of parameters" with "number of newly determined parameters". Newly determined parameters are those which have no predecessor in the evaluation. With this definition, it can be seen from Table 6, for example, that the number of parameters is 4, 0 and 1 for the steps no. 3 to 5 in the present evaluation.

The data used in the present evaluation were grouped in such a way that the zero correlation between **V** and **M** of Eq. (11) was always fulfilled. For the correlation of a new data set with a previous data set already included in the evaluation, a more general form of Eq. (11) is required. This can be done by replacing the middle term of Eq. (11) with

$$\begin{bmatrix} \mathbf{V} & \mathbf{C}^T \\ \mathbf{C} & \mathbf{M} \end{bmatrix}^{-1} \tag{19}$$

Due to the different dimensions of the matrices **V** and **M**, the matrix **C** describing the additional correlations is always a rectangular one. The minimalization of Eq. (11) with the term of Eq. (19) gives new equations for **P'** and **M'** which differ from Eqs. (8) and (9). However, the practical use of this modification is limited. In most cases, such an additional correlation concerns only a specific data set of the previous evaluation. The matrix **M**, however, represents the whole previous evaluation and thus the quantification of the matrix **C** becomes a difficult task. This means that it usually cannot be circumvented to repeat the whole evaluation to take previously unconsidered correlations into account. One thing which can be done to counter this disadvantage is to store the results of the sequential evaluation steps. This allows that part of the evaluation which is unimpaired by the new correlations to be conserved.

A final question which has to be answered is whether the evaluation result depends on the procedure. Instead of sequentially adding the data sets of Tables 1 to 5 to the evaluation, an alternative would be to do the whole evaluation in one run. The data vector $\mathbf{D}^0$ is then given by

$$\mathbf{D}^0 = (\mathbf{D}_1^0, \mathbf{D}_2^0, \mathbf{D}_3^0, \mathbf{D}_4^0, \mathbf{D}_5^0) \tag{20}$$

and the data covariance matrix is

$$\mathbf{V} = \begin{bmatrix} \mathbf{V}_1 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{V}_2 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{V}_3 & 0 & 0 \\ 0 & 0 & 0 & \mathbf{V}_4 & 0 \\ 0 & 0 & 0 & 0 & \mathbf{V}_5 \end{bmatrix} \tag{21}$$

$\mathbf{D}_i^0$ and $\mathbf{V}_i$ are the data sets given in Tables 1-5. When the same parameter estimate vector **P** and the same matrix **M**, as in the previous evaluation are used, the result then obtained from Eqs. (20) and (21) is different from that of step no. 5 of Table 6. The differences are small but they exist. At first glance

this result is surprising, but can easily be understood if one considers what has really been done. In the evaluation performed with the arrangement of Eqs. (20) and (21), the vector of the parameter estimates **P** is frozen for the whole evaluation. At the very beginning of the evaluation this vector contains only rough estimates of the final parameters with large uncorrelated uncertainties. In the sequential procedure of Table 6, knowledge of **P** is improved and refined step by step with the information resulting from the additional experiments. Thus in the context of "Bayesian learning", sequential evaluation is the better way to obtain a reasonable final result.

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APPROXIMATE METHODS FOR GENERATION OF COVARIANCE DATA FOR THE STRUCTURAL MATERIALS OF ENDF/B-VI

D. M. Hetrick, D. C. Larson, and C. Y. Fu
Oak Ridge National Laboratory
Oak Ridge, Tennessee, USA

ABSTRACT

The considerations that governed the development of cross section uncertainty files for the isotopes of Cr, Fe, Ni, Cu, and Pb in ENDF/B-VI are summarized. Four different approaches were used in providing the uncertainty information. Illustrative examples are given which show the resulting standard deviations as a function of incident energy and the corresponding correlation matrices.

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1. INTRODUCTION

Covariance data are required to assess uncertainties in design parameters of fusion reactors and to refine the use of nuclear data in reactor applications. The considerations which governed the development of the uncertainty files for the stable isotopes of Cr, Fe, Ni, Cu, and Pb in ENDF/B-VI are described in this paper. References to experimental data sets used in the evaluations were obtained primarily from CINDA but also from the literature. For each isotope, extensive model calculations were performed with the goal of simultaneously reproducing experimental data for all reaction channels with one set of parameters. The energy distributions of all product particles, including gamma-rays and heavy recoils, were given for each reaction in order to conserve energy within that reaction. The calculated cross sections for each reaction may be adopted for the evaluation, or individually adjusted, or replaced by those based on least-squares fit to experimental data, without disturbing the energy balance which is done following the choice of cross section values.

Four different approaches used in providing the uncertainty information, consistent with the above methods of cross-section evaluation, are reviewed. They are based on: (1) "Bayesian" analyses, (2) the scatter among data sets, (3) magnitudes of calculated cross sections if data are unavailable, and (4) derivations from covariance files for other reaction types when the cross sections themselves were obtained by additions and subtractions. Examples are given which show the standard deviations as a function of incident energy and the corresponding correlation matrices.

2. METHODS

Covariances are provided for all reaction cross sections given in file MF=3, including inelastic scattering (levels and continuum). At present, no covariance information is given for energy-angle distributions included in the evaluations (files MF=4 and 6), nor for resonance parameters or gamma-ray production. Four different approaches were used in providing covariance information, depending upon the quantity and quality of available experimental data.

In the first approach, when sufficient cross section data were available for a reaction (such as for the (n,p) reaction in ^{54}Fe, ^{56}Fe, and ^{58}Ni, the (n,2n) reaction for ^{63}Cu and ^{65}Cu, and the (n,a) reaction for ^{63}Cu), a Bayesian analysis using the GLUCS code[1] was done, using ENDF/B-V as the prior. GLUCS provides updated cross sections and covariances in ENDF/B-VI format. This method is the most rigorous of the four approaches used. Secondly, if insufficient data were available for a GLUCS analysis on a reaction, the scatter among cross section values in data sets selected for evaluation was estimated and used to construct the covariance file. For the third method, if the evaluated cross section depended primarily on TNG calculations,[2,3,4] uncertainties were assigned as shown in Table 1 in order to construct a covariance file.

Table 1. Assigned uncertainties for calculated cross sections.

Cross Section X (mb)	Standard Deviation
500 < X	10%
100 < X <500	15%
30 < X <100	20%
X < 30	>30%

This approach assumes that nuclear model codes are more reliable in their predictions for reactions which have large cross sections than for reactions which have small cross sections. A fourth approach was to describe the covariances in energy ranges where the cross sections in file MF=3 can be derived in terms of other evaluated cross sections in the same energy range for

which covariances are available. For example, this approach is often done to insure that correct correlations are obtained when the relatively large elastic and nonelastic uncertainties must be combined to be consistent with the relatively smaller uncertainties of the total cross section. Due to time constraints, methods that consider uncertainties of model parameters (e.g., see Kanda and Uenohara[5], Zhao et al.[6]) were not used for the present evaluations.

For most reactions the following algorithm was used to construct the covariance file, starting with the second and third approaches described above. Short-range (i.e., small energy intervals - typically 2 to 4 MeV) correlations using fractional components correlated within each energy interval were assembled using the "NI type" LB=1 sub-subsection in File 33.[7] The fractional components were assigned using either available data uncertainties from measurements or the assigned uncertainties listed in Table 1. The energy range of the correlation was based on experimental information, if available, or evaluator judgement. The short-range correlations were used to relay information primarily on the perceived uncertainty in the shape of the cross sections. An absolute component for the whole energy range from threshold to 20 MeV was included using the "NI type" LB=0 sub-subsection in File 33 if the reaction has cross section values varying with energy by orders of magnitude, such as often occur at total cross section minima, near thresholds, or at high incident energies. Typically, this absolute component was taken as a percentage of the smallest cross section value in the file for the reaction. For example, for ^{56}Fe, this percentage varied from 5% for reactions with "large" minimum cross sections to over 100% for reactions with very small minimum cross sections ($<<$ 1 mb). This component provides appropriately larger uncertainties for the smallest cross section values.

For the total (MT=1), nonelastic (MT=3), and capture (MT=102) cross sections, long-range (i.e., large energy intervals - typically 1 to 3 intervals from threshold to 20 MeV) correlations taken from available data (e.g., normalization effects, boundaries between different data sets, etc.) were assembled using the LB=1 sub-subsection. Long-range correlations were used to relay information about uncertainty in the absolute normalization of the whole cross-section curve within the range. If experimental information was unavailable, the short-range uncertainties were compiled first and the long-range covariance component (one energy interval from threshold to 20 MeV) was estimated by using one-half of the minimum value of the short-range components. The short range covariances were then divided by two to compensate for the effective removal of the estimated long-range correlations. It was desirable to have long-range correlations when no experimental information was available, and experience with measured data led to this method of estimating the long-range uncertainties from the assigned short-range uncertainties.

The required LB=8 sub-subsection[8] was derived from the resulting short-range correlations. A fraction F from the short-range covariance component (for each energy interval) was multiplied by the square of the cross section for the appropriate energy interval (from file MF=3) for inclusion into the LB=8 sub-subsection format. The resulting short-range values were then finalized by taking (1-F) times the initial short-range components. After testing this algorithm extensively by comparing results from this ad-hoc method to calculations from the GLUCS code[9] , the fraction F chosen for the method was 0.01 for the total, elastic, nonelastic, and capture cross sections and 0.10 for all other reactions. The smaller fraction was used for the total, elastic, nonelastic, and capture because of problems caused by small energy intervals and resulting discontinuities in the cross section file (see Hetrick et al.[10]).

The covariances for portions of the total, elastic, and nonelastic reactions are derived using the "NC type" sub-subsections.[7] A combination of explicit and derived uncertainties were used. The uncertainties for the total inelastic cross section (MT=4) were totally derived. Derived is used here in the context that cross sections for a reaction type (and therefore its covariances) may be determined by summing those for other reaction types. Note that for all reaction types with MT greater than four, only explicit uncertainties were used.

The scheme described below was used, consistent with the following considerations, to obtain uncertainty files for MT=1,2,3, and 4:

a. The total cross-section (MT=1) uncertainties are generally well known at thermal, in the resonance region, and up to 20 MeV.

b. The elastic-scattering cross-section (MT=2) uncertainties are generally well known at thermal and in the resolved resonance region, but not from the end of the resolved resonance region to several MeV due to structure which occurs as a result of obtaining the elastic cross section as the difference between the total and nonelastic cross sections.

c. The nonelastic cross-section (MT=3) uncertainties up to the threshold of the first reaction are generally given by the uncertainties for the capture cross section, and above the threshold are defined by data and optical model uncertainties to 20 MeV.

d. The total inelastic cross-section (MT=4) uncertainties may be estimated more accurately from the uncertainties for the nonelastic and other partial components of the nonelastic than obtained simply by summing uncertainties given for MT=51-91, which may be large. This is particularly true when data for the total inelastic cross section are available.

Thus, the uncertainties for MT=3 from 1.E-5 eV to the end of the resolved resonance region (or to the threshold of the first reaction in some cases) are derived by setting them equal to the capture (MF=33, MT=102). From this point to 20 MeV the uncertainties for MT=3 are given explicitly.

The uncertainties for MT=4 are derived from threshold to 20 MeV as [(MF=33, MT=3) - (MF=33, MT=16) - (MF=33, MT=22) - (MF=33, MT=28) - (MF=33, MT=102) - (MF=33, MT=103) - ...].

For the elastic cross-section (MT=2) uncertainties, from 1.E-5 eV to an arbitrary energy E_a between thermal and the first resonance (determined by where the smooth cross-section shape begins to be affected by the lowest resonance), the uncertainty is given explicitly. From E_a to the first reaction threshold the uncertainties are derived as [(MF=33, MT=1) - (MF=33, MT=102)], and from this threshold to 20 MeV the uncertainties are derived as [(MF=33, MT=1) - (MF=33, MT=3)].

The uncertainties for the total cross section (MT=1) from 1.E-5 eV to E_a are derived as [(MF=33, MT=2) + (MF=33, MT=102)], insuring correct uncertainties at thermal. From E_a to 20 MeV, the uncertainties are explicitly given, based on experimental data.

The above method of obtaining uncertainties for MT=1, 2, 3, and 4 generally achieves the goals noted above, and uses the concepts of derived and explicit uncertainties in a consistent manner. However, there is nothing unique about this scheme, and other methods to achieve the same goals can surely be developed.

3. RESULTS AND DISCUSSION

Tables 2-5 show results for the ^{65}Cu(n,2n), ^{56}Fe(n,2n), ^{60}Ni(n,2n), and ^{56}Fe nonelastic cross sections, respectively. The first approach (using GLUCS) described above was used in constructing the covariances for the ^{65}Cu(n,2n) cross sections. The second approach was used for ^{56}Fe(n,2n), while the third approach was used for ^{60}Ni(n,2n). For the ^{56}Fe nonelastic cross sections, both the second and fourth approaches were used.

The ^{65}Cu(n,2n) covariances are taken from the GLUCS calculation[9] in which this reaction was studied simultaneously with thirteen other dosimetry reaction cross sections correlated by ratio data (see Table 2).

The ^{56}Fe(n,2n) covariances shown in Table 3 are estimated from the scatter of the measured data and the file was constructed according to the method described in Section 2. The effect of the absolute component can be seen at energies close to threshold.

The ^{60}Ni(n,2n) cross section was calculated by TNG and no data were available, thus the uncertainties were assigned as a function of cross section magnitude. The short-range components were generated from Table 1, and the long-range component was obtained by taking one-half of the minimum of the short-range components. To preserve the total uncertainty at the energy where the uncertainty was the smallest, the short-range components were divided by two to compensate for the removal of the long-range component. Finally, the LB=8 components were "backed out" from the reduced short-range components by taking 10% from the LB=1 short-range values and multiplying by the appropriate cross section value from file MF=3, squared. The resulting standard deviations and correlation matrix are given in Table 4.

Note that in Table 5 the standard deviations for the ^{56}Fe nonelastic cross sections are large when the incident energy intervals (from MF=3) are small. This characteristic is directly related to the variance contribution from the LB=8 sub-subsection (see Hetrick et al.[10]). In this case, if the fraction F that was used (F=0.01) were larger, the standard deviations for energy ranges of 1.012-1.013, 1.013-1.014, and 1.298-1.299 MeV would be even larger than those shown in Table 5. Also, note that the covariances for the nonelastic cross section from 1.0E-5 to 8.6227E+5 eV are equal to the capture covariances. The blocks of zero correlations in the matrix reflect the fact that the experimental data are uncorrelated in these regions.

CONCLUSIONS

The methods described in this paper were used for the initial ENDF/B-VI release to construct the covariance files for most of the reactions for the isotopes of Cr, Fe, Ni, Cu, and Pb; a GLUCS analysis was used on relatively few reactions. The method is quite simple, but the goal for the first phase of these evaluations was reasonableness and consistency across isotopes and reactions for the structural materials, and this goal has been met. There are problems such as the idiosyncrasies caused by the LB=8 sub-subsection. It appears that including the LB=8 sub-subsection should be reconsidered in the future. However, the overall method is a significant improvement over what was commonly done in the past when only LB=1 sub-subsections were used, resulting in fully-correlated submatrices in the correlation matrix.

Vonach et al.[11] showed that, on average, cross-section uncertainties for the structural materials are highly correlated for energies differing by less than about 1 MeV, but for energies differing by more than 5 MeV little correlation was left. The method used here of estimating the long-range uncertainties as one-half of the minimum value of the short-range components may provide too large a long-range component. For example, the long-range correlations as seen in Tables 3-4 are larger than what would be produced using the approximate method of Vonach et al.

The next step towards improvement of the uncertainty files is to use methods that consider uncertainties of the most sensitive model parameters based on the scatter of measured data around the theoretical curves and the long-range correlation error of the data, such as the methods proposed by Kanda and Uenohara[5] and as was done for the F-19 evaluation.[6] Also, covariances should be included for the distributions in files MF=4 and 6, and options to accomplish this need to be studied. Finally, covariances for the important resonance parameters as well as for gamma-ray production need to be included.

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Table 2. Covariance information for the $^{65}Cu(n,2n)$ cross section

	Energy Range	σ	St Dev	Correlation Matrix																		
	(MeV)	(mb)	(%)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
1	10.063 - 10.50	12.43	0.00	0																		
2	- 11.00	84.26	10.31	0	100																	
3	- 11.50	220.74	4.88	0	9	100																
4	- 12.00	381.24	4.91	0	9	26	100															
5	- 12.50	541.86	4.94	0	9	26	26	100														
6	- 13.00	676.01	4.44	0	9	19	19	19	100													
7	- 13.50	778.14	4.44	0	9	19	19	19	25	100												
8	- 14.00	859.31	4.45	0	9	19	19	19	25	25	100											
9	- 14.50	922.08	2.86	0	4	8	8	8	15	15	15	100										
10	- 15.00	965.70	1.65	0	6	12	12	12	16	16	16	47	100									
11	- 15.50	997.83	1.65	0	6	12	12	12	16	16	16	47	16	100								
12	- 16.00	1021.80	1.65	0	6	12	12	12	16	16	16	47	16	16	100							
13	- 16.50	1046.70	2.39	0	3	5	5	5	7	7	7	21	37	37	37	100						
14	- 17.00	1067.00	1.78	0	4	6	6	6	9	9	9	27	50	50	50	44	100					
15	- 17.50	1073.40	1.88	0	3	6	6	6	9	9	9	25	45	45	45	46	53	100				
16	- 18.00	1083.50	3.43	0	2	3	3	3	5	5	5	14	25	25	25	23	33	33	100			
17	- 18.50	1084.00	2.27	0	3	5	5	5	7	7	7	21	38	38	38	34	43	44	-8	100		
18	- 19.00	1056.80	3.82	0	2	4	4	4	6	6	6	16	32	32	32	17	23	22	22	17	100	
19	- 20.00	997.83	5.51	0	1	2	2	2	3	3	3	9	18	18	18	11	15	15	13	13	27	100

Table 3. Covariance information for the $^{56}Fe(n,2n)$ cross section.

	Energy Range	σ	St. Dev.	Correlation Matrix																									
	(MeV)	(mb)	(%)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
1	11.402 - 11.50	1.12	564.78	100																								
2	- 11.60	4.92	129.02	100	100																							
3	- 11.70	11.40	56.33	99	99	100																						
4	- 11.80	20.13	32.91	96	97	99	100																					
5	- 11.90	31.26	22.46	91	93	96	99	100																				
6	- 12.00	43.71	17.45	84	87	91	96	99	100																			
7	- 12.20	64.29	14.90	67	68	71	73	74	74	100																		
8	- 12.40	95.12	12.37	54	57	60	64	66	68	87	100																	
9	- 12.60	129.08	11.25	44	47	51	55	59	62	85	92	100																
10	- 12.80	167.36	10.67	36	39	43	48	53	56	83	91	95	100															
11	- 13.00	205.55	10.36	31	33	38	43	48	52	81	90	94	96	100														
12	- 13.50	270.31	10.06	24	27	32	37	43	48	79	89	94	97	98	100													
13	- 14.00	359.86	9.92	19	22	26	32	38	44	76	87	93	96	98	99	100												
14	- 14.50	434.92	10.69	14	17	22	27	33	38	40	45	48	49	49	50	50	100											
15	- 15.00	493.85	10.48	13	16	20	26	32	37	40	45	48	49	50	50	50	86	100										
16	- 15.50	538.21	10.37	12	15	20	25	32	37	40	45	48	49	50	51	51	87	89	100									
17	- 16.00	569.92	10.31	12	15	19	25	31	37	40	45	48	49	50	51	51	88	89	90	100								
18	- 16.50	591.89	10.75	11	14	18	24	30	35	38	43	46	47	48	49	49	45	46	46	46	100							
19	- 17.00	605.93	10.71	11	13	18	24	30	35	38	43	46	47	48	49	49	45	46	46	46	84	100						
20	- 17.50	611.12	10.69	11	13	18	23	30	35	38	43	46	47	48	49	49	45	46	46	46	84	84	100					
21	- 18.00	610.69	10.69	11	13	18	23	30	35	38	43	46	47	48	49	49	45	46	46	46	84	84	84	100				
22	- 18.50	607.35	10.78	10	13	18	23	29	35	38	43	45	47	48	48	48	45	45	46	46	44	44	44	44	100			
23	- 19.00	601.19	10.80	11	13	18	23	29	35	38	43	45	47	48	48	48	45	45	46	46	44	44	44	44	83	100		
24	- 19.50	592.74	10.83	11	13	18	23	29	35	37	43	45	47	47	48	48	45	45	46	46	44	44	44	44	82	82	100	
25	- 20.00	581.64	10.87	11	14	18	24	29	35	37	43	45	47	47	48	48	44	45	45	46	44	44	44	44	82	82	82	100

Table 4. Covariance information for the ^{60}Ni(n,2n) cross section.

	Energy Range (MeV)	σ (mb)	St. Dev. (%)	Correlation Matrix 1	2	3	4	5	6
1	11.581 - 12.0	9.87	32.63	100					
2	- 13.0	94.35	21.40	65	100				
3	- 14.5	277.43	12.80	12	18	100			
4	- 16.0	441.11	12.50	12	19	95	100		
5	- 17.5	507.94	12.45	12	19	95	97	100	
6	- 20.0	500.22	10.02	15	23	39	40	40	100

Table 5. Covariance information for the nonelastic cross section of ^{56}Fe. For clarity, selected points have been deleted.

	E_n Range	σ	St. Dev.	Correlation Matrix																				
	(MeV)	(mb)	(%)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
1	1E-11 - 1E-9	7.15E4	7.21	100																				
2	- 1E-7	7150.0	25.67	9	100																			
3	- 1E-5	715.0	25.67	9	7	100																		
4	- 1E-4	85.0	69.40	3	3	3	100																	
5	- 1E-3	70.0	8.09	27	8	8	3	100																
6	- 0.01	50.5	12.17	0	0	0	0	0	100															
7	- 0.10	5.5	15.64	0	0	0	0	0	71	100														
8	- 0.60	7.5	20.88	0	0	0	0	0	14	11	100													
9	- 0.80	4.5	21.45	0	0	0	0	0	14	11	96	100												
10	.8627 - 0.863	29.4	4.79	0	0	0	0	0	0	0	0	0	100											
11	1.012 - 1.013	279.4	41.93	0	0	0	0	0	0	0	0	0	2	100										
12	- 1.014	305.4	38.41	0	0	0	0	0	0	0	0	0	2	1	100									
13	- 1.060	335.0	6.79	0	0	0	0	0	0	0	0	0	12	7	8	100								
14	1.298 - 1.299	597.6	20.00	0	0	0	0	0	0	0	0	0	4	2	3	15	100							
15	1.299 - 1.413	692.9	4.72	0	0	0	0	0	0	0	0	0	18	10	11	62	21	100						
16	1.583 - 1.749	854.6	4.58	0	0	0	0	0	0	0	0	0	18	10	11	64	22	92	100					
17	2.235 - 4.480	1138.8	4.46	0	0	0	0	0	0	0	0	0	19	2	2	13	4	19	20	100				
18	7.500 - 7.747	1438.8	5.11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100			
19	10.00 - 10.36	1424.6	5.24	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	34	100		
20	14.50 - 14.60	1376.8	5.89	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	30	29	100	
21	17.50 - 18.00	1289.4	5.20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	34	33	81	100
22	19.50 - 20.00	1244.6	5.22	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	34	33	81	91	100

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DIRECT COVARIANCE DATA FOR COUPLED ENERGY-ANGLE DISTRIBUTIONS

H. Vonach

Institut für Radiumforschung und Kernphysik,Universität Wien,
Boltzmanngasse 3
1090–Vienna, Austria

ABSTRACT

The paper discusses the need for direct covariance information of coupled energy angle distributions of secondary neutrons, charged particles and photons emitted in neutron induced reactions, the methods for obtaining such information and proposes a new format (MF 36) for covariances of evaluated coupled energy–angle distributions stored as MF 6 data.

1. Introduction

Coupled energy–angle distributions of secondary neutrons, charged particles and photons can be stored in file 6 (MF 6) within the ENDF/B–VI format and this new format has been used in many recent evaluations [1,2]. At present there is however no possibility to describe the covariances of these distributions within the ENDF/B format.

In this talk I will address the problem how this situation could be improved and present a proposal for a new format MF 36 for describing covariances of coupled energy–angle distributions of secondary particles stored in form of MF 6 data.

For this purpose I will first discuss the need for such covariance information in different application areas and especially the amount of detail which is needed to characterize the uncertainties of such distributions. Subsequently I will review the sources of information available to judge the accuracy of the secondary energy and angular distributions. Based on the above considerations I will finally present a detailed proposal for a format MF 36 suitable for describing the covariances of MF 6 data which is based on the following considerations:

a) The format should allow to present the covariance information in sufficient detail as to fulfill the need of all presently anticipated applications.

b) The format should be as simple as possible and should result in files of reasonable length.

c) The format should allow quick construction of such files MF 36 for existing evaluations by means of rough qualitative methods.

2. Needs for covariance information for secondary neutrons, charged particle and photon energy and angular distributions

2.1. Areas of application where those data are needed

The most important demand for covariances of secondary particle distributions occur in neutronic calculations for fusion reactor design. For the design of the next generation of tokomaks (NET/ITER) it is very important that the predictions of neutron transport calculations for the heating blanket and the various parts of the shielding of the superconducting coils are as accurate as possible and that it is possible to calculate quantities like nuclear heating and dpa values for the superconducting coils and other fusion reactor components with small uncertainty [3].

Such calculations depend in principle on the shapes of the energy – and angular distribution of secondary neutrons in the materials traversed by the neutrons. Without knowledge of the uncertainties of these distributions it is not possible to reliably estimate the uncertainty e.g. of the fast neutron flux and its spectral shape energy from a particular shield of the fusion reactor coils. Concerning nuclear heating in addition the uncertainties of the average energies of the charged particles from (n, charged particle) reactions in the respective materials and the uncertainties in the total and energy differential γ–production cross sections are needed.

In addition the uncertainties of secondary energy and angular distributions are needed for the design of shields of high energy accelerators especially of those needed for materials testing in fusion technology.

2.2 Amount of information needed

At first glance it might appear an enormous task to characterize the uncertainties of a three–dimensional distribution $d\sigma^2/dE_{n'}d\Omega$ $(E_n,E_{n'},\theta)$ as function of its three parameters, incident energy, secondary energy and angle.

If one takes a closer look, it becomes obvious, however, that the information needed is much less.

At first it has to be kept in mind that for neutron energies needed in fusion reactor technology, that is for $E_n < 14$ MeV, the angular distribution of all secondary particles can be well described by Legendre polynomials up to order two only [4] e.g.

$$d\sigma^2/dE_{n'}d\Omega = \sigma_{nn'}/4\pi\, f_o(E_n,E_{n'})\,[1 + b_1P_1(\cos\theta) + b_2P_2(\cos\theta)] \qquad (1)$$

that is the whole information on the angular distributions is contained in the two parameters $b_1(E_n,E_{n'})$ and $b_2(E_n,E_{n'})$; for photons in addition $b_1 = 0$ because of symmetries of compound nucleus decay. Even at higher neutron energies, where higher order Legendre polynomials become important, one can probably restrict the consideration of uncertainties to b_1 and b_2 as the importance of higher order Legendre contributions in neutron transport calculations decrease rapidly with increasing order l [5]; thus in most cases the uncertainty of the b_1 term will be the only important quantity. Thus instead of one distribution depending on three parameters we have to deal with two or at most three distributions (for f_o, b_1 and b_2) depending on only two parameters (E_n and $E_{n'}$).

Concerning the dependence of the distributions on E_n and $E_{n'}$ we may consider the problem of the transport of fusion neutrons ($E_n = 14$ MeV) through some shielding or neutron multiplier material. For this case the needed range of E_n and $E_{n'}$ is shown in fig. 1.

As the figure shows there is a relatively restricted range for E_n and $E_{n'}$. As inelastic neutron scattering with energy loss below a few MeV is described by excitation of discrete levels the range of incident energies of interest extends from 3 – 4 to 14 MeV. Within this range the energy bin around 14 MeV is most important as most of the 14 MeV fusion neutrons are transfered to rather low energies in their first nuclear interaction and only a relatively small part reaches the energy range where a second continuum inelastic scattering can occur. Thus it will be sufficient to use a very rough grid (5 groups) for the incident energy E_n. Outgoing neutron energy ranges from $E_{n'} = 0$ to $E_{n'} = E_n - U$, U being the energy range up to which inelastic scattering to resolved levels has been taken. These distributions can be well characterized by group structures with 10 – 20 groups [6] (see also fig. 2). Thus in practice it will be sufficient to characterize such coupled energy–angle distributions by typically $5 \times 15 \times 3 \approx 200$ numbers for which uncertainties have to be estimated.

For distributions of secondary charged particles and photons the amount of information is considerably less. For photons the angular distribution is symmetric to 90° and the relatively small P_2 term describing the deviation from isotropy is unimportant for transport calculations. Thus the only information needed concerns the uncertainties in the energy distribution of the photons as function of the incident neutron energy, again only for E_n above the region of resolved levels and most important at E_n = 14 MeV. Thus it will again be possible to use a 5 group structure for E_n and a 10 – 20 group structure for E_γ resulting in a total of only $\approx 5 \times 15 = 75$ elements to characterize the energy–distributions of the secondary photons for the whole neutron energy range of interest. In addition for each incident energy E_n an uncertainty of the total photon multiplicity is needed for a complete description.

For secondary charged particles the most important quantity of applied interest at present seems to be the average energy (e.g. for calculation of nuclear heating); a very crude description of the charged particle energy spectrum ($\approx$ 5 groups) will be sufficient for this purpose. This information is needed at E_n = 14 MeV and perhaps 2 lower energies as the cross sections for charged particle emission decrease very strongly with neutron energy for most materials.

Thus we may summarize. There is a need for covariances for coupled energy angle distributions for all materials important in fusion technology and neutron shielding, the amount of detail needed for the description of these (in principle 3–dimensional distributions) however is remarkably small and thus – as will be shown in section 4 – describable in conventional file structures.

For the most important application, fusion technology, it is important to keep in mind that the sensitivity to the data for 14 MeV is much higher than for the lower energies. At 14 MeV "quantitative" covariance information also for the distributions is needed, whereas for all lower energies rough "qualitative" estimates of the uncertainties are probably sufficient.

3. Sources of information for covariances for energy and angular distributions for secondary neutrons and photons

3.1. Incident neutron energy = 14 MeV

There exists considerable experimental information on double–differential secondary neutron spectra for many materials [6,7]. Concerning the angle–integrated secondary neutron spectra this information has been evaluated for 10 important elements at the Institut für Radiumforschung und Kernphysik, University of Vienna [7]. From this work the shapes of these distributions are now known to better than 5 – 10% (see fig. 2). The shapes of the angular distributions at incident energies up to 14 MeV are well

described by Legendre polynomials of first and second order as already discussed in section 2 (see equ. 1).

An evaluation of the coefficients $b_1(E_{n'})$ and $b_2(E_{n'})$ for Pb has recently been completed [8], an extension to all of the materials covered in ref. 1 and 2 is planned at our institute within the Coordinated Research Program of the IAEA on double-differential neutron emission cross sections.

Furthermore the experimental results show that the cross sections $d\sigma/dE_{n'}$ $(E_{n'})$ and angular distributions coefficients $b_1(E_{n'})$ and $b_2(E_n)$ vary rather smoothly with mass number at least for nuclei with A > 50. Thus at 14 MeV we have experimental information for reliable assessment of covariances for all medium and heavy nuclei. For important light nuclei [^{7}Li, ^{6}Li, ^{9}Be, Al, Si] there are also experimental results [9,10] which however have not yet been combined into sets of recommended values.

From this information it will in general be straightforward to estimate the covariances of evaluations of angle-energy distributions of secondary neutrons at 14 MeV incident energies.

3.2. Incident neutron energies below 14 MeV

For energies below 14 MeV we have new measurements performed at the Argonne National Laboratory [11] for incident neutron energies in the range 7 - 9 MeV for a number of elements which can be used to assess the uncertainties at that incident energy and by means of inter- and extrapolation it should be possible to estimate the uncertainty of evaluated energy-angle continuum distribution for all incident neutron energies of interest below 14 MeV.

Alternatively for many materials of importance covariances of secondary angle- and energy distributions can be estimated from the dispersion of recent evaluations [12]. An example for this is shown in fig. 3.

For elements for which we have neither experimental data nor several new incident evaluations estimates on the uncertainties of angular and energy distributions of secondary neutrons can be estimated by calculation of these quantities using different codes like GNASH [13], TNG [14] or codes based on FKK [15] with parameters adjusted to reproduce the experimental data at 14 MeV.

4. Proposal for new format MF 36 for description of covariances of coupled energy-angle distributions (MF 6 data)

Our format proposal for MF 36 data is given in table 1. As far as possible the proposal makes use of existing format structures, especially MF 33 and MF 35 used for characterizing the covariances of MF 3 (cross sections) and MF 5 (secondary energy distribution) data.

It is proposed that each of the MF 36 files consist of two parts

a) One first part has exactly the form of a MF 33 file and describes the covariance of the particle multiplicities. This can be omitted if the corresponding multiplicities are integers without uncertainty.

b) The second part actually describes the covariance of normalized coupled energy-angle secondary particle or photon distributions. It is very similar to MF 35, which describes the covariance of normalized angle-integrated secondary energy distributions.

The main difference is the introduction of a new control parameter, which may have values 0, 1 or 2 depending on how much covariance information for the angular part of the distributions is to be stored. Values of 0, 1 or 2 mean that covariances of the angle-integrated distributions only or also of the coefficients of the Legendre

polynomial P_1 or of those of P_1 and P_2 (see equ.1) are to be stored. Depending on the value of this control parameter each of the covariance matrices of our MF 35 file is replaced by a sequence of one, two or three covariance matrices describing the uncertainties of the quantities in equ.1. It is proposed that this description be in form of LB = 6 sub-subsections. For the uncertainties of the angle-integrated energy distributions restriction to this type of sub-subsections is necessary as the constraints imposed by the normalization condition can be handled most easily by this type of sub-subsection. For the covariance matrices describing the coefficients of the P_1 and P_2 terms, description in form of LB = 1 sub-subsection would probably be better as there are no normalization conditions and existing information on the non-diagonal elements of these matrices is very poor anyway. In my proposal LB = 6 type subsections are generally required for keeping the format as simple as possible, but this advantage has of course to be judged versus the disadvantage of unnecessarily increasing the length of the files.

The present proposal of course imposes severe restrictions on the type of correlations admitted in the description of covariances.

It is assumed that there are no correlations between the quantities describing the energy distributions (f_0) and those describing the P_1 and P_2 part of the angular distributions and also there is no correlation possible between energy-angle distributions belonging to different incident neutron energies. Both restrictions appear reasonable if the covariances are estimated by means of the qualitative methods outlined in section 3. In our experimental data base there are no significant correlations between the $d\sigma/dE_{n'}(E_n E_{n'})$ values describing the energy distributions and the values describing the energy-dependent shapes of the secondary angular distributions.

Concerning the second point there are of course strong correlations between the uncertainties of the distributions if the incident neutron energies are only slightly different. These correlations, however, can be accounted for approximately if the incident energy intervals in the file 36 description are chosen sufficiently large e.g. 1 - 2 MeV.

Concerning the number of elements in such files we get the following rough estimates:

$$N = N_{E_n}(N_{E_{n'}}^2/2) \cdot L$$

using 10 incident energies, on average about 8 secondary energies within each distribution, and the maximum value of 3 for NL, we get a total of $\approx$ 1000 elements for the covariance matrix of a coupled energy-angle distributions of secondary neutrons which is only a rather small fraction of the overall file length. For charged particle and photons the demands on details of covariance information are even less (see section 3) and thus the corresponding number of elements will accordingly be a few 100 in most cases.

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Table 1: Proposal for a new format MF 36 for covariances of energy-angle coupled distributions stored as MF 6 data

File 36

	ZA	AWR	O	O	NK	O	MAT	36	MT	NS
cov.matrix of	ZAP_1	AWP_1	LI=0	0	0	0	-- " --	- "-	- " -	- " -
multiplicity	0.0	0.0	LS=1	LB=5	NT	NE	-- " --	- "-	- " -	- " -
				$\{E_n\}, \{F_{KK'}\}$ LIST						
covariance	ZAP_1	AWP_1	LI=1	0	NL	0	-- " --	- "-	- " -	- " -
information	E_1	E_2	LS=1	LB=7	NT	NE	-- " --	- "-	- " -	- " -
for secon-				$\{E_{n'}\}, \{G_{KK'NL}\}$ LIST						
dary energy-										
angle	ZAP_1	AWP_1	LI=1	0	NL	0	-- " --	- "-	- " -	- " -
coupled	E_2	E_3	LS=1	LB=7	NT	NE	-- " --	- "-	- " -	- " -
distributions				$\{E_{n'}\}, \{G_{KK'NL}\}$ LIST						
for (n-1)										
incident	ZAP_1	AWP_1	LI=1	0	NL	0	-- " --	- "-	- " -	- " -
energy	E_{n-1}	E_n	LS=1	LB=7	NT	NE	-- " --	- "-	- " -	- " -
intervalls				$\{E_{n'}\}, \{G_{KK'NL}\}$ LIST						

same for all other emitted particle types including photons

NK = total number of subsections
= (number of incident energy intervals for particle 1+1) + (number of incident energy intervals for particle 2+1) + ...+ (number of incident energy ranges for particle n+1)

LI = flag LI=0 covariance information refer to particle multiplicities
LI=1 refers to covariance information for coupled energy-angle distributions

NL = number of l-values to be concidered for the coupled energy-angle distributions
(NL)min = 1 (no angular distribution information)
(NL)max = 3 (covariance information up to P2 coefficient of angular distribution)

NE = number of energy intervals +1
= number of entries in $\{E_{n^*}\}$ or $\{E_{n'}\}$

NT = total number of entries in $\{F_{KK'}\}$ or $\{E_{n'}\}$ + $\{G_{KK'NL}\}$

a) for LI=0 (multiplicities)
NT = NE + (NE-1)*(NE)/2 = (NE+1)*(NE)/2

b) for LI = 1 (angle-energy coupled distribution)
NT = NE + NL*[(NE-1) (NE)/2]

Table 1 (continued):

$\{ G_{KK'NL} \} = \{ F_{KK'0} \} , \{ F_{KK'1} \} , \{ F_{KK',(NL-1)} \}$

= sequences of covariance matrices for Legendre coefficients of energy-angle coupled distributions up to the order (NL-1)

$F_{KK'L} = \mathrm{cov}[f_{L-1}(E_K,E_{K'}) * f_{L-1}(E_K,E_{K'})]$

$F_{KK'}$ = relative covariance matrix for particle multiplicities

$$= \frac{\mathrm{cov} (y(E_K) , y(E_{K'}))}{y(E_K) * y(E_{K'})}$$

with $\frac{d\sigma}{dE'd\Omega} = \frac{\sigma}{4\pi} y(E_n) \Sigma f_l(E_n,E'_{n'})(2l+1)*P_l(\cos\Theta)$

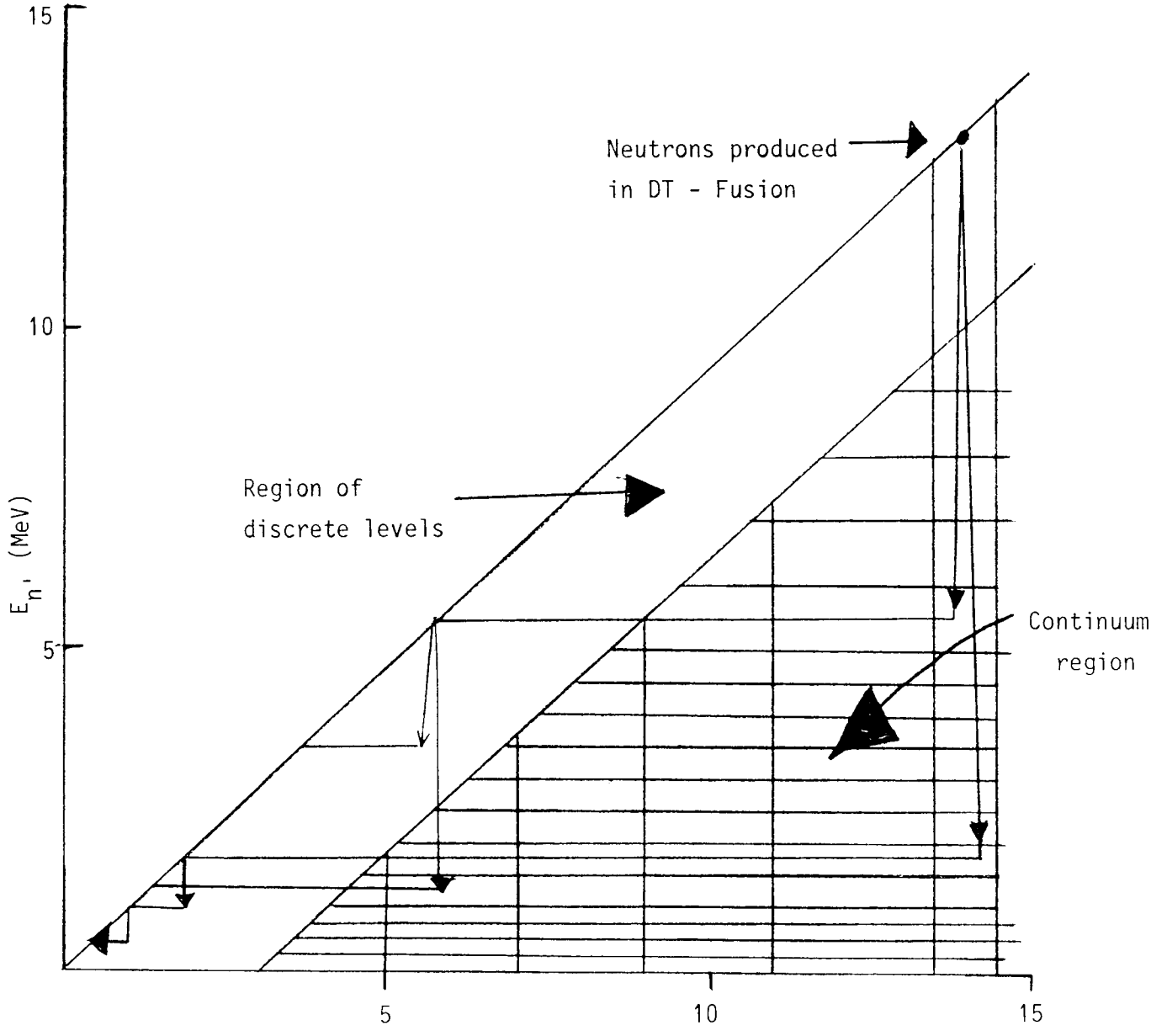

Figure 1: Continuum region (range in E_n and $E_{n'}$) needed for fusion neutrons calculation grid indicates possible bin structure for the description of the continuum

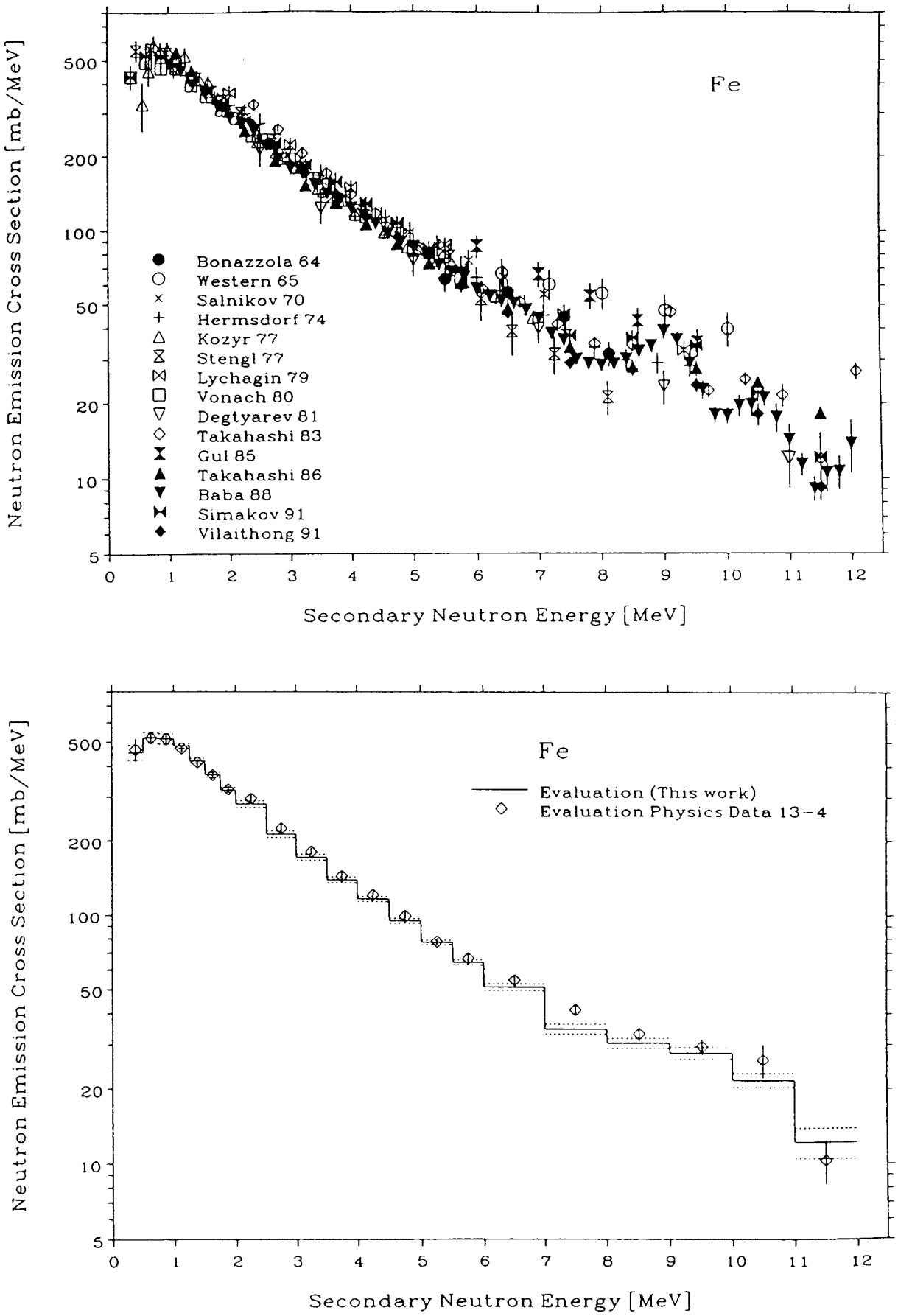

Figure 2: Angle-integrated neutron emission spectrum from the interaction of 14 MeV neutrons with iron:
a) experimental data (Fig. 1 of Ref. 7)
b) evaluated cross sections derived from the data shown in a) (Fig. 4 of Ref. 7)

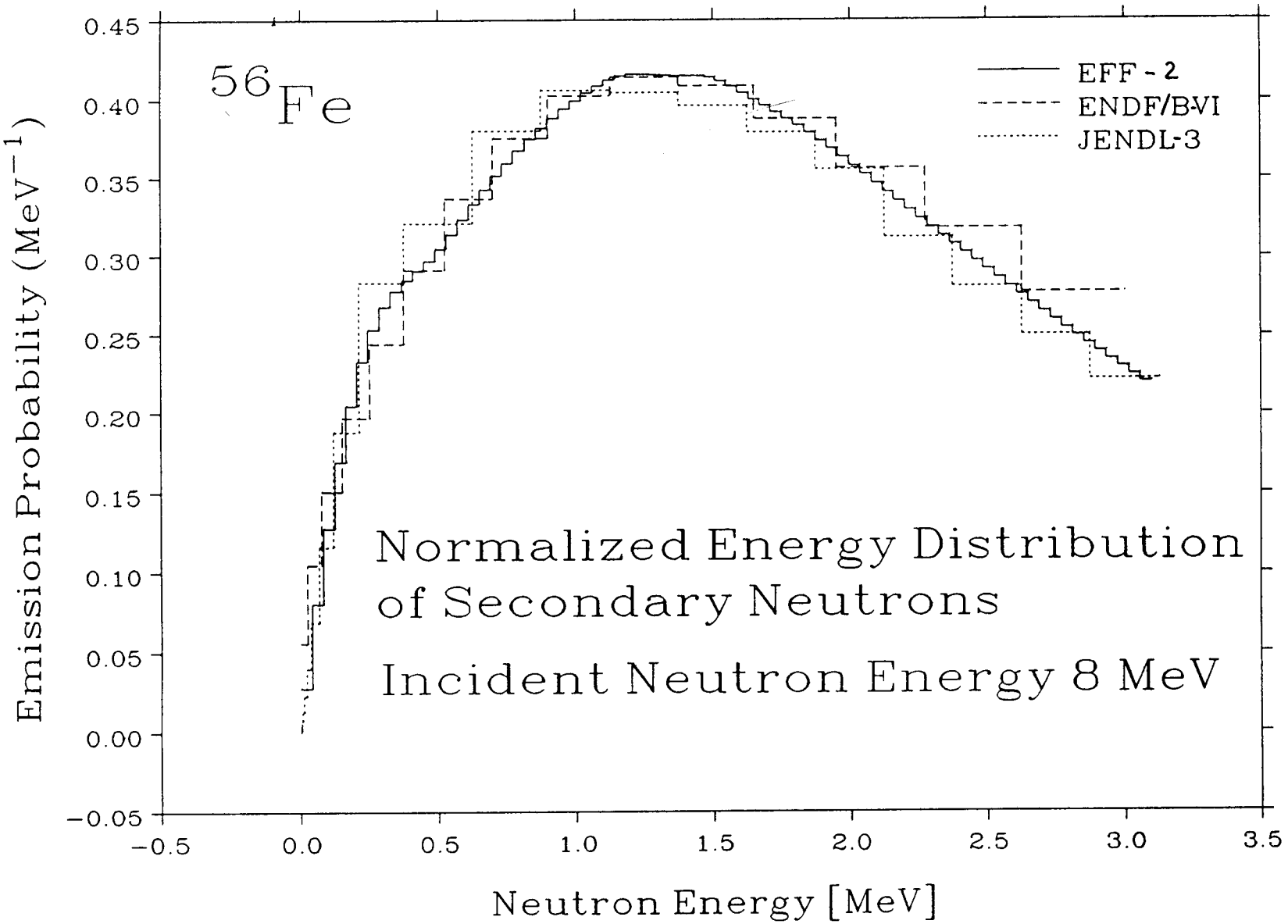

Figure 3: Comparison of the normalized energy–distributions of secondary neutrons in different recent evaluated data files at E_n = 8 MeV (Fig. 69 of ref. 12)

DESCRIPTION OF COVARIANCES OF EMISSION SPECTRA USING ENDF FILE 30

D. W. Muir

Nuclear Theory and Applications Group
Theoretical Division
Los Alamos National Laboratory
Los Alamos, NM 87545
U. S. A.

ABSTRACT

The ENDF File-30 format provides a means of recording completely, yet reasonably compactly, any type of nuclear data covariances that can be formally separated into (a) a fairly small set of parameters with known covariances and (b) tabulated derivatives of the nuclear data with respect to the parameters. In this paper, we discuss the potential usefulness of File 30 for describing the covariances of emission spectra. In particular, it will be shown that, relative to older approaches such as "SED/SAD", the greater fundamental clarity of the File-30 approach will facilitate the work of both the data evaluator and the data user. To place the topic of such factored covariances into perspective, we also briefly review relevant aspects of the generalized method of least squares and the new technology of computer calculus.

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1. Statement of the Problem

An important unresolved problem in the production of data evaluations with formatted data covariances is the description in a physically correct, yet compact, way the covariances of the angle- and energy-distributions of emitted particles and gamma rays, especially the products of nuclear interactions of high-energy neutrons.

This problem has remained intractable over the years because it brings one directly up against the awkward fact that, whereas there are typically 10^6 data points in a modern nuclear data evaluation, there are also, associated with those data points, 5×10^{11} potentially non-trivial correlation coefficients. Most of the data points contributing to the bulk of these data files are included in order to describe *emission* properties, such as gamma-ray and charged-particle energy spectra, correlated angle-energy distributions of neutrons and charged particles emitted in the continuum region, etc.

Older technologies for addressing this problem (especially, the so-called "SED-SAD" approach) resorted to a crude energy and angle binning of the emission properties prior to defining covariances of the bin-integrated data. There are two fundamental problems with this approach. First, it is difficult to see how to evaluate the uncertainty in bin-integrated quantities without some prior uncertainty information. Secondly, it is difficult to see how to process correctly such coarse-bin data into arbitrary, user-specified group structures without any knowledge of the within-bin covariance structure.

Both objections stem from the fact that coarse-bin covariances already constitute processed information. Before one can meaningfully create such binned covariances, one must have a least a rough knowledge of the underlying energy- and angle-dependent behavior of the covariances. Whether the evaluator's understanding of this underlying behavior be qualitative or quantitative (see later Sections of this paper), it would be much better to put the data evaluator's understanding of the underlying covariances directly into the basic data files than to put in a filtered version of this information. Binning into coarse structures, as is often required in applications, is more appropriately done at the multigroup processing stage.

Within the framework of the approved, version-6 format of the Evaluated Nuclear Data File (ENDF-6) [1], File 30 was created with the primary goal of overcoming this difficult problem of preserving the energy- and angle-dependent details of this covariance information without, at the same time, destroying the usefulness of the files by adding impractical bulk. The approach used in File 30 is based on the fortunate coincidence that, exactly in the neutron energy region where the particle-emission properties of nuclei are the most complicated (E_n above about 5 MeV), the bulk of the data in the files are predominantly the output of nuclear-model computer programs.

The uncertainties of most computed results can be adequately described as being the result of uncertainty in a relatively small number of model input parameters (perhaps 10-50). This leads one to consider a transition at the higher neutron energies away from the usual representation in the data files of the covariances of the actual data, replacing them with the covariances of the underlying nuclear parameters that are responsible for uncertainties in the emission properties (and other nuclear data). These underlying covariances can be supplemented with numerical files of sensitivity coefficients that give the relationship between parameter changes and nuclear-data changes. Together, the parameter covariances and data sensitivities provide a description of nuclear data uncertainties that is both physically sound and reasonably compact.

Before discussing the mechanical devices used in File 30 to represent these parameter covariances and their sensitivities, it is useful to review the fundamental issues that affect the

process of evaluating nuclear model parameters and their associated covariances by the method of least squares, given a set of measured nuclear data and nuclear model programs appropriate for their analysis. In this review, we shall focus on the special problems introduced by the use of nuclear model programs as an intrinsic part of this evaluation process.

2. Partitioned Least Squares

2.1. Minimum-Variance Estimation

Many problems in the general field of data evaluation reduce to the need to improve upon an existing set of raw measurements by taking into account the theoretical relationships that are known to exist among the quantities being measured. A very useful tool for combining information from multiple sources to obtain improved estimates (i.e., evaluations) of the relevant data types is the method of correlated linear least squares. The power and general applicability of the least-squares method have led to its wide use. In particular, considerable progress has been made in the application of least squares to the goal of quantifying the uncertainty of the results of nuclear model calculations. (See, for example, Refs. [2-9].)

In a number of applications, including the present one, the measured quantities naturally segregate into two groups, namely "parameters" and "data". In our case, the first group forms a complete set of numerical information (ground state masses and spins, discrete-level properties including decay schemes, strength functions, average level spacings, level densities vs. spin and excitation energy, fission barrier heights, optical model parameters, etc.) required as input for the theoretical computation of nuclear data. In the present terminology, then, nuclear models read in "parameters" and write out "data".

At the starting point of an uncertainty analysis, some of the parameters will have been measured in the traditional sense (for example, discrete-level properties), while others will probably have been measured only in the sense of having been estimated from general systematic trends. Nevertheless, we shall refer to the initial set of parameters and data collectively as the "measured quantities" or simply as the "measurements", and we shall assume that it is possible to at least roughly estimate all of their uncertainties.

When measurements can be partitioned into the classes of parameters and data, as in the present case, one no longer requires the full generality of the standard Normal equations, as given for example in Ref. [10], because the sensitivity matrix relating the total set of measurements to the parameters to be estimated then has a special "partitioned" structure. The sensitivity matrix for the parameter portion of the measurement pool is just the identity matrix. It is only the sensitivity matrix for the data portion of the measurement pool that is non-trivial. It is possible to take advantage of this special partitioned structure of the total sensitivity matrix to reduce significantly the matrix-inversion requirements, relative to solving the Normal equations, while still retaining full minimum-variance guarantees. This matrix reduction approach can be called the method of "partitioned least squares".

We refer the reader to Ref. [11] for a rigorous, "non-Bayesian" derivation of the partitioned least squares method that consistently employs the viewpoint of minimum-variance estimation, avoids any assumptions on the shape of underlying probability distributions, and avoids any assumptions on the extent of measurement correlations.

2.2. Problem Set-up

We suppose that there exists a parameter set $\{v_j, j=1,k\}$ corresponding to the measurement or estimation of k different nuclear-model parameters having (unknown) true values c_j. In each case, the measurements are assumed to be perturbed from the true values by random error e_j. We consider v_j, c_j and e_j to be elements of column vectors **v**, **c** and **e**, respectively, so that

$$\mathbf{v} = \mathbf{c} + \mathbf{e} .$$

The errors are assumed to have zero mean,

$$\langle \mathbf{e} \rangle = \mathbf{0} ,$$

(the symbol $\langle\ \rangle$ denoting the expectation operator) so that

$$\langle \mathbf{v} \rangle = \mathbf{c} . \tag{2.1}$$

It is also assumed that the errors e_j have finite second moments. These second moments form the elements of the covariance matrix $D(\mathbf{v})$,

$$D(\mathbf{v}) \equiv \langle \mathbf{e}\, \mathbf{e}^* \rangle ,$$

where the * symbol indicates the matrix transpose.

We now introduce the measured data $\{w_i, i=1, m\}$. The measurements of the w_i are again assumed to be perturbed from the true values of the measurements y_i by random errors f_i,

$$\mathbf{w} = \mathbf{y} + \mathbf{f} ,$$

where, as for the parameters,

$$\langle \mathbf{f} \rangle = \mathbf{0} ,$$

$$\langle \mathbf{w} \rangle = \mathbf{y} , \tag{2.2}$$

and

$$D(\mathbf{w}) \equiv \langle \mathbf{f}\, \mathbf{f}^* \rangle .$$

Cross-covariance matrices, describing uncertainties and correlations between the parameter and data measurements, are defined analogously;

$$C(\mathbf{v},\mathbf{w}) \equiv \langle \mathbf{e}\, \mathbf{f}^* \rangle .$$

2.3. Linear vs. Nonlinear Functions

We consider that each of the elements of the data vector **y** in Eq. (2.2) is a known function of the elements of the parameter vector **c**,

$$y_i = y_i(\mathbf{c}) . \tag{2.3}$$

Usually these functions are not known analytically but rather are evaluated numerically using a large nuclear-model program. In the case of nuclear-model calculations, these functions can be quite nonlinear, but we shall assume here that the most important functions can all be "linearized". That is to say, we assume

(1) that it is possible by some means to locate a set of parameters $\mathbf{c}_0$ that is close to the true value **c**, and

(2) that near this point in parameter space, all of the functions $y_i(\mathbf{c})$ can be calculated accurately enough for evaluation purposes using only a first-order Taylor-series expansion.

These two assumptions can be summarized as follows:

$$\mathbf{y}(\mathbf{c}) \cong \mathbf{y}(\mathbf{c}_0) + \mathbf{R}(\mathbf{c}_0)\,(\mathbf{c} - \mathbf{c}_0) , \tag{2.4}$$

where the ij-th element of the rectangular matrix $\mathbf{R}(\mathbf{c}_0)$ contains the partial derivative of $y_i(\mathbf{c})$ with respect to parameter c_j, evaluated at $\mathbf{c}_0$,

$$\mathbf{R}(\mathbf{c}_0) \equiv \left. \frac{\partial \mathbf{y}}{\partial \mathbf{c}} \right|_{\mathbf{c}_0} . \tag{2.5}$$

The assumption just made, that the functions $y_i(\mathbf{c})$ can be linearized, requires further

discussion. The general problem of nonlinearity is illustrated in Fig. 1. The functional dependence $\mathbf{y(c)}$ is illustrated there for the simplest case of a single function y_i of a single parameter c_j, or y(c) for short. Here, v is the measured value of the parameter having the unknown true value c, and w is the measured value of the function having true value y(c). As is usual in the case of nuclear model calculations, the curve y(c) is shown with a significantly nonlinear shape. As we shall see in the next paragraphs, there is an interesting connection between the degree of nonlinearity that can be tolerated in y(c) and the accuracy of the available measurements v and w.

First of all, the converged least-squares solution point will lie somewhere on the curve y(c), which is a consequence of the unbiased character of the least-squares solution. Because of the minimum-variance properties of the solution, the solution will also approach as close as possible the measured values v and w. It is convenient to define the a-priori "error ellipse", as a region centered on the measurement point (v,w) and covering the region within which the true values of c and y can be expected to be found (with some specified confidence), given the uncertainties Δv and Δw. This is illustrated in Fig. 1 by the shaded cigar-shaped region. Unless v and w are very unlikely samples from the underlying error distributions, the curve y(c) will pass through a portion of this error ellipse. This means that the converged solution point will be somewhere on the segment of the curve that falls within the shaded region. The validity of the least-squares solution requires only that the function y(c) be reasonably linear over the segment that crosses the error ellipse. If the function is measured quite accurately (that is, if Δw is small, as illustrated in the figure), the segment over which the curve is required to be linear can be, as shown, quite short.

The method of accommodating nonlinearity within the linear least-squares method is illustrated in Fig. 2. In effect, one replaces the true curve y(c) with a linear line-segment tangent to the curve at the initial reference point $c = v = c_0(0)$ (see upper filled circle in Fig. 2). One then employs the resulting solution a'(0) for the parameters, obtained for example from Eq. (3.1) below, to locate an improved reference point ($c = c_0(1)$ in the figure) that is used, in turn, to obtain a second least-squares solution. Iterating this process leads to a calculational scheme, called "Newton iteration", that nearly always converges rapidly to a stable solution, where $c_0(n) \cong c_0(n\text{-}1)$. The only major effect of strong curvature outside the error ellipse is to slow the convergence of the Newton-iteration process. Pathological behavior can be avoided by using a reasonable initial parameter set, preferably one obtained by earlier fits to similar data types.

The functional form of Eq. (2.4) above suggests that considerable simplification can be achieved by introducing a modified set of parameters and data that are equal to the ones discussed up to now, but offset by the constant values $\mathbf{c}_0$ and $\mathbf{y}(\mathbf{c}_0)$, respectively. To achieve this simplification, we now introduce the modified quantities **x**, **a** and **b**, where, recalling Eqs. (2.1) and (2.2),

$$\mathbf{x} \equiv \mathbf{c} - \mathbf{c}_0 , \tag{2.6}$$

$$\mathbf{a} \equiv \mathbf{v} - \mathbf{c}_0 = (\mathbf{c} - \mathbf{c}_0) + \mathbf{e} , \tag{2.7}$$

$$\mathbf{b} \equiv \mathbf{w} - \mathbf{y}(\mathbf{c}_0) = [\, \mathbf{y}(\mathbf{c}) - \mathbf{y}(\mathbf{c}_0) \,] + \mathbf{f} , \tag{2.8}$$

with expectation values correspondingly offset,

$$\langle \mathbf{a} \rangle = \mathbf{c} - \mathbf{c}_0 , \tag{2.9}$$

$$\langle \mathbf{b} \rangle = \mathbf{y}(\mathbf{c}) - \mathbf{y}(\mathbf{c}_0) \cong \mathbf{R}(\mathbf{c}_0)\,(\mathbf{c} - \mathbf{c}_0). \tag{2.10}$$

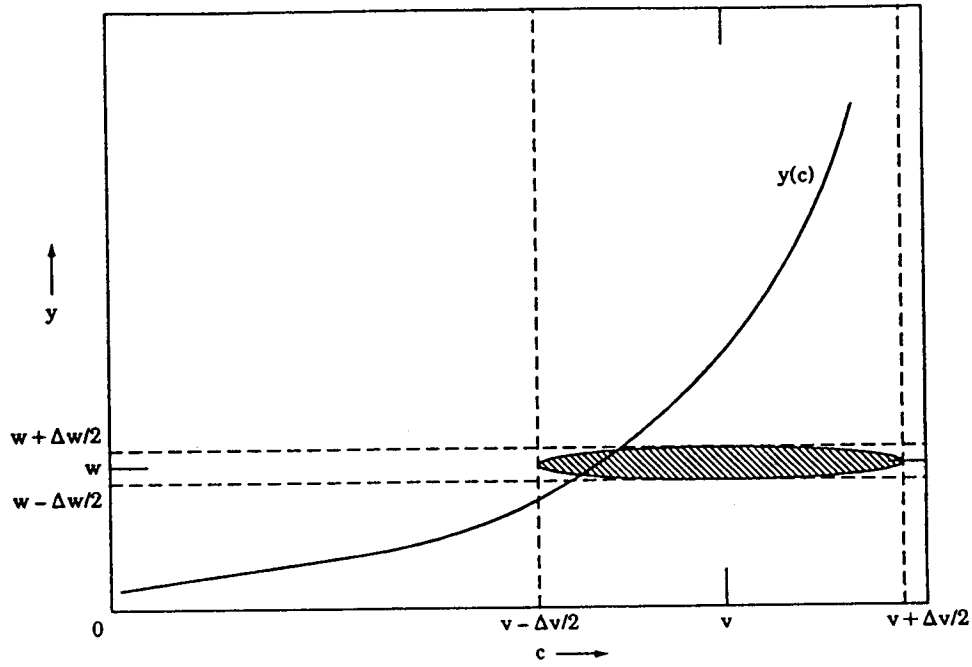

Fig. 1. Accuracy vs. Nonlinearity. Illustration of the relationship between the degree of nonlinearity of y(c) and the accuracy of the parameter and data measurements.

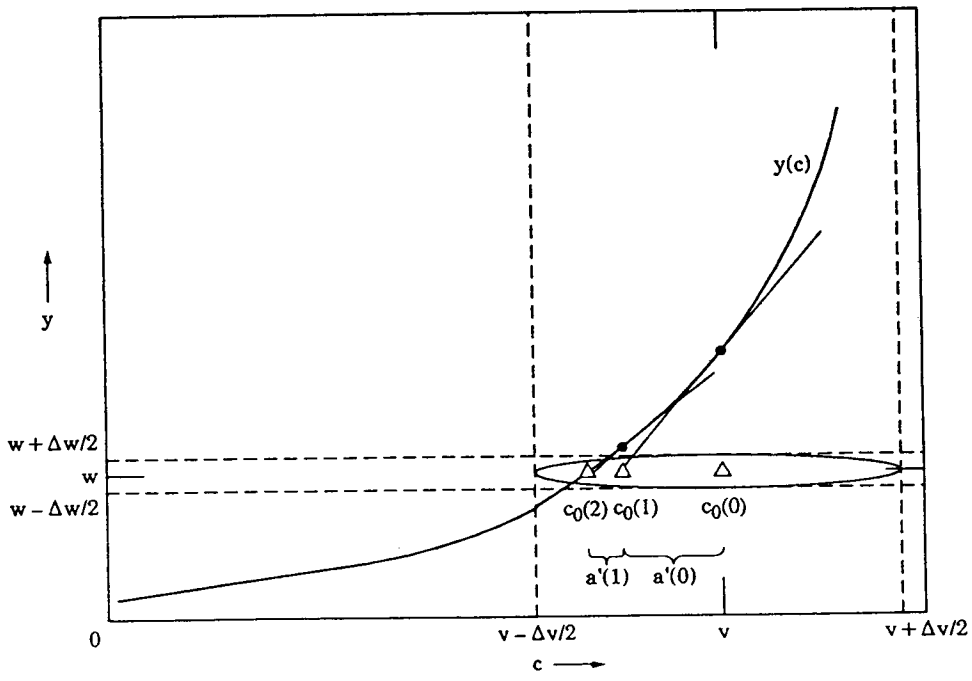

Fig. 2. Newton Iteration. The main effect of strong curvature outside the error ellipse is to slow the convergence of the Newton-iteration process.

In the last equation, we have invoked the linearization relation, Eq. (2.4). It should be emphasized that Eq. (2.10) is the *only* point in the derivation of the method of partitioned least squares where one has to invoke this approximation.

Now substituting from Eqs. (2.6) into Eqs. (2.9) and (2.10), we obtain the following important results:

$$\langle \mathbf{a} \rangle = \mathbf{x} \tag{2.11}$$

$$\langle \mathbf{b} \rangle = \mathbf{R}\,\mathbf{x}\,. \tag{2.12}$$

Since the same additive constant $\mathbf{c}_0$ appears in both **a** and $\langle \mathbf{a} \rangle$, for example, the transformation of Eqs. (2.6) - (2.8) does not influence the parameter and data covariance matrices at all. Independent of the point $\mathbf{c}_0$ where the Taylor expansion is actually performed, then,

$$C(\mathbf{a}, \mathbf{a}) = \langle \mathbf{e}\,\mathbf{e}^* \rangle = C(\mathbf{v},\mathbf{v})\,, \tag{2.13}$$

$$C(\mathbf{b}, \mathbf{b}) = \langle \mathbf{f}\,\mathbf{f}^* \rangle = C(\mathbf{w},\mathbf{w}), \tag{2.14}$$

$$C(\mathbf{a}, \mathbf{b}) = \langle \mathbf{e}\,\mathbf{f}^* \rangle = C(\mathbf{v},\mathbf{w})\,. \tag{2.15}$$

We can therefore simplify the mathematics considerably, good examples being Eqs. (2.11) and (2.12), without making any changes to the covariance matrices. For this reason, in the following discussions we shall focus on **x**, **a** and **b** as the primary quantities of interest.

We have now converted the original nonlinear problem into a linear one (in fact, a linear one without explicit additive constants) in the region of the converged solution point. Agreement between the original functions and the linearized ones in this neighborhood is crucial, because it guarantees that the *fitted* values of the parameters and data will be consistent with one another in the context of the original functions $y_i(\mathbf{c})$, even if the linearized functions should differ considerably from the original ones in parts of parameter space far from the solution point.

In order to proceed, we shall have to make the additional assumption that such mismatches between the distant behavior of the linearized and original functions may be neglected in calculating variances. This permits one to use the law of propagation of errors to propagate the covariances of the parameters forward into the covariances of the data.

3. Summary of the Method of Least Squares

It is shown in Ref. [11] that the minimum-variance, linear, unbiased estimates $\mathbf{a}'$ of the nuclear model parameters, the estimates that derive the maximum benefit from the provided experimental and theoretical information, are given by

$$\mathbf{a}' = \mathbf{a} - C(\mathbf{a}, \mathbf{p})\,\mathbf{G}\,\mathbf{p}\,, \tag{3.1}$$

$$D(\mathbf{a}') = D(\mathbf{a}) - C(\mathbf{a}, \mathbf{p})\,\mathbf{G}\,C(\mathbf{p}, \mathbf{a})\,, \tag{3.2}$$

where we have introduced the important concept of the "discrepancy" vector **p**,

$$\mathbf{p} = \mathbf{b} - \mathbf{R}\,\mathbf{a}\,, \tag{3.3}$$

and the corresponding "information matrix" **G** and covariance matrix $D(\mathbf{p})$,

$$\mathbf{G}^{-1} \equiv D(\mathbf{p}) = C(\mathbf{p}, \mathbf{p})\,. \tag{3.4}$$

By the usual rules of covariance algebra,

$$D(\mathbf{p}) = D(\mathbf{b}) - C(\mathbf{b},\mathbf{a})\,\mathbf{R}^* - \mathbf{R}\,C(\mathbf{a},\mathbf{b}) + \mathbf{R}\,D(\mathbf{a})\,\mathbf{R}^*\,, \tag{3.5}$$

and

$$C(\mathbf{a}, \mathbf{p}) = C(\mathbf{a}, \mathbf{b}) - D(\mathbf{a})\,\mathbf{R}^* \,. \tag{3.6}$$

A second interesting set of quantities is a linear combination of the parameters, $\mathbf{z} = \mathbf{L}\,\mathbf{a}$. As shown in Ref. [11], the minimum-variance estimate of $\mathbf{z}$ is simply $\mathbf{z}' = \mathbf{L}\,\mathbf{a}'$, which is the Gauss-Markov theorem for the partitioned case. Thus the minimum-variance estimate $\mathbf{a}'$ of the parameters can be used directly to calculate the least-squares (minimum-variance) estimate of arbitrary linear functions of the parameters, without actually repeating the least-square exercise. By the law of propagation of errors, the covariances of $\mathbf{z}'$ are given by

$$D(\mathbf{z}') = \mathbf{L}\,D(\mathbf{a}')\,\mathbf{L}^* \,. \tag{3.7}$$

Thus for any linear (or linearizable) function of the fitted nuclear model parameters, and in particular the computed output of a nuclear model program, the covariances of the computed data are related to the covariances of the best-fit parameters by the familiar law of propagation of errors.

4. Model Deficiency

Another important aspect of the uncertainty of nuclear-model calculations is the treatment of deficiencies in the models themselves. By approaching nuclear-data evaluation as an empirical science, one does not need to dwell on the conceptual questions raised when two or more rather different nuclear models can be made to give reasonable fits to the same measured data, causing model uncertainty and parameter uncertainty, in some absolute sense, to become "hopelessly intertwined", to use D. L. Smith's expression. (Sec. 9.2.5. in Ref. [12]). The reason for our relaxed attitude is that the evaluator, in such a case, is free simply to choose among these models the one that he prefers, on either physical or practical grounds, and to move forward with an uncertainty analysis. The covariances that he obtains in the end will describe the uncertainties in his own evaluation, as performed with his own chosen model.

A much more important problem, from our present viewpoint, is the situation where, *even after completion of a least-squares adjustment of parameters*, the best available model still gives poor fits to the data. In discussing this important case, we first must distinguish between "discrepancies" and "inconsistencies".

Discrepancy is a normal state of affairs, referring to the existence of differences between the predictions and the measurements that are comparable to the estimated uncertainties of these predictions and measurements. In fact, as discussed in Sections 2 and 3, the whole point of the least-squares procedure is that discrepancies between predictions and observations can be viewed as a valuable new source of information about the magnitude of the parameters.

Inconsistency, on the other hand, is an entirely different matter. Inconsistency can be compactly defined as a case where the discrepancies are statistically unlikely. Inconsistency is clearly a property of the entire network of input information, namely the a-priori parameters $\mathbf{a}$ and data $\mathbf{b}$, their respective covariances, and the model-based sensitivities $\mathbf{R}$. In order to derive a quantitative measure of the inconsistency in a set of data, we first examine the magnitude of the discrepancy vector,

$$\mathbf{p} = \mathbf{b} - \mathbf{R}\,\mathbf{a} \,. \tag{4.1}$$

Unlike $\mathbf{b}$ and $\mathbf{a}$, the true value of $\mathbf{p}$ is actually known:

$$\langle \mathbf{p} \rangle = \langle \mathbf{b} \rangle - \mathbf{R} \langle \mathbf{a} \rangle = \mathbf{R}\,\mathbf{x} - \mathbf{R}\,\mathbf{x} = \mathbf{0} \,.$$

The unique value of $\mathbf{p}$ for the purposes of consistency analysis is that we are able to directly compare the *actual error* of the discrepancy vector,

$$\mathbf{p} - \langle \mathbf{p} \rangle = \mathbf{p}$$

with the *expected error*, as contained in D(**p**),

$$D(\mathbf{p}) = \langle (\mathbf{p} - \langle \mathbf{p} \rangle) (\mathbf{p} - \langle \mathbf{p} \rangle)^* \rangle = \langle \mathbf{p}\, \mathbf{p}^* \rangle . \tag{4.2}$$

Recalling Eq. (3.5), the covariance matrix of **p** is given in terms of the input data to a least squares study by the following relation:

$$D(\mathbf{p}) = D(\mathbf{b}) - C(\mathbf{b},\mathbf{a})\, \mathbf{R}^* - \mathbf{R}\, C(\mathbf{a},\mathbf{b}) + \mathbf{R}\, D(\mathbf{a})\, \mathbf{R}^* . \tag{4.3}$$

For reasons that will become clear shortly, the most useful measure of consistency is obtained from the specific matrix product

$$\chi^2 = \mathbf{p}^*\, \mathbf{G}\, \mathbf{p} , \tag{4.4}$$

where, as above, $\mathbf{G}^{-1} = D(\mathbf{p})$. Note that χ^2 is a scalar quantity, a single number.

If **p** were repeatedly sampled from a distribution with covariances D(**p**), χ^2 would also display a distribution of values. The expected value of χ^2 obtained by averaging over this distribution is just

$$\langle \chi^2 \rangle = m \tag{4.5}$$

where m is, as before, the dimension of the vector **p**. The validity of this important result, Eq. (4.5), is shown below in a proof adapted from Hamilton [13]. The proof rests on an interesting theorem involving the trace (sum of diagonal elements) of a square matrix: If **r** and **s** are two arbitrary column vectors of equal dimension, then it is easy to show that $\mathbf{s}^*\, \mathbf{r} = \text{trace}(\mathbf{r}\, \mathbf{s}^*)$. Proceeding then with the proof,

$$\begin{aligned}
\langle \chi^2 \rangle &= \langle \mathbf{p}^*\, \mathbf{G}\, \mathbf{p} \rangle \\
&= \langle \text{trace}(\mathbf{p}\, \mathbf{p}^*\, \mathbf{G}) \rangle \\
&= \text{trace} \langle \mathbf{p}\, \mathbf{p}^*\, \mathbf{G} \rangle \\
&= \text{trace} \langle \mathbf{p}\, \mathbf{p}^* \rangle \mathbf{G} \\
&= \text{trace}\, D(\mathbf{p})\, \mathbf{G} \\
&= \text{trace}\, \mathbf{I}_{m,m} \\
&= m .
\end{aligned}$$

Therefore if χ^2/m greatly exceeds unity for a particular set of predictions and observations, then it is highly unlikely that **p** was actually sampled from a distribution with the claimed covariances D(**p**), and the network of input information has been shown to be inconsistent.

How should one react to inconsistency? One must first eliminate the possibility that the inconsistency is due to a simple blunder or mistake in the handling of the data. Also, one must be alert to the possibility that experimentalists have underestimated the uncertainties in their quoted results, **a** and **b**. After eliminating these other possible explanations, one is lead to a strong indication of deficiencies in the model itself.

Rather than interpreting a large χ^2 as a failure, probably most theorists view it as an opportunity. For it is *only* when χ^2/m is large (and no alternative explanations can be found) that theorists have a clear signal from the laboratory that something is missing from their model. Such a signal is often the prelude to the emergence of entirely new insights.

In order to acquire this important new information about the model, Eq. (4.4), it is necessary to carry the uncertainty analysis, exactly as described in the preceding Sections, up to the point just before the final step of parameter adjustment. For example, compare Eqs. (4.1) - (4.4) with the parameter adjustment relation, Eq. (3.1). Thus, there is little difference, both in terms of the detailed mathematical formalism employed and the work required to prepare the input information, between (a) performing a proper assessment of the consistency between a given model and a set of measurements, and (b) performing a least-squares fit to those measurements. Thus the possibility of encountering inconsistency is not a reason to avoid performing a least-squares fit but, rather, a good reason to perform one.

5. Model Sensitivities from Computer Calculus

In previous Sections we demonstrated a methodology for improving nuclear models and their associated parameters. The basic recommended approach is to compare model predictions with measurements and to extract the maximum possible amount of information from the comparisons using partitioned least squares. For a given set of experimental data selected for normalization purposes, the least squares method provides a unique best estimate $\mathbf{a}'$ of the parameters and their covariances $D(\mathbf{a}')$. Both the $\mathbf{a}'$ and all linear functions of the $\mathbf{a}'$ have minimum variance, relative to other estimates based on the same data. Thus, subsequent calculations performed with the revised parameters, even those involving unmeasured data types, will benefit from this gain in information.

The theoretical calculation of nuclear data can be characterized as the computation of a set of dependent variables y_i (the data), as functions $y_i(\mathbf{c})$ of several independent variables c_j (the parameters). As noted in Section 2.3, y_i is determined by executing a large computer program, containing typically ten thousand statements, so the functional forms are known in practice only via tables or graphs. On the other hand, a primary requirement for the use of the least squares approach is the availability of numerical values of the derivatives of the output data with respect to the input parameters, that is, sensitivities.

For the simpler models such as the spherical optical model, it is possible (and common practice) to include explicit coding in the computer programs for the purpose of calculating sensitivities as part of an integrated calculation-plus-parameter-search package [14]. However, in all (or nearly all) published studies related to Hauser-Feshbach and coupled-channel calculations, and other calculations of comparable complexity (for example, Refs. [7] and [14]), sensitivities have been approximated by "pseudo-derivatives", obtained by repeating each calculation with slightly altered input for one parameter and taking the ratio of the resulting differences. The main problem with pseudo-derivatives is that, for each parameter-datum *pair*, it must be tediously verified that the change in the parameter is large enough to be numerically significant, but small enough to avoid major nonlinearities. This fundamental difficulty has discouraged the wider use of the least squares approach to parameter adjustment for the more complex models.

In this Section, we shall discuss a more sophisticated approach that is capable of adding "exact" derivative-computing logic to an arbitrarily complicated FORTRAN program, with only a modest amount of user intervention in the program-conversion process. Following Oblow [15], we call this approach "computer calculus". Through the use of computer calculus, the input parameters for almost any nuclear model can be optimized through the use of least squares, with all of the attendant benefits mentioned in the preceding Sections.

We are only interested in models where one actually can define partial derivatives $R_{ij} = \partial y_i/\partial c_j$ over at least some range of parameter values about the nominal ones $\mathbf{c}_0$. There may exist nuclear models that violate this criterion, for example, because some of the y_i are highly discontinuous functions of certain c_j. Upon encountering such a situation, one can adopt the

viewpoint that nuclear-data evaluation is still an empirical science and simply reformulate the model in order to circumvent the difficulty. Such reformulations, made for calculational convenience, are both logical and appropriate.

In the computer-calculus approach [15,16,17], a pre-compiler searches a FORTRAN computer program for arithmetic statements and constructs from them the additional statements required for the calculation of numerical values of the derivatives R_{ij} at the point $\mathbf{c}_0$ in parameter space. The calculation of pseudo-derivatives by finite differences is not involved in this approach, so the computed sensitivities should be as accurate as any other computed quantity. The interested reader is referred to Ref. [18], where he will find a review of the theoretical basis of computer calculus, as well as some preliminary results for the application of the GRESS system [16] to the task of creating a sensitivity-analysis version of the GNASH statistical-preequilibrium program [19].

The final phase of this work, namely the incorporation of this sensitivity version of GNASH into the framework of a conventional nonlinear least-squares analysis, as described in the preceding Sections, is now in progress. There appear to be no major obstacles to prevent the achievement of the twin goals of generating optimized model-parameter sets and computing defendable covariances of computed quantities.

The availability of computed covariances from the new sensitivity version of GNASH, as well as from the existing EDA program [20] and other resonance-analysis codes such as those discussed in Ref. [5] , have imparted new significance to the development of the new ENDF File-30 format to store very compactly the computed covariances from model codes. This new format is described in the next Section.

6. FILE 30: AN ENDF FORMAT FOR DATA COVARIANCES FROM PARAMETER COVARIANCES AND SENSITIVITIES

6.1. General Description

Within the framework of the internationally endorsed ENDF format [1], File 30 is provided as a means of numerically describing the covariances of reaction cross sections, multiplicities, and energy-angle distributions that result from propagating the covariances of a set of underlying parameters (including, but not limited to, the input parameters of a nuclear-model code), using an evaluator-supplied set of parameter covariances and parameter sensitivities. File 30 can be used to describe data covariances of any origin, so long as they can be formally separated into a set of parameter covariances and an accompanying set of data sensitivities.

The need for a covariance format of this type has been suggested in connection with the R-matrix analysis of the ENDF/B-VI light-element standards [21]. The key parameters here are the parameters of a few high-energy resonances in the relevant compound systems. As discussed in the preceding Sections, an area where the File-30 format is expected to find even wider application is in representing the covariances of cross sections and secondary-particle emission spectra and angular distributions due to neutron interactions in the range above 5 MeV, when the data are obtained primarily from the optical model and statistical-preequilibrium nuclear theory. Relevant parameters here include the optical parameters, level-density parameters, preequilibrium matrix elements, and gamma-ray strength functions.

It is shown below that multigroup averages of parameter sensitivities are identical to the parameter sensitivities of the corresponding multigroup data. It is the latter that are actually needed in most applications. (See Section 6.5.) To take maximum advantage of this equivalence, sensitivity information is represented in File 30 in a format that is as close as possible to the format for storage of the corresponding nuclear data, so that the sensitivities can be retrieved and integrated by processing codes, such as the covariance processing modules of

NJOY [22], with the least possible modification.

To limit the bulk of the files and to minimize processing costs, evaluators are encouraged to reduce (if possible) the number of parameters and the number of sensitivities per parameter to the minimum necessary to describe data uncertainties of practical importance. This is not as large a restriction as it may seem, however, because that is exactly how an evaluator adjusts parameters, namely, by focusing his efforts on the most significant uncertainties and sensitivities.

In defining the format for File 30, no attempt was made to prejudge the types of parameters or the forms of nuclear theory that may be most appropriate or useful. Discussion of such points is obviously encouraged in the printed documentation, but the format itself was deliberately kept totally general. One advantage of this generality is that the results of a wide variety of evaluation methodologies can be described using a single format.

Although correlations between the covariances in File 30 and those in the other ENDF-formatted covariance files are not permitted, the fact that File 30 is so general can be used to advantage to describe any such correlations that may exist. By introducing appropriate "artificial" parameters and sensitivities, covariance data from other ENDF files can be "promoted" to File-30 format, in which case full correlation possibilities will exist.

6.2. Definitions

In the context of File 30, the word "sensitivity" is defined as the derivative of an evaluated quantity, y, with respect to the logarithm of a parameter, a_i,

$$y'_i \equiv \partial y/\partial(\ln a_i) = a_i \, \partial y/\partial a_i \, . \qquad (6.1)$$

An advantage of employing such derivatives is that y'_i is expressed in exactly the same units as y, whether it be an actual cross section or a distribution (energy distribution, angle distribution, double-differential quantity, etc.). This means that integrations over energy and angle can be performed with minimal changes in multigroup processing codes. The use of derivatives with respect to the logarithms of the parameters also meshes nicely with the use of relative parameter-covariance matrices, as shown below in Eq. (6.7).

As discussed in detail in Chapter 30 of Ref. [1], a subsection of one section of File 30 is employed to store the sensitivities of the data in one section (called the *referenced* section) of a file elsewhere in the material of interest. (For definitions of "file", "section", and "subsection" and other ENDF nomenclature, the interested reader should consult the Preface of Ref. [1].)

It should be emphasized that normally there will not be a direct, one-to-one correspondence between the energy or angular grid in a subsection of File 30 and that used in the referenced section. This follows from the fact that the derivatives in File 30 are not actually the derivatives of individual data values appearing elsewhere in the evaluation. Rather, the collection of data in one such subsection of File 30 should form an adequate representation of the energy-and angle-dependence of the relevant derivative *function*, making effective use of the standard interpolation laws.

File 30 does not permit the representation of the uncertainty in independent variables (the floating-point numbers that define the energy and angle grids of an ENDF section). This would seriously complicate the calculation of the uncertainty in averaged quantities, as discussed below. Further, if y is thought of as the output of a model calculation, quantities such as the incident energy or outgoing angle are *specified* by the model-code user and have no meaningful uncertainty. In addition, File 30 may not be used to represent uncertainty of any integer, nor the uncertainty of stand-alone (not tabulated) quantities that affect energy or angle grids, such as masses, Q-values, and the boundaries of energy ranges. Thus, it is understood

that the data fields normally used to store probability information (cross sections, multiplicities, or normalized distributions) are used in File 30 to record sensitivity information, but that other quantities have standard (File n, where $n \neq 30$) ENDF definitions.

6.3. Treatment of Various Data Types

Following the general guidelines stated above, subsections of File 30 describing cross-section (as opposed to multiplicity or distribution) sensitivities would have the same mechanical structure as sections of the cross-section file, File 3. Of course, since sensitivities are derivatives, many more negative numbers would appear in the data fields than one normally expects to see in a cross-section file.

Some interesting points arise with respect to distributions, for example tabulated data in the angular distribution file, File 4, for elastic scattering. If the derivatives of the normalized angular distribution $h(\theta)$ with respect to a given parameter are large, these derivatives should be included in File 30. Note that since $h(\theta)$ integrates to unity by definition, the angle integral of the sensitivities (equal to the parameter-derivative of the angle integral) should be zero.

A second important aspect of the use of two separate functions to build the actual desired data is that, in order to build the corresponding sensitivities, the product rule is employed. For example, the differential elastic cross section $\gamma(\theta)$ (barns/steradian) at angle θ is formed as a product,

$$\gamma(\theta) = dy/d\Omega = y\ h(\theta)\,, \tag{6.2}$$

so that

$$\partial\gamma(\theta)/\partial a_i = y\ \partial h(\theta)/\partial a_i + h(\theta)\ \partial y/\partial a_i\,. \tag{6.3}$$

Multiplying both sides of Eq. (6.3) by a_i, and recalling the notation of Eq. (6.1), one gets,

$$\gamma'_i(\theta) = y\ h'_i(\theta) + y'_i\ h(\theta)\,. \tag{6.4}$$

Eq. (6.4) shows, then, how the sensitivity $\gamma'_i(\theta)$ is constructed from the data in two different subsections (y'_i and h'_i) of a section of File 30, plus data (y and h) from Files 3 and 4, respectively. The generalizations needed to treat three or more separate factors are obvious.

Both to reduce the bulk and to reduce processing costs, evaluators are encouraged to omit reference to sections in the main evaluation (File n, $n \neq 30$) that exhibit little sensitivity to a given parameter. Such omissions will be treated as if zeros had been entered explicitly. For example, if the angular distributions are omitted from File 30, then the first term on the right in Eq. (6.4) will be omitted.

Just as one is permitted to employ a Legendre representation of $h(\theta)$ in File 4, one is permitted in File 30 to use a Legendre expansion to represent $h'_i(\theta)$. In fact, if it reduces the size of the files, it is preferable to use Legendre moments for $h'_i(\theta)$, even if $h(\theta)$ itself is given in tabular form. As mentioned above $h'_i(\theta)$ must integrate to zero, so the magnitude of the implied zero-th Legendre moment of $h'_i(\theta)$ is zero, not unity. These considerations of File 4-type sensitivities can be extended in an obvious way to treat neutron spectra (in File 5), isomer-ratios, photon-production multiplicities, fission-product yields, and so on.

No fundamental new problems are introduced by considering double-differential data, as

represented in File 6. In that case, the emission probability h becomes a function $h(E',\theta)$ of both the final energy and angle of the outgoing particle. The only complication that this adds is that h'_i in Eq. (6.4), for example, is also doubly differential, $h'_i = h'_i(E',\theta)$. In fact, it is conceivable that $h'_i(E',\theta)$ for some parameter exhibits more severe angle-energy correlations than $h(E',\theta)$ itself, so it is permitted to represent the emission sensitivities for a given reaction in File-6 format in File 30, even though the angle and energy distributions for that reaction are given as separable functions in Files 4 and 5. Conversely, for the sake of compactness, one may choose to represent uncertainties in File-6 correlated angle-energy distributions with separable functions in File 30.

6.4. Multigrouped Sensitivities

Multigroup operations on the data in an evaluation can be summarized as the performance of certain weighted integrations over incident energy, secondary particle type, secondary energy, and secondary angle. Although these operations are very complicated, there is no connection between the variables (or limits) of integration and the nuclear-model parameters of concern in File 30. One can take advantage of this in calculating the derivatives of multigroup-averaged data with respect to nuclear-model parameters. If we introduce g as a generic group-averaged quantity (such as a single Legendre moment of one element of a scattering matrix), which corresponds to a differential quantity γ, then

$$g = \int dE\, dE'\, d\Omega\ \gamma(E,E',\theta)\ \omega(E,E',\theta)\ , \tag{6.5}$$

where ω is some weighting function. As discussed below, one frequently is interested in the uncertainty in such multigroup quantities, and to obtain this uncertainty, one will first need to calculate the derivative of g with respect to the parameter a_i:

$$\begin{aligned} g'_i &= \partial g/\partial(\ln a_i) = a_i\, \partial g/\partial a_i \\ &= \int dE\, dE'\, d\Omega\ a_i\ \partial\gamma(E,E',\theta)/\partial a_i\ \omega(E,E',\theta)\ , \\ &= \int dE\, dE'\, d\Omega\ \gamma'_i(E,E',\theta)\ \omega(E,E',\theta)\ . \end{aligned} \tag{6.6}$$

Comparing Eqs. (6.5) and (6.6), we obtain the useful result that the sensitivity of a multigroup value to a given nuclear-model parameter is equal to the multigroup average of the (energy- and angle-dependent) parameter sensitivity. Thus an ENDF processing program that calculates multigroup cross sections, as in Eq. (6.5), can be used with few modifications to calculate the parameter sensitivity of the multigroup constants, Eq. (6.6). As mentioned in Section 6.1., this is the motivation for storing the sensitivities γ'_i in a format that is as close as possible to the format of the data γ. The reader who wishes to construct a covariance file in the File-30 format should consult Chapter 30 of Ref. [1] for the details of the actual data-storage format.

6.5. Multigroup Applications of Parameter Covariances

To help place the above material in perspective, we conclude this Section with a few remarks about the applications of covariances stored in File-30 format. Given relative covariances,

$$RC(a_i, a_j) \equiv C(a_i, a_j) / a_i\, a_j\ ,$$

from File 30, and the multigrouped parameter sensitivities g'_{mi} from Eq. (6.6), it is straightforward to obtain the covariance between one multigroup datum g_m and another g_n. It is necessary to add the additional index to keep track of the multiplicity of data types. Making the usual approximation that g_m is not an extremely nonlinear function of the parameters, we expand in a Taylor series and retain only the first term,

$$C(g_m, g_n) = \sum_{i,j} \partial g_m/\partial a_i \; \partial g_n/\partial a_j \; C(a_i, a_j)$$

$$= \sum_{i,j} a_i \; a_j \; \partial g_m/\partial a_i \; \partial g_n/\partial a_j \; C(a_i, a_j) \; / \; a_i \; a_j$$

$$= \sum_{i,j} g'_{mi} \; g'_{nj} \; RC(a_i, a_j) \, . \qquad (6.7)$$

Eq. (6.7) gives the desired multigroup covariance matrix in terms of the multigrouped (logarithmic) sensitivities, as calculated in Eq. (6.6), and data read directly from File 30.

In addition to providing a direct route to the calculation of the uncertainty of multigroup cross sections due to parameter uncertainties, data provided in File-30 format have the potential for additional kinds of application, which do not involve straightforward application of Eq. (6.7). Since these issues relate to computing requirements, it is necessary to deal with specific examples. In situations presently foreseen, the number of nuclear parameters might be in the range of 10 to 100, so we take 50 as typical. On the other hand, it is very common in neutronics applications that the number of individual multigroup constants substantially exceeds 10 000. In such cases, the data covariance matrix $C(g_m, g_n)$ becomes prohibitively large (10^8 items), while the sensitivity matrix g'_{mi} (containing 500 000 items) and parameter covariance matrix $RC(a_i, a_j)$ (with 2 500 items) remain fairly manageable. Since, according to Eq. (6.7), all of the covariance information is already contained in the latter two items, it seems likely that multigroup libraries for high-energy neutronics applications will store these items separately, rather than in the product form.

Further efficiencies are possible if the ultimate aim is to calculate the uncertainties in a set of predicted responses (dose, radiation damage, fuel-breeding ratio, etc.), which can be denoted by a column vector **r**. A typical number of such quantities might also be around 50. The covariance matrix D(**r**) for the integral quantities is related (again in the first-order approximation) to the cross section covariance matrix D(**g**), with elements given by Eq. (6.7), by the propagation of errors relation,

$$D(\mathbf{r}) = \mathbf{H} \; D(\mathbf{g}) \; \mathbf{H}^* \, ,$$

where **H** is the 50 (row) × 10 000 (column) sensitivity matrix relating the integral quantities **r** to the multigroup cross sections **g**. **H** can be obtained from standard, perturbation-theory based neutronics analyses.

If we introduce a 10 000 × 50 matrix **R** relating the multigroup cross sections to the nuclear parameters, that is, having elements $\partial g_m/\partial a_i$, then the first line of Eq. (6.7) can be rewritten in matrix form,

$$D(\mathbf{g}) = \mathbf{R} \; D(\mathbf{a}) \; \mathbf{R}^* \, .$$

Eq. (6.8) then becomes

$$D(\mathbf{r}) = \mathbf{H} \; [\, \mathbf{R} \; D(\mathbf{a}) \; \mathbf{R}^* \,] \; \mathbf{H}^* = \mathbf{P} \; D(\mathbf{a}) \; \mathbf{P}^* \, . \qquad (6.8)$$

The product matrix **P** = **H R**, which contains the direct sensitivity of the integral data to the nuclear-model parameters, is very compact, having about the same size as the covariance matrix D(**a**). Note that if one *only* needs the uncertainties of the responses D(**r**), one never actually has to calculate the full 10 000 × 10 000 cross-section covariance matrix.

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ASPECTS OF INTERNAL CONSISTENCY OF COVARIANCE DATA

S. TAGESEN
Institut für Radiumforschung und Kernphysik
University of Vienna, Boltzmanngasse 3, A-1090 Vienna, Austria

ABSTRACT

The "Evaluated Nuclear Data Files" (ENDF) contain – due to existing physical relations – large portions of data which are not independent. There exist either connections caused by common features of experimental arrangements or built in "redundancies" caused by physical constraints due to relations between the cross sections contained in the files. Both facts can lead to the loss of consistency each time when new experimental information is added.

Some important aspects concerning covariance information in this context, as well as general precautions in the "design" of covariance matrices are summarized and discussed.

1. Introduction

Covariance data, as given in files 30 of the ENDF-6 specifications[1] have become increasingly important due to more demanding requirements in the prediction of dimensions of components for highly specialized facilities as, e.g., the planed NET/ITER fusion reactor. Accordingly considerable emphasis has been put on the generation of such data. Experience in this field is, however, still rather poor and consequently evaluators have to be especially careful in view of the important consequences in which any deficiencies might result

Evaluators have started to generate covariance information for the cross sections with highest technical importance in a way which treats them as rather isolated data sets. One must, however, be aware that as a consequence of the historical growth of the underlying database there exist numerous coherences which, if not properly reflected in the uncertainty files, will considerably mislead predictions based on those data.

In addition the ENDF-6 files contain in several places redundant information. This is highly desirable from the users point of view as it may save a lot of processing. It is clear, however, that special care must be taken to ensure, that uncertainties for those quantities be defined and stored in a unique and correct way.

Some of the inherent dangers of the evaluators business will be discussed in the following sections.

2. The covariance matrix

2.1. General properties

Let X be a particular input value contributing to an evaluation, e.g. of a reaction cross section at incident particle energy E. Several of those data from different measurements are distributed according to a (normalized) density function f(X). The expected ("true") value is then given by (this treatment is closely following the presentation given by R. Peelle[2])

$$\langle X \rangle = \int X\, f(X)\, dX \qquad (1)$$

and this is the number given in an ENDF. If we take two results $\langle X \rangle$ and $\langle Y \rangle$, e.g. cross sections of different reactions or/and at different incident particle energies, we can define

$$COV(X,Y) = \iint (X - \langle X \rangle)\,(Y - \langle Y \rangle)\, f(X,Y)\, dX\, dY \qquad (2)$$

the covariance between X and Y,

$$VAR(X) = COV(X,X) = \langle (X - \langle X \rangle)^2 \rangle \qquad (3)$$

the variance,

$$s(X) = (VAR(X))^{1/2} \qquad (4)$$

the standard deviation or uncertainty in $\langle X \rangle$ and

$$COR(X,Y) = COV(X,Y) / (s(X)\, s(Y)) \qquad (5)$$

the correlation between X and Y.

It is important to note at this point, that all the defined quantities depend on the density function f(X,Y), which in turn is given by the design of all the individual experiments contributing data to the particular evaluation. From this we can draw our

consistency statement #1:
An evaluation (defined by the contributing experimental or other data) and its covariance information belong together, they may not reasonably be used separately.

In particular, one should never take the covariance file from one ENDF and use it for a different one.

Further general properties of covariance matrices are
- they are by definition symmetric
- they are positive (semi)definite

The latter is a consequence of the fact, that variances of any function of physical quantities must be non-negative and are usually not zero.

This property may be used to test whether a proposed covariance matrix is "well behaving". The most rigourous test in this respect would be transformation of the matrix to diagonal form to find out if any of the eigenvalues were zero or negative.

2.2. Precautions in the design of covariance matrices

The general properties of a data covariance matrix which have been pointed out in section 2.1. are normally correctly produced when such a matrix has been derived by including correct and complete uncertainty information into an evaluation by means of a code like, e.g., GLUCS[3]. If due to the lack of complete information approximate methods have to be used for the assignment of covariances, special precautions should be taken to avoid the occurrence of effects that must be excluded because of underlying physics or definitions, e.g. negative weights or correlation > 100%.

Apart from the requirements outlined in section 2.1. there is an additional aspect which sometimes has received insufficient attention. If one is to construct a covariance matrix in the way indicated by (2), then if VAR(X) << VAR(Y) or vice versa and one uses a high correlation component for some reason, it may happen that COV(X,Y) > VAR(X) or COV(X,Y) > VAR(Y), because with 100% correlation COV(X,Y) = s(X)*s(Y). Such a situation must be avoided since it produces the assignment of negative weights[4] and leads with correct uncertainty propagation to mean values outside the range given by <X> and <Y>. The arguments that justify the bounds

$$COV(X,Y) < VAR(X) \text{ and } COV(X,Y) < VAR(Y) \qquad (6)$$

are the following: If uncertainty components for different evaluated data points are combined correctly, then they contribute either to both variances (correlated) or to one of them only. Consequently 100% correlation can normally occur only with equal variances, because otherwise there must be an uncorrelated additional component in one of the data points.

Sufficient attention should be devoted also to aspects facilitating future updates. Especially important is a reasonable balance between long-range and short-range correlations. Due to the state of the art of modern experiment technology uncertainty components with purely statistical behaviour are among the least important. If the covariance matrix is dominated by long-range correlated components, this may give rise to severe consistency problems in future updates due to shape "rigidity". Similar problems would arise with a too broad energy group structure for the covariance matrix because all cross sections belonging to one group are treated as fully correlated.

3. Correlations between reactions

Only a small part of reaction studies have been carried out as "direct" (absolute) measurements, that is, the result is determined completely by physical and apparatus constants and decay properties of the isotope under study. Usually nuclear reactions are measured "relative" to some other "reference" or "standard" reaction, which is agreed on to be known with high accuracy. This has led in course of time to numerous interrelations and dependencies which rarely are reflected in the ENDF's.

As long as there were numerous data sets with low correlation (high statistical uncertainty component), dependencies between different reactions did not play an important role in uncertainty calculations for applications of evaluated nuclear data. Meanwhile statistical uncertainty components were successively reduced due to progress in experimental techniques while correlated uncertainty components in some cases not even have been identified (e.g. same sample used in different experiments etc.).

Already in 1979 an indication of the magnitude of correlations between reactions has been given in an evaluation carried out at the IRK[5]. At that time the overall uncertainties were still rather large and inclusion of correlations between reactions into ENDF's did not appear to be necessary in view of the minor influences on any derived results compared to the large storage requirements. Considering the recent demands on accuracy of uncertainty estimates the topic should be recalled to attention now. It is, of course, not necessary to ask for interreaction covariances for all reactions. Most of these matrices would in fact contain elements close to zero only. Some reactions, however, which have been used frequently as "references" in ratio measurements should be examined and covariance matrices given. An example for a relatively large correlation from the mentioned evaluation[5] is given in table 1.

Table 1. Relative correlations [%] for the reactions $^{24}Mg(n,p) - {}^{64}Zn(n,p)$

E-GROUP	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	
1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.00 E-5
2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	28	31	40	39	36	37	38	36	48	40	27	21	0	0	45	42	43	4.60 E+6
3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	28	31	40	39	36	37	38	36	48	40	27	21	0	0	45	42	43	5.20 E+6
4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	28	31	40	39	36	37	38	36	48	40	27	21	0	0	45	42	43	5.60 E+6
5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	17	19	24	24	22	22	23	22	29	24	16	13	0	0	27	25	26	5.80 E+6
6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	19	21	27	27	24	25	26	25	33	27	18	15	0	0	31	29	30	6.10 E+6
7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	23	26	33	32	30	31	32	30	40	34	22	18	0	0	38	35	36	6.30 E+6
8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	17	18	24	23	21	22	23	22	29	24	16	13	0	0	27	25	26	6.50 E+6
9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	17	19	25	25	22	23	24	23	30	25	17	13	0	0	28	26	27	6.70 E+6
10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	18	20	26	25	23	24	25	24	31	26	17	14	0	0	30	27	28	6.90 E+6
11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	20	22	28	28	25	26	27	26	34	29	19	15	0	0	32	30	31	7.10 E+6
12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	20	22	29	28	26	27	27	26	35	29	19	16	0	0	33	30	32	7.31 E+6
13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	18	20	25	25	23	24	24	23	30	26	17	14	0	0	29	27	28	7.51 E+6
14	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	18	20	26	25	23	24	24	23	31	26	17	14	0	0	29	27	28	7.70 E+6
15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	25	28	35	35	32	33	34	33	43	36	24	19	0	0	40	37	39	7.90 E+6
16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	19	21	27	26	24	25	25	24	32	27	18	14	0	0	30	28	29	8.11 E+6
17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	28	31	40	39	36	37	38	36	48	40	27	21	0	0	45	42	43	8.50 E+6
18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	28	31	40	39	36	37	38	36	48	40	27	21	0	0	45	42	43	9.50 E+6
19	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	27	30	39	38	35	36	37	35	46	39	26	21	0	0	44	41	42	1.00 E+7
20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	28	31	40	39	36	37	38	36	48	40	27	21	0	0	45	42	43	1.05 E+7
21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	24	27	35	34	31	32	33	32	42	35	23	19	0	0	39	37	38	1.15 E+7
22	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.22 E+7
23	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	8	9	12	12	11	12	12	11	15	13	8	7	0	0	14	13	14	1.24 E+7
24	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5	4	2	2	2	3	4	2	0	1.26 E+7
25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.28 E+7
26	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.30 E+7
27	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	8	7	4	3	4	6	6	3	0	1.32 E+7
28	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.34 E+7
29	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	4	5	5	4	4	5	4	9	7	5	4	1	2	8	7	5	1.36 E+7
30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.38 E+7
31	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	2	3	3	3	3	3	3	4	3	2	1	0	0	3	3	3	1.40 E+7
32	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	1	1	0	0	1.42 E+7
33	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	1	1	0	0	1.44 E+7
34	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	2	3	3	3	3	3	3	4	3	2	1	0	0	3	3	3	1.46 E+7
35	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	3	3	3	3	3	3	3	6	5	3	2	0	1	5	4	4	1.48 E+7
36	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	3	4	4	4	4	4	4	5	4	3	5	0	0	5	4	5	1.46 E+7
37	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	10	8	5	4	5	8	8	4	0	1.48 E+7
38	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6	6	3	2	3	5	5	3	0	1.50 E+7
39	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7	6	3	2	3	5	5	3	0	1.55 E+7
40	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	9	11	14	13	12	13	13	13	23	20	13	10	3	5	21	18	15	1.60 E+7
41	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	14	15	20	19	18	18	19	18	34	29	19	15	5	7	31	25	22	1.70 E+7
	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	12	13	17	16	15	16	16	15	20	17	11	9	0	0	19	18	18	1.80 E+7
	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	13	14	19	18	17	17	18	17	22	19	12	10	0	0	21	20	20	1.90 E+7
E-SCALE	1.0	9.2	1.2	1.5	1.7	2.0	2.2	2.5	2.7	3.0	3.2	3.5	3.7	4.0	4.2	4.5	5.0	5.2	5.5	5.7	6.0	7.0	8.0	9.0	1.0	1.3	1.4	1.4	1.4	1.5	1.6	1.7	1.8	
	E-5	E+5	E+6	E+6	E+6	E+6	E+6	E+6	E+6	E+6	E+6	E+6	E+6	E+6	E+6	E+6	E+6	E+6	E+6	E+6	E+6	E+6	E+6	E+6	E+7	E+7	E+7	E+7	E+7	E+7	E+7	E+7	E+7	

It might even be useful to indicate explicitly if such correlations in some cases turned out to be negligibly small. One element covering the whole energy range would suffice and users would be safe from unpleasant surprises since ENDF-6 specifications state that no covariance information in the files does not indicate no existing correlations.

If covariances between reactions are entered into an ENDF, e.g. by means of a LB=6 sub-subsection in file 33, one has to take precautions to maintain consistency in future updates. Such a covariance matrix should always be given in the files of both materials affected. Covariance information is not mandatory up to now and there is no easy way to find out where in all the tapes and materials might possibly exist interreaction covariances. This implies on the other hand, that evaluators also update such information in both places if it is changed.

consistency statement #2:
If information on covariances between reactions is created/modified, the data have to be stored/updated always in the files of both reactions.

4. Redundant reactions

The ENDF-6 format specifications[1] define a number of reaction types designated by their MT number as redundant, i.e. they may be calculated by summing other reactions:

MT	Meaning; components
1	total; 2, 4, 5, 16, 17, 18, 22-37, 41-42, 102-116
3	nonelastic; 4, 5, 16-18, 22-37, 41-42, 102-116
4	inelastic (total of neutron levels); 50-90
18	total fission; 19-21, 38
103	total of proton levels; 600-649
104	total of deuteron levels; 650-699
105	total of triton levels; 700-749
106	total of He-3 levels; 750-799
107	total of alpha levels; 800-849

Correspondingly in file 33 provision has been made to indicate by so called NC-type sub-subsections, that uncertainties for those cross sections have to be derived by propagation of uncertainties of the components.

In fact certain experiments are capable of providing much more accurate information on some of these cross sections, than would be available by summing up the indicated components. This has led to the situation, that evaluators take the above specified relations only as a constraint for the sum of all component cross sections, but give covariances in a NI-type sub-subsection without any information on existing correlations between sum and components. Even worse for future evaluations, though very reasonable from the practical point of view at the present situation, is a "mixture" of NC and NI-type sub-subsections for one particular MT. Such a procedure states that uncertainties for a part of the energy range are derived, creating implicitly covariance matrices between reactions for that energy range, while uncertainties in other energy ranges are treated as generated independently. When entering new data one then has to be extremely careful not to miss any implicitly existing correlations.

Generally, if experimental data belonging to one of the above specified redundant MT types are entered with their full covariance information into an evaluation procedure, this will automatically create a whole system of excitation functions

connected by interreaction covariance matrices. This has been done recently at the IRK for the most important neutron cross sections of ^{56}Fe and the results have been presented at this meeting[6]. Fig. 1 displays an overview over the full covariance information generated, broken down into submatrices connecting all participating reactions.

MT#	1	103	28	51	52	53	851	852	853	91	16	107
1												
103	0											
28	4	1										
51	12	0	0									
52	1	0	0	20								
53	2	0	0	38	6							
851	4	0	0	47	13	28				851=54 to 58		
852	3	0	0	28	19	12	29			852=59 to 65		
853	4	0	2	22	12	16	24	54		853=66 to 83		
91	10	5	33	45	8	12	21	16	92			
16	2	0	85	0	0	0	0	0	1	37		
107	1	0	27	0	0	0	0	0	0	17	9	

Fig. 1: "Blocked" full covariance matrix for ^{56}Fe reactions. Numbers indicate maximum correlation within block in %

As can be seen there are considerable correlations in some areas whilst in others they are negligible. However, as this is in fact a result of the evaluation, one should keep this information in the least "expensive" way as indicated already in section 3 for users and future evaluation updates. It is clear that once such a "system" has been established, one never again should treat one of the member reactions independently, since not only covariances but also cross sections will mutually react to changes in some position of the whole system.

consistency statement #3:
In evaluations always all existing (known) correlations have to be taken into account and updated to keep the integrity of the whole system.

A further implication of the emergence of connected systems is that other quantities given explicitly for the users convenience, e.g. photon production cross sections in file 13, have to be treated in accordance with other data that represent the same information. In case of file 13 a "one way" data flow for update information would be required between corresponding materials in file 3 MT's 51 – 90 plus possibly some components of MT's 103 – 107.

5. Strategy for future development

As discussions in sections 2, 3 and 4 have illustrated we are actually starting to establish numerous connections and relations within already existing very large data bases. While doing so we have to make sure that this is done in a consistent manner and in addition we have to realize well in time the consequences on future evolution. With very powerful computersystems nowadays available, with rapidly increasing storage and data manipulation capabilities, we will not primarily run into volume problems. We should devote much more attention to maintaining consistency to preserve the data bases capability of providing reliable basic information for critical technical applications. I will therefore close my talk with some strategical comments and proposals in this direction.

In section 2 the connection between experimental characteristics influencing data uncertainties and deduced covariance information have been pointed out. It is therefore extremely important to know which data have already contributed to a particular ENDF. Accurate "bookkeeping" of input data as an integrated component of ENDF's (file 1) is the only reliable means of avoiding duplication of data with disruption of covariance information.

The urgent requirement to have "complete" ENDF's for highly complicated technical applications, and at the same time very limited funds which prohibit thorough evaluation work on all required materials, have led to the practice to adopt certain data considered as "good" from one ENDF into others. It is clear from the arguments in section 3 that doing so will inevitably destroy consistency, since data are combined which have not been evaluated together and in fact originate from different experimental and/or theoretical data bases.

It is clear that in constructing the covariance information in the files numerous approximations have been made. Consequently one might argue that violation of the strict propagation of interreaction covariances to a certain extent would be tolerable. Can we agree to generally treat interreaction correlations below a certain percentage (<10%?) as negligible? This would permit decoupling of large parts of the database and justify adoption practices.

Concerning the arguments in section 4 the already mentioned recent evaluation of ^{56}Fe at the IRK[6] may propose a possible solution. For this purpose the program GLUCS[3] has been extended by the capability of treating experimental data from reactions defined as redundant correctly by entering the formula for the component MT's. This method guarantees the adherence to all specified constraints on sum rules for cross sections as well as the correct update of covariance information. Making use of this procedure would permit a standardized definition which reaction should be treated as independent and which as redundant. Nevertheless one would not loose the advantage of profiting from high accuracy measurements of reactions which are defined as redundant. Such an agreed and used standard would greatly facilitate the evaluators' task of maintaining consistency because this would then be achieved almost automatically.

Finally I would like to add a recommendation to designers of experiments. As we have seen, the amount of attention and precautions in using data is strongly increasing when high correlations exist. The best "investment" is therefore to spend the highest possible effort on the identification and minimisation of correlated uncertainties. Experimental data exhibiting an extremely low uncorrelated uncertainty component due to marvellous counting statistics will almost certainly cause problems because of shape inconsistencies with other data sets. Therefore, decreasing statistical uncertainties much below the level of correlated uncertainties, is no good strategy.

6. Acknowledgements

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COVARIANCES AS INPUT TO AND OUTPUT FROM RESONANCE ANALYSES

N. M. Larson

Oak Ridge National Laboratory
Oak Ridge, Tennessee, USA

ABSTRACT

Accurate data analysis requires understanding of the roles played by both data and parameter covariance matrices. In this paper the entire data reduction/analysis process is examined, for neutron-induced reactions in the resonance region. Interrelationships between data and parameter covariance matrices are examined and alternative reduction/analysis methods discussed.

1. Introduction

The use of covariance matrices in resonance parameter analysis is a topic with many facets. This paper explores only a few in depth, and suggests areas where more work is needed. In Section 2 the "conventional" approach to resonance analysis is discussed, and the roles of both data and parameter covariances are examined. Alternative, possibly superior, methods are suggested in Section 3, including (1) fitting to raw data and (2) using a hybrid approach which fits to reduced data but involves the data-reduction parameters as part of the analysis process. Comparisons are made of results produced by the various methods.

Additional aspects of the title topic are presented in Section 4, with suggestions about how those questions might be studied.

2. Conventional Data Analysis

The usual procedure for analysis of resonance data involves two distinct steps. First is the data-*reduction* process, in which the raw data (counts per channel) are reduced to physically meaningful quantities (e.g., cross sections). Concurrently, uncertainties are determined for each data point, and the data covariance matrix is generated. The second step is the data-*analysis* process itself, in which the parameters of the theory (e.g., R-matrix) are adjusted to fit the reduced data. This step requires initial (or "prior") estimates for parameter values and for the parameter covariance matrix, and generates the output (or "posterior") parameter values and covariance matrix. We now examine each step of this procedure.

2.1 Preparation of the data

2.1.1 Reduction of raw data to physically meaningful quantities

The raw data $\{r_i\}$ produced by an experiment are a series of numbers (counts), each of which is independent of the others, and for which the statistical uncertainties are known. These data are reduced to physically meaningful quantities by well-defined mathematical operations involving "data-reduction parameters" (e.g., normalization constants). That is, the reduced data $\{d_j\}$ may be written in terms of the raw data $\{r_i\}$ and of the parameters $\{q_k\}$ as

$$d_j = \boldsymbol{D}_j(q_1, q_2, q_3, \ldots, r_1, r_2, r_3, \ldots) \qquad (1)$$

where the specific form of the function $\boldsymbol{D}$ can be determined from the precise mathematical operations used to reduce the data. The expression for d_j may involve only one raw data point, or, as in the case of transmission experiments for example, may involve a ratio of two data points. The number of data-reduction parameters changes from experiment to experiment.

A detailed description of the data reduction process for a natural nickel transmission experiment is presented in a report by D. C. Larson et al.[1] In that experiment, the data-reduction process included corrections for detector dead time, for pulse-to-pulse variation in beam intensity, and for several different types of background. These corrections were applied to both sample-in and sample-out data before

transmissions were obtained as the normalized ratio of sample-in to sample-out counts. A total of 30 data-reduction parameters were involved.

2.1.2 Generating the data covariance matrix

Because each raw datum is independent of every other, the covariance matrix for the raw data is diagonal, with the value of the diagonal element being equal to the square of the uncertainty. Unfortunately, the same is not true of the reduced data, for which the covariance matrix generally has many non-zero off-diagonal elements.

The covariance matrix associated with the reduced data can be derived using the method of "propagation of errors". This involves generating the partial derivative of $\boldsymbol{D}$ with respect to each independent variable (r or q), multiplying by small increments in that variable, squaring, and taking expectation values. Explicitly, a small increment in the reduced datum is related to increments in each component via

$$\delta d_i = \sum_k \partial D_i / \partial q_k \; \delta q_k + \sum_k \partial D_i / \partial r_k \; \delta r_k \tag{2}$$

Squaring and taking expectation values gives the equation for the covariance matrix v for the reduced parameters

$$\begin{aligned} v_{ij} = < \delta d_i \; \delta d_j > = & \sum_{k,\ell} \partial D_i / \partial q_k \; \partial D_j / \partial q_\ell \; < \delta q_k \; \delta q_\ell > \\ & + \sum_k \partial D_i / \partial r_k \; \partial D_j / \partial r_k \; < (\delta r_k)^2 > \end{aligned} \tag{3}$$

in which terms with zero expectation values (i.e., terms which are uncorrelated) have been dropped.

Using the method described above, it is a straight-forward mathematical operation to generate the covariance matrix v for the reduced data. It can nevertheless be a formidable task, since it requires knowledge of the specific form for Eq. (1) and for its derivatives, as well as considerable "bookkeeping" to take care of all the subscripts. The computer code ALEX[2] was developed for performing this task: in ALEX all the bookkeeping is accomplished internally within the code, so the user needs to supply programming only for those features which are unique to the particular experiment.

For the natural nickel transmission experiment,[1] ALEX was used to generate not the full data covariance matrix, since the size of such a matrix would be unmanageable ((60000 × 60000)/2), but rather the coefficients of the various components of the uncertainty on each data point. These coefficients could then be used in an analysis code to generate the covariance matrix elements as needed.

2.2 Preparation of the model parameters

2.2.1 Estimating initial values

The goal of data analysis is to determine "best" values for parameters of the R-matrix theory (e.g., energy and widths for each resonance, channel radii). As input to the analysis, an initial ("prior") value must be chosen for each parameter. These initial values are normally obtained from the literature, or may be estimated from an examination of the data.

2.2.2 *Estimating the input parameter covariance matrix*

The analysis code SAMMY,[3] which will be used for all examples presented here, uses Bayes' equations for the fitting procedure. Bayes' equations, unlike least squares, require the input of a prior parameter covariance matrix as well as prior values for the parameters.[4] (Readers unfamiliar with Bayes' equations are referred to the appendix of this paper and to references 3 and 4.)

In the case where a good estimate of the value of a parameter is known, that information should be used for the prior. For example, if a resonance energy is well-known from earlier work as 1.15 ± 0.01 keV, the diagonal element of the covariance matrix should be set at $(0.01)^2$ keV^2. Information about relationships between parameters should also be included, as off-diagonal elements of the parameter covariance matrix. For example, the sum of two fission widths might be known but not the individual components, so the correlation between the two would be -100%.

When the value of a parameter is not well known, or when the analyst has no knowledge about how well the value is known, the true "non-informative prior" is infinite uncertainty. That is, the least-squares equations should be used, since those equations are the limiting case of Bayes' equations with no information about the uncertainties.

Since a good estimate may be available for the uncertainty on some parameters, and no information available for others, the equations used for the fitting procedure should reflect that situation; i.e., one should use a combination of Bayes' and least squares. This, however, would be complicated to implement, and is not done in SAMMY. Instead only Bayes' method is used, since the many advantages of this approach far outweigh any difficulties.

The procedure used in SAMMY to approximate the non-informative prior is as follows: initial uncertainties are set at relatively large values, and changes in those uncertainties due to analysis of the data are studied. If the decrease in the uncertainty for a given parameter is large (say, an order of magnitude), then the initial uncertainty was effectively infinite. If the change is very small (a few percent), there are two possibilities which the analyst will wish to investigate: The parameter may be unaffected by this data, in which case the initial uncertainty is essentially irrelevant. Alternatively, this choice for the uncertainty may be much too small, being a greater constraint on the parameter's value and uncertainty than the data are, in which case a larger number should be used for the prior uncertainty.

In practice, SAMMY users have found that a prior uncertainty of 10 to 20% of the value of the resonance widths is generally large enough to avoid unduly constraining the value, and small enough to avoid computational problems. For resonance energies, the prior uncertainty must be small enough to constrain the energy-ordering of the resonances. (Such values for the prior uncertainties are default input for SAMMY.) For a parameter whose prior value is very small, experience has shown that it is best to assign an absolute uncertainty rather than accepting the default 10% value. For example, one might suspect a constant background to be present, but the estimated prior value for that background is zero; here the assigned prior uncertainty would be based on the analyst's judgement of how large a background *might* be present in the data.

If the uncertainty on any parameter is *increased* significantly (more than a few percent) during the course of the analysis, it is generally safe to assume that a problem exists! Spin assignments may be wrong, a decimal point may have been misplaced in

typing the input, the chosen resolution function may not properly describe the experimental conditions, a previously unsuspected contaminant may be present, ...

2.3 The analysis

Once the data and data covariance matrix are prepared, and prior values have been determined for the parameters and parameter covariance matrix, the analysis can proceed. Usually this is an iterative process, with the analyst examining the output from one run, making appropriate changes in the input, and re-running the analysis code.

2.4 The output parameter values and covariance matrix

2.4.1 Reporting values and covariances

The output from analysis codes such as SAMMY includes a listing of both parameter values and the associated covariance matrix. While parameter uncertainties are regularly given in publications reporting the outcome of analyses, the full off-diagonal covariance matrix seldom is, primarily because of size limitations. However, the matrix should be made available; in particular, ENDF/B-VI has formats for reporting that information.

2.4.2 Example

What can be learned by studying the parameter covariance matrix provided as part of the output from the data analysis? To answer this question, consider an example from a SAMMY analysis[5] of ^{58}Ni transmission data. The short run reported here included data from 490 to 498 keV only, although resonance parameters were included from 0 to 800 keV; starting values have been deliberately changed to give a rather poor fit to the data. The data, with initial and final fits, are shown in Fig. 1. Table 1 shows initial and final values and uncertainties for the resonance energies E, capture widths Γ_γ, and neutron widths Γ_n for each of the 9 resonances whose parameters were varied in this particular run. Table 2 gives the lower half of the correlation matrix, times 100, for these parameters; correlations are defined in terms of covariances as

$$corr_{ij} = cov_{ij} / (cov_{ii}\, cov_{jj})^{1/2} \qquad (4)$$

The first thing to notice about the output is that posterior values and uncertainties for all gamma widths are essentially unchanged from the prior values. This is what one expects with Bayes' method, since transmission data are insensitive to these parameters, but this is *not* what would happen with a least-squares analysis. Correlations between the gamma widths and all other parameters are likewise zero (or nearly so), as seen in Table 2 (in which only non-zero correlations are printed).

From Table 1 we note that posterior uncertainties on resonance energies and on most of the neutron widths are much smaller than prior uncertainties, indicating that the data can indeed determine those quantities. The exceptions are the neutron widths for resonances number 4, 5, and 8, all of which have quite small values and therefore are not well determined by transmission data.

Table 1. Prior and posterior values for resonance parameters and uncertainties in the 490-498 keV region of ^{58}Ni, for the analysis reported in Section 2.4 of this text. Parameter numbers are listed in the second column; see Table 2 for correlation matrix for these parameters.

Resonance number	Parameter number		Initial value	Initial unc.	Final value	Final unc.	ratio of initial to final uncertainties
1 = s1/2							
	1	E (eV)	491900.	20.	491819.	4.	0.20
	2	Γ_γ (meV)	1000.	100.	1002.	100.	1.00
	3	Γ_n (meV)	180000.	18000.	170490.	4462.	0.25
2 = s1/2							
	4	E (eV)	496300.	40.	496301.	7.	0.18
	5	Γ_γ (meV)	2000.	200.	2006.	200.	1.00
	6	Γ_n (meV)	1500000.	150000.	1422800.	16619.	0.11
3 = p1/2							
	7	E (eV)	493200.	30.	493175.	4.	0.14
	8	Γ_γ (meV)	1000.	100.	1002.	100.	1.00
	9	Γ_n (meV)	600000.	60000.	406850.	8684.	0.14
4 = p1/2							
	10	E (eV)	496000.	101.	496056.	8.	0.08
	11	Γ_γ (meV)	1000.	100.	1000.	100.	1.00
	12	Γ_n (meV)	16000.	1600.	16084.	1594.	1.00
5 = p1/2							
	13	E (eV)	496500.	108.	496472.	18.	0.16
	14	Γ_γ (meV)	1000.	100.	1001.	100.	1.00
	15	Γ_n (meV)	30000.	3000.	25917.	2450.	0.82
6 = p1/2							
	16	E (eV)	496800.	30.	496853.	5.	0.18
	17	Γ_γ (meV)	1000.	100.	1000.	100.	1.00
	18	Γ_n (meV)	280000.	28000.	225200.	5416.	0.19
7 = p3/2							
	19	E (eV)	491600.	137.	491472.	3.	0.02
	20	Γ_γ (meV)	1000.	100.	1002.	100.	1.00
	21	Γ_n (meV)	90000.	9000.	88728.	1764.	0.20
8 = d3/2							
	22	E (eV)	495300.	97.	495355.	4.	0.04
	23	Γ_γ (meV)	1000.	100.	1000.	100.	1.00
	24	Γ_n (meV)	9000.	900.	9181.	899.	1.00
9 = d5/2							
	25	E (eV)	493700.	20.	493744.	3.	0.15
	26	Γ_γ (meV)	1000.	100.	1003.	100.	1.00
	27	Γ_n (meV)	90000.	9000.	88605.	1821.	0.20

Table 2. Lower half of the posterior parameter correlation matrix from the analysis described in Section 2.4 of this text. Correlations are multiplied by 100, and only non-zero values are printed. Parameter numbers (along the top and left-hand side) refer to parameter numbers as listed in Table 1. Divider lines separate resonances; see Table 1 for definitions of parameters.

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27
1	100																										
2		100																									
3	-6	1	100																								
4	-1		-1	100																							
5					100																						
6	7			1		100																					
7	2		5	-2		6	100																				
8								100																			
9	1		-37	-13		46	29		100																		
10	1			-40	1	12	1		10	100																	
11										-1	100																
12				3		-2			-1	43		100															
13	1		1	-37		8			-18	13		-1	100														
14														100													
15			-1	51		11	-1		-1	-17		3	-1		100												
16	-1		3	-52		-24	-3		-9	16		-4	35		-26	100											
17																	100										
18				46	1	7	2		-6	-15		3	-32		8	-27		100									
19	38	-1	-14	1		-5	-1			-1			-1			1			100								
20																				100							
21	5	-1	51	-1		12	3		-21	2			2						-4	-1	100						
22	2		-1	-14		25	1		12	9		1	7		-4	1		-3	-1		3	100					
23																							100				
24				-1		3			1	2			1									-62		100			
25	1		-8	-6		18	33		37	4		-1	3		-1	-3		-2	-1		-4	5		1	100		
26																										100	
27	1		10	3		6	-47		-51				-1		1	1		8			11	2			-27	-1	100

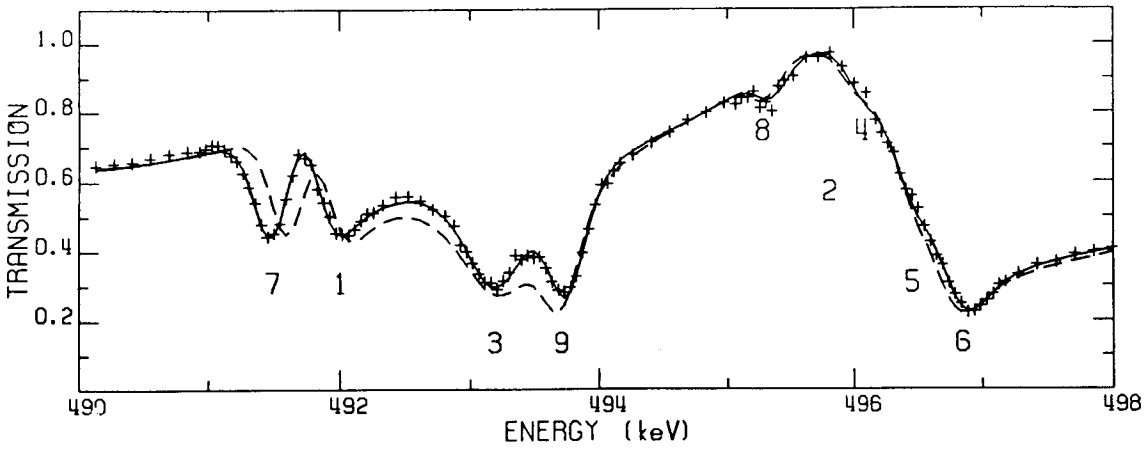

Figure 1. Data (+), prior theoretical transmission calculations (dashed curve), and posterior theoretical transmissions (solid curve) for the ^{58}Ni analysis described in Sec. 2.4. Numbers in the figure refer to resonances numbers as listed in Table 1.

(Correlations involving parameters which are not well determined by the data should be discounted, even when they appear large. The data simply contain no information about those parameters, so no conclusions can be drawn about correlations involving those parameters.)

Examination of the correlation matrix shows fairly large values connecting the parameters of resonance number 1 (R1) with those of R7; this is not surprising since R1 is an *s*-wave and therefore will have influence away from its peak. Similarly, the correlations for (R2,R3) and (R2,R6) are rather large.

2.5 Sequential analyses

One strength of Bayes' method is a direct consequence of including the prior parameter covariance matrix as input to the analysis: Output parameter values and parameter covariance matrix from analysis of one data set may be used as input for a subsequent analysis of another data set, and the results from that second analysis are equivalent to those which would have been obtained if both data sets had been analyzed simultaneously. This makes it possible, for example, to divide very large data sets into subsets of manageable size, without degrading the quality of the results. Similarly, different experiments can be analyzed separately (sequentially) rather than requiring a computer code capable of including all data sets simultaneously.

2.5.1 Example

Sequential analyses of this type were performed by F. G. Perey[6] as part of the NEANDC task force to investigate discrepancies in the parameters of the 1.15-keV resonance in ^{56}Fe. [Results quoted here should not be taken as definitive, since they are based on Perey's preliminary work.] The analyses involved three sets of transmission data, all taken at ORELA, on three different samples. The first and third measurements were made at room temperature, the second used a sample cooled to liquid-nitrogen temperature.

A total of fourteen parameters were varied in this analysis, including the energy and particle widths for a second resonance, the two temperatures and three sample thicknesses, the R-matrix matching radius, and three resolution-broadening parameters. Values for the parameters for the 1.15 keV resonance are shown in Table 3. Note that in each case, changes made to the capture and neutron widths from the previous values are well within the standard deviation of the previous results.

Data and fits from this analysis are shown in Fig 2.

Table 3. Resonance parameters for the 1.15-keV resonance in ^{56}Fe. The first row gives input values, and the other three give results after SAMMY analyses of the first, second, and third data sets.

	Energy (eV)	Γ_γ (meV)	Γ_n (meV)
BEGIN	1151.00 ± 5.00	600.0 ± 300.0	62.00 ± 15.00
ONE	1151.11 ± 0.06	584.0 ± 129.0	59.16 ± 6.87
TWO	1151.03 ± 0.04	581.7 ± 42.6	62.14 ± 1.05
THREE	1151.03 ± 0.04	575.7 ± 40.3	61.63 ± 0.87

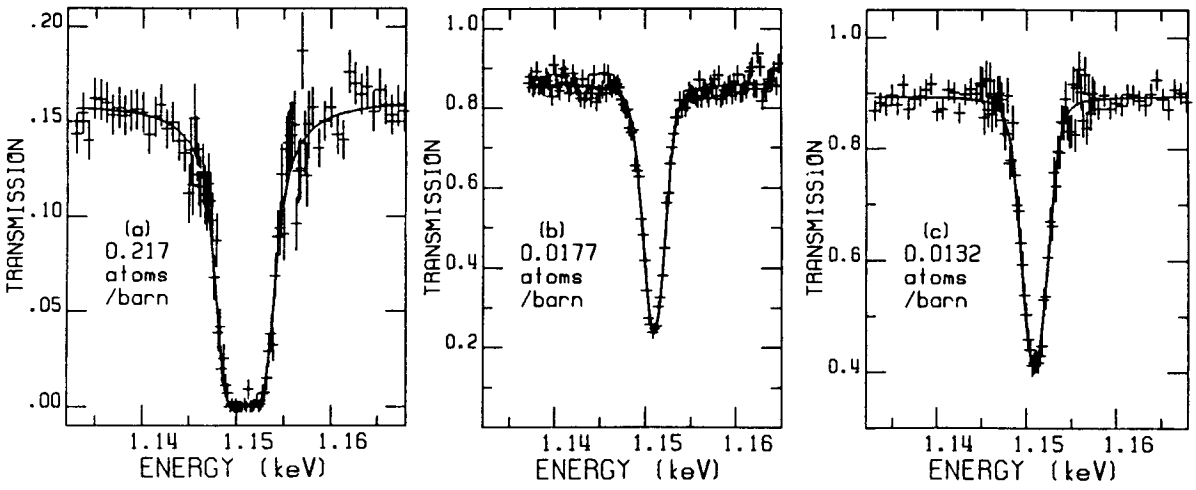

Figure 2. Results from a pseudo-simultaneous fit to three ^{56}Fe transmission measurements.

2.5.2 Caveat

At this point it should be noted that there are cases where it is *not* proper to use the output covariance matrix from one analysis as input to the next. This is true when *re-*running the analysis code with the *same* data, a procedure which is often undertaken during the early stages of an analysis. Upon viewing a plot of the fit provided by the first run, the analyst may decide to start over with different initial values or different spin assignments. In any case of re-examination of data already analyzed, the initial (non-informative) prior should be used as input to the second computer run, rather than using the output covariance matrix. To use the output covariance matrix from an earlier run when changes are made in values or assignments introduces inconsistencies, and to do so when no changes are made suggests that these data are twice as informative as they in fact are.

3. Modified data analysis

The approach to data analysis as outlined above works well in most cases; however, there are difficulties associated with it. In this section we will explore alternatives which may eliminate some of those difficulties while perhaps introducing a few others.

3.1 Problems with the data covariance matrix

The data covariance matrix may not be particularly easy to generate; this problem is eased, if not solved, by using a semi-automated code such as ALEX to assist the effort. However, the matrix may also not be particularly correct if the data-reduction parameters and their uncertainties are not well understood. In addition, the data covariance matrix is often so large as to be unmanageable, and many data analysis codes are ill-equipped to handle the full data covariance matrix.

A variety of solutions have been posed for these problems. One commonly (mis)used solution is to simply drop the off-diagonal terms of the data covariance matrix; we shall see later that this can lead to inaccurate parameter values. Another possible solution is to use group covariances as in ENDF/B-VI;[7] this author has little experience with this option so will not address it here except to suggest it as a possible solution.

3.2. Alternative formulations

3.2.1 Fit to raw data

The most reliable method to use in any data analysis is to fit to the raw data directly, rather than fitting to the reduced data. That is, the raw data are not reduced by, e.g., subtracting backgrounds and applying normalizations. Rather, those corrections are applied to the theoretical calculation to which the data are to be fit. The data-reduction parameters are added to the list of fitting parameters (which includes resonance widths and energies, Doppler temperature, resolution parameters, etc.); measured values and uncertainties (and correlations) for the data-reduction parameters are used as prior

values for those parameters. Data-reduction parameter values and uncertainties are *not* used in generating the full data covariance matrix, since the data covariance matrix to be used in the fitting procedure is the matrix associated with the *raw* data.

This technique has several advantages, not least of which is that the covariance matrix associated with the raw data is diagonal. In addition to eliminating the need to store and manipulate a very large matrix, use of the uncorrelated raw data gives the analyst the liberty to treat subsets independently (which cannot be done with the correlated reduced data).

3.2.2 Hybrid method of fitting

A third possibility exists, which combines desirable features of both the raw-data and the reduced-data method. First, reduce the data in the usual manner but treat data-reduction parameters as though they are absolute, i.e., as though they have zero uncertainties. Then introduce additional parameters into the data analysis process, whose values are such as to have no effect on the value of the theoretical calculation but whose uncertainties reflect the true experimental uncertainties on the data-reduction parameters.

A simple example may serve to explain this process. Let the raw data $\{r_i\}$ consist of a cross section normalized by an energy-independent constant whose measured value is $a \pm \delta a$, to which is added an energy-independent background whose measured value is $b \pm \delta b$.

The reduced data $\{d_i\}$ are related to the raw data via

$$d_i = a r_i + b \tag{5}$$

where the values for a and b are as measured, but both are considered to be exact, i.e., to have zero uncertainty. Thus the uncertainty on d_i is only that due to r_i,

$$\delta d_i = a \, \delta r_i \tag{6}$$

and the off-diagonal covariance matrix elements for the reduced data are zero.

The theoretical expression which will be used to fit this raw data is of the form

$$t_i(E, p_1, p_2, \ldots p_N, p_{N+1}, p_{N+2}) = \sigma(E, p_1, p_2, \ldots p_N)\, p_{N+1} + p_{N+2} \tag{7}$$

in which the first N parameters are from the R-matrix theory, and the last two parameters represent the normalization and background respectively. The prior value for p_{N+1} is 1.00 and for p_{N+2} is 0.00; the prior uncertainty for p_{N+1} is δa and for p_{N+2} is δb.

3.3 Comparison of methods

To determine the relative accuracies of the various analysis methods, comparisons were made using artificial "raw" data generated as follows: experimental fission cross section data for ^{241}Am from 0.018 eV to 1.72 eV were multiplied by a normalization factor (1.030), and a constant background (4.97) was added. The resulting numbers $\{r_i\}$ are assumed to be proportional to the number of counts in our artificial experiment, so the uncertainties δr_i may be specified as proportional to the square root of r_i; we

somewhat arbitrarily assign $\delta r_i = 0.1\sqrt{r_i}$. Our artificial experimenter also measured the normalization and background at 1.031 ± 0.006 and 4.97 ± 1.00, respectively.

These data were then analyzed using five different methods:

(1) Fit to the raw data, using normalization and background as fitting parameters with the known values (1.031 ± 0.006 and 4.97 ± 1.00) as priors.
(2) Use the hybrid method described in Section 3.2.2.
(3) Reduce the data, carefully including systematic uncertainties in the data covariance. Use the full off-diagonal data covariance in the analysis, and do not include normalization and background as fitting parameters.
(4) Reduce the data and include no uncertainties due to normalization and background in the data covariance matrix (as for method 2 above). Analyze without regard to normalization or background.
(5) Reduce the data properly and obtain the correct diagonal data covariance matrix elements but ignore off-diagonal elements. Again analyze without regard to normalization or background.

Finally, this entire set of five analyses was repeated, with "wrong" values of the normalization (0.95 ± 0.006) and background (1.00 ± 1.00).

Only method 1 is precisely correct, while the others involve various approximations. Intuitively one might expect that method 2 would give equivalent results, and the results from method 3 should also be close, provided the "known" values of the normalization and background are nearly correct. Neither method 4 nor method 5 would be expected to give consistently reliable results (in spite of the fact that method 5 appears the most generally used!).

In order to judge the relative merits of the five analyses, it was necessary to first design a criterion for comparison of results. [The naive use of χ^2 clearly will not work, since it involves division by the diagonal data covariance matrix element, which varies considerably over the five methods.] Since method 1 is known to be correct, the goal for the other methods is to reproduce the results of method 1; therefore the sum of the squares of the relative differences in the resonance parameters should give a reliable measure of the quality of the method. We define a quantity c as

$$c = \sum_{i=1}^{N} ((p_i - p_i^{raw})/p_i^{raw})^2 \qquad (8)$$

and evaluate c for each method. Low values of c correspond to good agreement with the "correct" results from method 1, and high values indicate poor agreement.

Results from these analyses are summarized in Table 4. Note that results from method 2 agree nearly perfectly with results from method 1. When "measured" values for the data reduction parameters are very close to the true values, all methods appear to work fairly well. This is definitely not true, however, when "measured" values are not close to the true values. In this case only method 2 (the hybrid method) and method 3 (using reduced data with the full covariance matrix) give reasonable agreement with results obtained by method 1.

Table 4. Comparison of results from four approximate data analysis procedures with results from fitting to raw data. Lower values of c indicate good agreement.

Method	c with "good" prior values for norm and background	c with "bad" prior values for norm and background
2	0.000000	0.000006
3	0.000125	0.020197
4	0.000211	91.934166
5	0.028188	13.263780

Though not reflected in our criterion c, the parameter covariance matrices generated by methods 2 and 3 also agree nearly perfectly with that generated by fitting the raw data.

Erroneous results produced by dropping the off-diagonal elements of the data covariance matrix (method 5), in the case where the prior values are "wrong", are shown in Fig. 3a. Note the distortion in the shape of the calculated cross section (solid curve). Fig. 3b shows the curve generated by method 3; here the calculated cross section (dashed curve) is displaced from the reduced data (+) but nevertheless has the correct shape. The solid curve through the data is the dashed curve displaced by 4.233 barns, and appears in good agreement with the data.

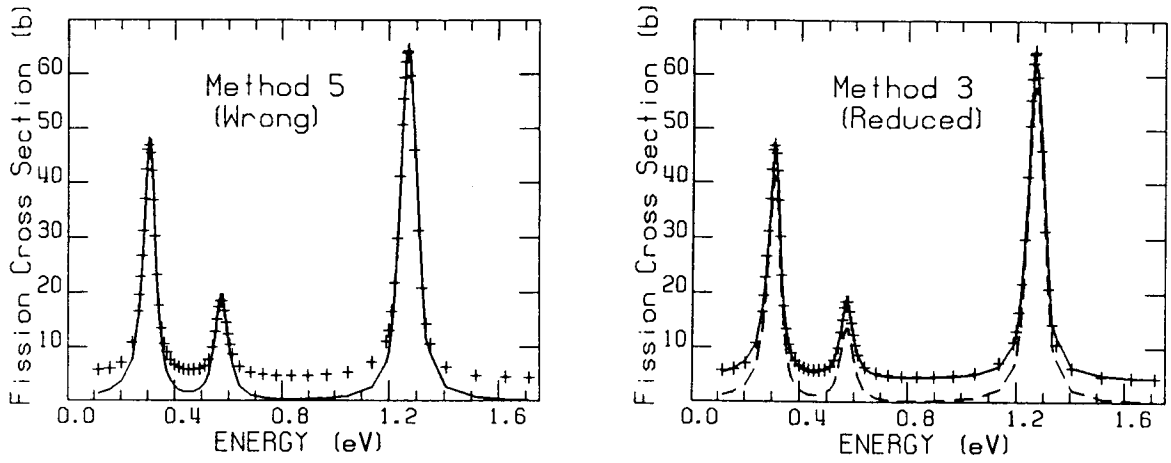

Figure 3. Results obtained from analysis of the (artificial) reduced data described in Section 3.3, first (part a, method 5) dropping the off-diagonal data covariances and second (part b, method 3), using the full off-diagonal data covariance matrix. The dashed curve in part b gives the calculated cross section, the solid curve shows the same line displaced by 4.233 barns.

4. Additional topics

Bayes' equations describing the fit to the raw data with $N+1$ parameters can be converted directly to Bayes' equations describing the fit to the reduced data with N parameters, provided certain approximations and assumptions are valid. Essentially, the

initial values for all $N+1$ parameters must be very close to the correct values For the reader interested in mathematical detail, equations describing that conversion are available from the author.

ENDF/B-VI permits the use of "group covariances" to describe the relationships among the data. A careful study of the mathematics underlying such a formulation should be undertaken, to ascertain the conditions and extent of validity. [If this has been done, the author would be interested in learning about it.]

Left unexplored by this study is the question of disengaging parameter values (and covariances) from the experimental conditions under which those values were obtained. For example, the apparent width of a resonance is greatly affected by the Doppler and resolution broadening that occurs in the course of the experiment; values for the neutron widths extracted via the analysis process then are coupled with the resolution and Doppler parameters. How great an effect is this, and if it is large how can it be overcome? This author's intuition is that, while this effect may be important for a single experiment, multiple experiments under a variety of conditions will serve to isolate the parameter values independent of experimental conditions.

Also largely unexplored here is the effect of incorrect assumptions about the experimental conditions. How are parameter values and covariances affected by using a Gaussian resolution function, for example, when the actual experimental resolution is highly skewed?

In the "ideal" analysis of resonance data, every possible parameter (both resonance parameters and data reduction parameters) will be varied and the "best" value chosen by the fitting procedure. In actual analyses, this is not practical; values of some parameters must be fixed. How does this affect the values and covariances of those that are varied? Does the magnitude of the uncertainty on a varied parameter increase or decrease (or neither) as fewer parameters are varied?

How well can posterior uncertainties (and covariances) be believed? Are parameter uncertainties output by SAMMY and other resonance analysis codes too small, as some analysts believe? If so, what is lacking in our understanding of the analysis process? Are we missing a major source of uncertainty?

The subject of patterns in the posterior parameter covariance matrix has not been carefully addressed here. Here are several questions[8] related to this subject that should be explored:

(1) What patterns are obvious, first in the case of good data with isolated resonances and then in the more general case?
(2) Are some types of parameters (e.g., resonance energies) correlated only among nearby resonances?
(3) Which parameters are correlated over long range?
(4) How does inclusion of specific experimental uncertainties affect covariances between resonance parameters?
(5) If one energy region is fit very poorly, how are parameter values and covariances in nearby regions affected?

(6) Can examination of the posterior parameter covariance matrix provide information about systematic errors that have not been recognized beforehand?

5. Conclusions

In this paper the generation and use of both data and parameter covariance matrices in data reduction and resonance analysis have been explored. The ramifications of fitting to reduced data vs. fitting to raw data was explored in some detail; the recommended method is a hybrid between those two extremes. Some comments were made about intelligence to be gained by examining the posterior parameter covariance matrix, but this subject was not investigated in depth. Suggestions were made of other areas where further work is needed.

6. Acknowledgments

The author is indebted to D. C. Larson for many helpful conversations and for carefully reviewing this paper. Thanks also go to R. W. Peelle for providing a list of suggested topics; many of the "additional topics" proposed in Section 4 came from that list. Research sponsored by the Office of Energy Research, Division of Nuclear Physics, U. S. Department of Energy, under contract DE-AC05-84OR21400 with Martin Marietta Energy Systems, Inc.

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APPENDIX A

Bayes' Equations

A derivation of Bayes' equations from Bayes' theorem (using three additional hypotheses regarding distributions and linearity) is given in Ref. 3; the reader interested in details of that derivation is referred to that paper. The equations themselves, in several forms, are presented in this appendix.

Let p represent the vector of prior parameter values, and m the associated covariance matrix. Let d represent the measured (or derived from measurement) data, and v the associated covariance matrix. Let t represent the theoretical calculation of the quantity for which d is the measurement, and g the derivative of t with respect to the parameters p. Then the posterior values for parameters p' and covariance matrix m' are given, in matrix form, by

$$p' = p + m g^t (n+v)^{-1} (d-t) \tag{A.1a}$$

$$m' = m - m g^t (n+v)^{-1} g m \tag{A.1b}$$

where

$$n = g m g^t \tag{A.1c}$$

This is the form in which Bayes' equations are usually encountered; note that this form requires inversion of a matrix whose dimensions are (*Ndat* × *Ndat*), where *Ndat* is the number of data points.

An alternative formulation is

$$p' = p + m (i+q)^{-1} g^t v^{-1} (d-t) \tag{A.2a}$$

$$m' = m (i+q)^{-1} \tag{A.2b}$$

where

$$q = g^t v^{-1} g m \tag{A.2c}$$

and i is the identity matrix. In this form, Bayes' equations require two separate inversions, first of v (*Ndat* × *Ndat*) and secondly of $(i+q)$, whose dimensions are (*Npar* × *Npar*) where *Npar* is the number of parameters. Therefore in general this form is not as useful as the first. However, the data covariance matrix is often diagonal, in which case inversion of v is straightforward. If in addition the number of data points is

much larger than the number of parameters (as is generally true for resonance analyses), then this second formulation of Bayes' equations is the preferred method.

The usual least-squares equations can be derived directly from Bayes' equations, most easily in the form of Eq. (A.2), by taking the limit as the diagonal elements of m become infinite and the off-diagonal become zero. In this case Eq. (A.2b) takes the form

$$\lim_{m\to\infty} m' = \lim_{m\to\infty} m\,(i+g^t v^{-1} g m)^{-1} = \lim_{m\to\infty} (m^{-1}+g^t v^{-1} g)^{-1} = (g^t v^{-1} g)^{-1} \tag{A.3}$$

which is the familiar least-squares equation for the posterior parameter covariance matrix. Substituting this expression for the quantity $m(i+q)^{-1}$ in Eq. (A.2a) gives the familiar least-squares equation for posterior parameter values.

Finally, we note that Bayes' equations are strictly correct only if the theory is a linear function of the parameters. Since this is rarely true, iterative forms of Bayes' equations have been derived to compensate for non-linearities. The iterative form of the first formulation of Bayes' equations is

$$p^{(k+1)} = p^{(0)} + m\,g^{(k)t}\,(n^{(k)}+v)^{-1}\,(d-t^{(k)}-g^{(k)}(p^{(0)}-p^{(k)})) \tag{A.4a}$$

$$m^{(k+1)} = m - m\,g^{(k)t}\,(n^{(k)}+v)^{-1}\,g^{(k)}\,m \tag{A.4b}$$

where

$$n^{(k)} = g^{(k)}\,m\,g^{(k)t} \tag{A.4c}$$

Here $p^{(0)}$ represents the initial or prior values of the parameters, and $p^{(k)}$ represents the k-th iterated values. The theory $t^{(k)}$ and derivatives $g^{(k)}$ are evaluated at the k-th iterated values $p^{(k)}$.

Similar equations can be written for the iterative form of the second formulation of Bayes' equations.

PROCESSING OF RESONANCE PARAMETER COVARIANCE FILES

B. L. Broadhead
Oak Ridge National Laboratory
Oak Ridge, Tennessee USA

ABSTRACT

The prudent use of resonance parameter covariance information requires the availability of a means of error propagation from the resonance parameters to the cross sections. This work presents an approach to obtaining these so-called resonance parameter sensitivities.

The resonance parameter sensitivity methodology developed herein generally provides accurate results when compared with direct recalculations using existing and well-known cross-section processing codes. However, it has been shown in several cases that self-shielded cross sections can be very nonlinear functions of the basic parameters. For this reason, caution must be used in any study that assumes that a linear relationship exists between a given self-shielded group cross section and its corresponding basic data parameters.

The study also has pointed out the need for more approximate techniques that will allow the required sensitivity information to be obtained in a more cost-effective manner.

This paper is a synopsis of major work that was completed nearly ten years ago. However, due to the lack of additional development in the field, it remains essentially the current state of the art in resonance parameter sensitivities.

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INTRODUCTION

Current generation cross-section adjustment procedures involve the combination of differential nuclear data measurements (i.e., evaluated cross sections such as ENDF/B) with integral data measurements (i.e., k_{eff}, fission ratios, central worths, etc.) to obtain "newly evaluated" or "adjusted" cross-section data and integral data. This combination procedure is the so-called least-squares adjustment procedure. The steps required to perform such an analysis are generally (1) processing of uncertainty information about the differential nuclear data, (2) calculating detailed sensitivity information that will allow propagation of the differential data uncertainties to the integral data values, and (3) the calculation of the integral data values with the differential nuclear data values. Thus, the differential data measurements and the integral data measurements are "combined" with this procedure to produce the "best" estimates of each in the least-squares sense. The mathematics of this technique are bounded on Bayes Theorem and are detailed in many places.[1-4] However, current generation cross-section adjustment procedures have some inherent limitations. All techniques to date assume that the so-called shielding factors (both energy and spatial) have no uncertainty. The impact on the cross-section adjustment is the implication that the infinitely dilute cross section can be changed without affecting the shielding factors. Even though this approximation is good outside the resonance range, when near resonances, it breaks down. Greenspan[5] has shown that the uncertainty in the energy shielding factors is only about 10% of that due to the infinitely dilute cross sections in the unresolved region. Therefore, most of the adjustment studies done prior to this work have been for fast reactors in which the primary area of interest is in the unresolved region.

In the resolved resonance range, the primary region of interest for thermal reactors, Greenspan has shown that uncertainties in the energy shielding factors are in some cases equal to the uncertainty in the infinitely dilute cross sections. Thus, it would appear that the inclusion of self-shielding effects in an uncertainty analysis and data adjustment for thermal reactors is very important.

The resonance-parameter sensitivity technique presented herein will allow for several improvements over current technology. First, the remaining approximations in the region of fast-reactor interest (unresolved region) can be removed. The use of adjustment techniques will also now be feasible for use on thermal and intermediate reactors (LWR, HWR, HTGR, etc.). These techniques can be used either to obtain adjustments in the energy self-shielding factors or to obtain adjustments in the resonance parameters (RP). Both procedures adjust the group cross sections outside the resonance region and produce the same results, although in a slightly different form. Also new in this work is the representation of the uncertainties in the spatial self-shielding effect.

SENSITIVITY COEFFICIENTS TO BASIC NUCLEAR DATA METHODOLOGY

Several methods have been outlined for the calculation of basic nuclear data sensitivities:[5] (1) the consistent bilinear method, where a generalized perturbation theory approach is used, and (2) the consistent flux method, where either direct perturbations are made or analytical methods are used. The method employed in this work falls into the consistent flux class, with several improvements over earlier work.[6] Further discussion of this method will consider the resolved and unresolved regions separately.

In the resolved region, the following single-level Breit-Wigner (SLBW) equations represent the pointwise infinitely dilute cross sections at zero K:[7]

$$\sigma_t(E) = \sum_\ell \sigma_t^\ell(E) = \text{total cross section} , \tag{1}$$

where

$$\sigma_t^\ell(E) = (2\ell + 1)\frac{4\pi}{k^2}\sin^2\phi_\ell + \frac{\pi}{k^2}\sum_J g_J \sum_\lambda \frac{N_\lambda}{D_\lambda} ,$$

$$N_\lambda = \Gamma_{n\lambda}^2 \cos 2\phi_\ell - 2\Gamma_{n\lambda}(\Gamma_{\gamma\lambda} + \Gamma_{f\lambda})\sin 2\phi_\ell + 2(E - E'_\lambda)\Gamma_{n\lambda}\sin 2\phi_\ell ,$$

$$D_\lambda = (E - E'_\lambda)^2 + 1/4\Gamma_\lambda^2 ,$$

$$\sigma_c(E) = \sum_\ell \sigma_c^\ell(E) = \text{capture cross section} , \tag{2}$$

where

$$\sigma_c^\ell(E) = \frac{\pi}{k^2}\sum_J g_J \sum_\lambda \frac{N_\lambda^c}{D_\lambda} ,$$

$$N_\lambda^c = \Gamma_{n\lambda}\Gamma_{\gamma\lambda} ,$$

$$\sigma_f(E) = \sum_\ell \sigma_f^\ell(E) = \text{fission cross section} , \tag{3}$$

where

$$\sigma_f^\ell(E) = \frac{\pi}{k^2}\sum_J g_J \sum_\lambda \frac{N_\lambda^f}{D_\lambda} ,$$

$$N_\lambda^f = \Gamma_{n\lambda}\Gamma_{f\lambda} ,$$

$$\sigma_e(E) = \sum_\ell \{\sigma_t^\ell(e) - \sigma_c^\ell(E) - \sigma_f^\ell(E)\} = \text{elastic cross section} , \tag{4}$$

where

$$g_J = \frac{2J + 1}{2(2I + 1)} ,$$

$$\Gamma_{n\lambda} = \frac{P_\ell(E)\Gamma_{n\lambda}^o}{P_\ell(E_\lambda)} = \text{the neutron width for resonance } \lambda ,$$

$\Gamma_\lambda = \Gamma_{n\lambda} + \Gamma_{\gamma\lambda} + \Gamma_{f\lambda}$ = the total width for resonance λ ,
E_λ = the resonance energy of resonance λ ,
$\Gamma_{\gamma\lambda}$ = the capture width for resonance λ ,
$\Gamma_{f\lambda}$ = the fission width for resonance λ ,

$$\Gamma_{n\lambda}^o = \Gamma_{n\lambda}(E_\lambda) ,$$

J = the spin of the compound nucleus ,
I = the spin of the target nucleus ,

$$E'_\lambda = E_\lambda + \frac{S_\ell(E_\lambda) - S_\ell(E)}{2P_\ell(E_\lambda)}\Gamma_{n\lambda}(E_\lambda) ,$$

$k = 2.196771 \times 10^{-3}\ A/(A + 1.0)\ \sqrt{E}$,
A = ratio of mass of particular isotope to that of a neutron ,
S_ℓ = the shift factor ,
P_ℓ = the penetration factor ,
$\phi_\ell = \phi_\ell(\hat{a})$ = the phase shift ,
$\hat{a}$ = the effective scattering radius.

The initial objective is to analytically obtain the partial derivatives of the above equations to the basic parameters, $\Gamma_{\gamma\lambda}$, $\Gamma_{f\lambda}$, $\Gamma^o_{n\lambda}$, σ_o, and $\hat{a}$. The equations for the capture cross-section derivatives follow:

$$\frac{\partial \sigma'_c(E)}{\partial \Gamma_{\gamma\lambda}} = \frac{\pi}{k^2} g_J \left[\frac{\Gamma_{n\lambda}}{D^c_\lambda} - \frac{\Gamma_{n\lambda}\Gamma_{\gamma\lambda}\Gamma_\lambda}{2(D^c_\lambda)^2} \right], \tag{5}$$

$$\frac{\partial \sigma'_c(E)}{\partial \Gamma_{f\lambda}} = -\frac{\pi}{k^2} g_J \left[\frac{\Gamma_{n\lambda}\Gamma_{\gamma\lambda}\Gamma_\lambda}{2(D^c_\lambda)^2} \right], \tag{6}$$

$$\frac{\partial \sigma'_c(E)}{\partial \Gamma^o_{n\lambda}} = \frac{\pi}{k^2} g_J \left[\frac{Y\Gamma_{\gamma\lambda}}{D^c_\lambda} - \frac{\Gamma_{n\lambda}\Gamma_{\gamma\lambda}}{(D^c_\lambda)^2} \{2(E - E'_\lambda)Z + 0.5\,\Gamma Y\} \right], \tag{7}$$

$$\frac{\partial \sigma'_c(E)}{\partial \sigma_o} = \frac{\partial \sigma'_c(E)}{\partial \hat{a}} = 0 , \tag{8}$$

where

$Y = P_\ell(E)/P_\ell(E_\lambda)$,

$Z = \partial E'_\lambda / \partial \Gamma^o_{n\lambda}$.

The equations for fission cross sections are of the same form, with $\Gamma\gamma$ replaced by Γ_f. The equations for the total cross sections take on a slightly different form. The elastic cross-section derivatives are similar to the total, but, in most cases, have additional terms.

The next step is to Doppler-broaden these pointwise derivatives. We begin by writing the free-gas model equation for Doppler broadening.[8]

$$\sigma_x(E,T_2) = \frac{1}{2E}\sqrt{\alpha/\pi} \int_0^\infty dE_r\, E_r^{1/2}\, \sigma_x(E,T_1) \times \left[e^{-\alpha(E^{1/2} - E_r^{1/2})^2} - e^{-\alpha(E^{1/2} + E_r^{1/2})^2} \right], \tag{9}$$

with

$\alpha = A/k\ (T_2 - T_1)$,
E_r = relative energy .

By differentiating Eq. (9) with respect to the RP of interest, q_k, we obtain

$$\frac{\partial\sigma_x(E,T_2)}{\partial q_k} = \frac{1}{2E}\sqrt{\alpha/\pi}\int_0^\infty dE_r E_r^{1/2}\frac{\partial\sigma_x(E_r,T_1)}{\partial q_k}\times\left[e^{-\alpha(E^{1/2}-E_r^{1/2})^2} - e^{-\alpha(E^{1/2}+E_r^{1/2})^2}\right]. \quad (10)$$

The method used to solve Eq. (10) is similar to that used in the MINX cross-section processing code.[9] The method involves assuming a linear interpolation between tabulated values of the derivative. This approach differs from that of Greenspan[5] who uses psi- and chi-type formalism to perform the Doppler broadening. This method is more accurate than Greenspan's approach, especially in the wings of the resonance where large errors can occur using the psi and chi functions.

The next step in the development of the RP sensitivities is to group-average and resonance self-shield the Doppler-broadened point values. This step is accomplished via the so-called Bondarenko method,[10] where the weighting function for the cross-section averaging process is represented as

$$\phi(E,T,\sigma_0) = \frac{C(E)}{\sigma_t(E,T) + \sigma_0}\ , \quad (11)$$

where C(E) is a continuous, slowly varying function (normally 1/E), and σ_0 is the background cross section used to incorporate varying degrees of resonance self-shielding. The value for the group cross section using this weight function is then

$$\sigma_{xg}(\sigma_0,T) = \frac{\int_g \phi(E,T,\sigma_0)\sigma_x(E,T)dE}{\int_g \phi(E,T,\sigma_0)dE} = \frac{N_g}{D_g}\ . \quad (12)$$

Now taking derivatives of the above equation with respect to the RP results in the following equation:

$$\frac{\partial\sigma_{xg}(\sigma_0,T)}{\partial q_k} = \frac{1}{D_g}\left[\int_g\left\{\phi(E,T,\sigma_0)\frac{\partial\sigma_x(E,T)}{\partial q_k} + \sigma_x(E,T)\frac{\partial\phi(E,T,\sigma_0)}{\partial q_k}\right\}dE\right]$$
$$\left[-\sigma_{xg}(\sigma_0,T)\int_g\frac{\partial\phi(E,T,\sigma_0)}{\partial q_k}dE\right]. \quad (13)$$

In practice, the σ_0 and T dependence are usually represented in a so-called f-factor, where

$$f_{xg}(\sigma_0,T) = \frac{\sigma_{xg}(\sigma_0,T)}{\sigma_{xg}(\infty,T)} , \qquad (14)$$

where $\sigma_{xg}(\sigma_0,T)$ is the shielded group cross section, and $\sigma_{xg}(\infty,T)$ is the infinitely dilute group cross section. Thus, the following expression is obtained:

$$\frac{q_k}{f_{xg}(\sigma_0,T)} \times \frac{\partial f_{xg}(\sigma_0,T)}{\partial q_k} = \frac{q_k}{\sigma_{xg}(\sigma_0,T)} \times \frac{\partial \sigma_{xg}(\sigma_0,T)}{\partial q_k} - \frac{q_k}{\sigma_{xg}(\infty,T)} \times \frac{\partial \sigma_{xg}(\infty,T)}{\partial q_k} . \qquad (15)$$

These f-factor sensitivities [Eq. (15)] are tabulated at various values of σ_0 (i.e., 10^{-1}, 10^0, 10^1, 10^2, 10^3, 10^6, 10^{10}). The sensitivities corresponding to a given value of σ_0 for a particular system being modeled can then be interpolated using methods similar to the methods used for the cross sections. The most promising of these options appears to be a power method interpolation scheme developed by N. M. Greene.[11]

The unresolved resonance region offers a considerable amount of complexity due to the statistical nature of the cross-section representation. The development in the unresolved region follows closely that of the resolved region. The reader is referred to ref. 12 for further details.

CALCULATION OF RESONANCE PARAMETER SENSITIVITIES

As a test of the validity and usefulness of the RP sensitivity methodology, the theory described previously was programmed into a computer code, DEFUNCT.[12] In order to validate the results of the DEFUNCT code calculations, a dummy ^{238}U ENDF/B-like file (^{28}DUM) was created using 36 resolved resonances. The validations were performed by making direct perturbations in the RPs and using the NJOY cross-section processing code to obtain reference and perturbed ^{28}DUM cross-section values. The perturbations in the resolved RPs were, in all cases, 10%. In Tables 1 and 2 comparisons between NJOY "actual" and DEFUNCT "predicted" RP sensitivities are shown for the 6.67- and 20.9-eV resonances of ^{28}DUM, respectively, at a temperature of 300 K and σ_0 = 100 barns. The disagreement ranges from 1 to 5% for capture to Γ_γ, 4 to 15% for capture to Γ_n RP sensitivities, and 1 to 70% for elastic to Γ_n. The 70% discrepancy in the elastic to Γ_n RP sensitivity in the group from 29.0 to 37.3 eV for the 20.9-eV resonance is not of major concern since it is not a significant contributor to the total group sensitivity. This error is attributed to the difficulty in adequately representing the rapid variations in the pointwise resonance profiles in this range.

As an additional verification of the methodology developed herein and to evaluate a proposed alternative RP sensitivity method, additional results for ^{238}U are given in Table 3 for two different values of self-shielding, σ_0 = 10^{10} and 22 barns, and two temperatures, T = 0 and 300 K. The relative sensitivity results are given for ^{238}U capture for all resonances in a group spanning 167 to 214 eV. Table 3 compares the results of this method (labeled DEFUNCT), Perey's method[13] (developed by F. G. Perey, designed to operate on resonances greater than 100 eV), and direct recalculations using the MINX code for the sensitivities of ^{238}U capture cross sections to the Γ_γ and Γ_n RPs. The resonances selected for direct recalculations were chosen first on their high sensitivity, and second on apparent discrepancies between the Perey and DEFUNCT results. In

Table 1. Resonance parameter sensitivity comparisons for 6.67-eV resonance in ^{28}DUM cross sections

Group boundaries (eV)	Capture to Γ_γ sensitivity		Capture to Γ_n sensitivity		Elastic to Γ_n sensitivity	
	Actual[a]	Predicted[b]	Actual[a]	Predicted[b]	Actual[a]	Predicted[b]
3.06	20.51	20.54	306.0	306.6	-562.9	-632.6
3.93	39.50	39.80	596.0	594.2	-794.7	-909.5
5.04	345.3	361.4	5172.0	5431.0	-1603.0	-1964.0
6.48	639.1	665.3	8874.0	9355.0	4570.0	4972.0
8.32	20.15	20.30	300.0	302.3	755.0	855.8
10.7	4.083	4.080	60.93	60.88	344.4	406.4
13.7	1.332	1.308	19.87	19.53	192.1	243.7
17.6						

[a]The sensitivity obtained from a direct recalculation using NJOY.
[b]The sensitivity as calculated using DEFUNCT.

Table 2. Resonance parameter sensitivity comparisons for 20.9-eV resonance in ^{28}DUM cross sections

Group boundaries (eV)	Capture to Γ_n sensitivity		Elastic to Γ_n sensitivity	
	Actual[a]	Predicted[b]	Actual[a]	Predicted[b]
3.06	5.93	5.90	-58.3	-66.2
3.93	5.93	5.86	-59.3	-70.1
5.04	4.94	5.57	-54.3	-75.6
6.48	-9.88	-8.41	-98.8	-87.0
8.32	8.40	8.37	-94.9	-99.6
10.7	12.7	12.9	-119.0	-129.0
13.7	34.6	35.2	-187.0	-211.0
17.6	524.0	613.0	632.0	634.0
22.6	48.6	53.6	287.0	350.0
29.0	9.88	10.2	69.2	118.0
37.3	<0.98	1.10	79.1	56.9
47.9				

[a]The sensitivity obtained from a direct recalculation using NJOY.
[b]The sensitivity as calculated using DEFUNCT.

Table 3. Relative sensitivity comparisons for ^{238}U capture group cross section (167 to 214 eV) to all resonances contained in the group

Resonance energy (eV)	Γ_γ (D)[a]	Γ_γ (P)[a]	Γ_n (D)[a]	Γ_n (P)[a]
189.6	0.534	0.543	0.0753	0.0761
			(0.0654)[b]	
208.5	0.266	0.258	0.123	0.119
			(0.114)[b]	
173.2			1.68-3	1.78-3
194.8			1.41-3	1.41-3
			(1.31-3)[b]	
200.7			1.57-3	1.54-3
203.1				
		$\sigma_0 = 10^{10}$, T = 0.0 K		
189.2	0.499	0.469	0.0388	0.0515
			(0.0346)[b]	
208.5	0.314	0.274	1.70-3	0.0102
			(-0.0113)[b]	
173.2			0.0255	0.0328
194.8			0.0133	0.0261
			(0.0139)[b]	
200.7			0.0186	0.0283
203.1			0.0122	0.0173
		$\sigma_0 = 22.2$, T = 300 K		

[a](D) = DEFUNCT method; (P) = Perey method.
[b]Direct recalculation at +10% change in parameters.

Table 3, a cut-off of 1.0×10^{-3} is used for all the relative sensitivities so that insignificant sensitivities are omitted from the comparison. Shown in the top half of the table are the relative sensitivities for ^{238}U infinitely dilute capture cross sections (i.e., $\sigma_0 = 10^{10}$). In the case for infinitely dilute cross sections, the Perey method is nearly exact. This is verified by the good agreement between the DEFUNCT, Perey, and direct recalculation (for a 10% variation) relative sensitivity values. Two comparisons can be made here: (1) agreement between the DEFUNCT and Perey methods partially validate the DEFUNCT methodology since the Perey method is nearly exact for the infinitely dilute case, (2) comparison of the DEFUNCT and Perey methods with direct recalculations can also be used to validate both methods. However, in some cases, as shown later, the direct perturbations contain nonlinear terms so that a direct comparison is not possible.

A good example of this is seen in the bottom half of Table 3 for ^{238}U-capture cross sections at a self-shielding value of $\sigma_0 = 22$ barns and temperature of 300 K. The relative sensitivities for Γ_n at the 208.5-eV resonance show wide variation between the three values indicated. The presence of nonlinear terms is confirmed by making a -10% direct recalculation and again estimating the relative sensitivity value. In this case, the predicted relative sensitivity value is -1.73×10^{-3}, which is quite different from the positive 10% value. At $\sigma_0 = 100$ barns and a temperature of 300 K, this effect is not seen, and the DEFUNCT result agrees very well with the direct recalculations (i.e., DEFUNCT = -6.1×10^{-2}; 10% direct recalculation = -6.2×10^{-2}; -10% direct recalculation = -6.5×10^{-2}). For other resonances in Table 3, it appears that the DEFUNCT values agree very well with the direct recalculations, while the Perey value agreements are much less satisfactory.

In summary, the simple and very quick Perey method seems to give quite good results at infinite dilution. For heavily self-shielded cases, the Perey method gives excellent to good results for the most important Γ_γ relative sensitivities and, in general, very poor results for the Γ_n relative sensitivities. Also, as a caution, these results are given only for the capture cross sections. Other cross sections have not been tested, and the results could possibly be different.

COVARIANCE GENERATION

The RP sensitivities shown in the last section can be used to obtain detailed resonance region covariances as well as covariances for self-shielded cross sections. This section gives examples of infinitely dilute, energy-shielded, and spatial-shielded cross-section covariance matrices generated in ref. 12.

The resonance shielding methodology assumed in this study processes the basic cross-section data into an application-independent, infinitely dilute cross section. The treatment of spatial- and energy-resonance self-shielding is accounted for by f-factors that represent the shielded cross sections divided by the infinitely dilute cross sections. The covariance matrices plotted in Figs. 1–3 give the standard deviation and correlation matrices (correlation values shown range from 0 to +1) for ^{238}U infinitely dilute capture cross sections and the energy and spatial self-shielding f-factors in the resolved and unresolved resonance regions. The cross-section uncertainty information contained in these matrices is directly due to uncertainties in the underlying basic nuclear data parameters. Currently, additional uncertainty data outside the resolved and unresolved

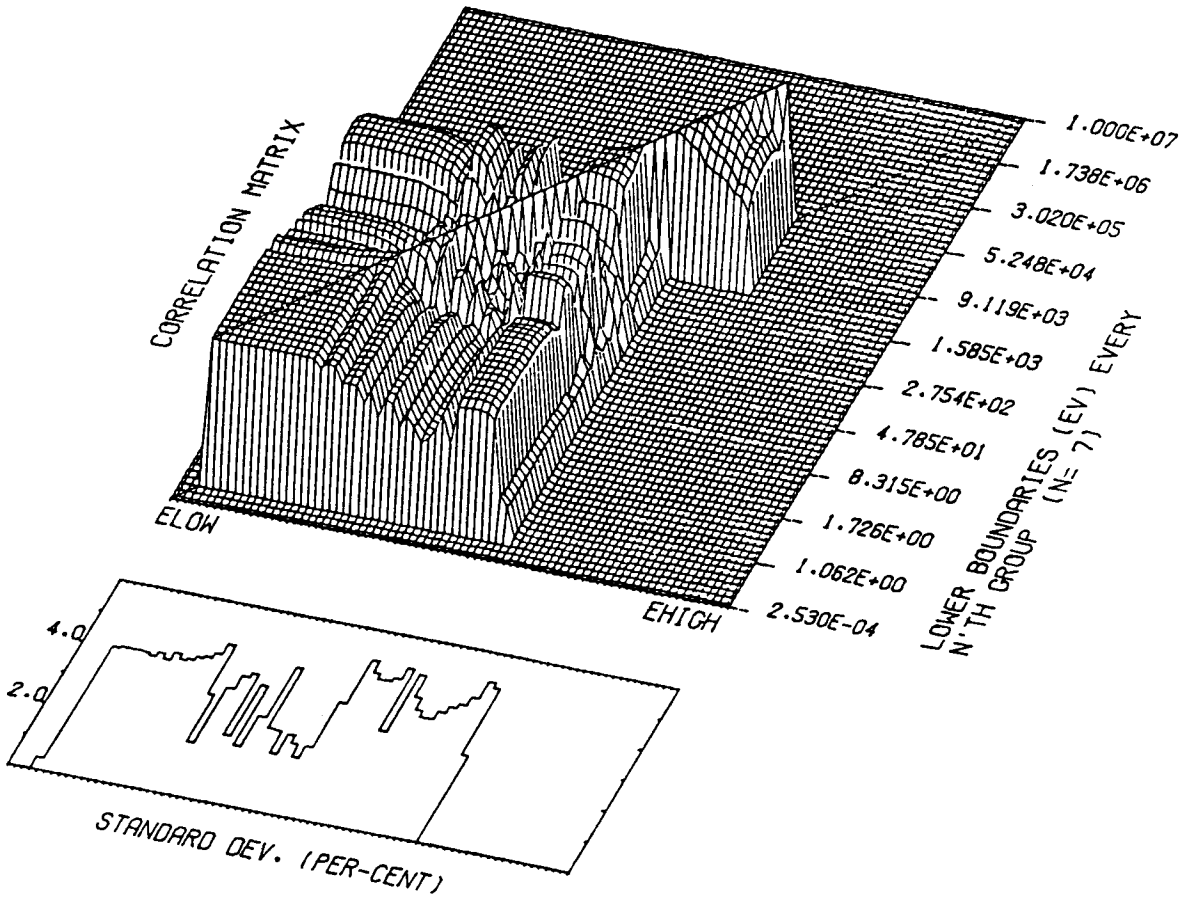

Fig. 1. Correlation matrix and standard deviation plots for ^{238}U infinite dilute capture cross sections in the resolved and unresolved ranges.

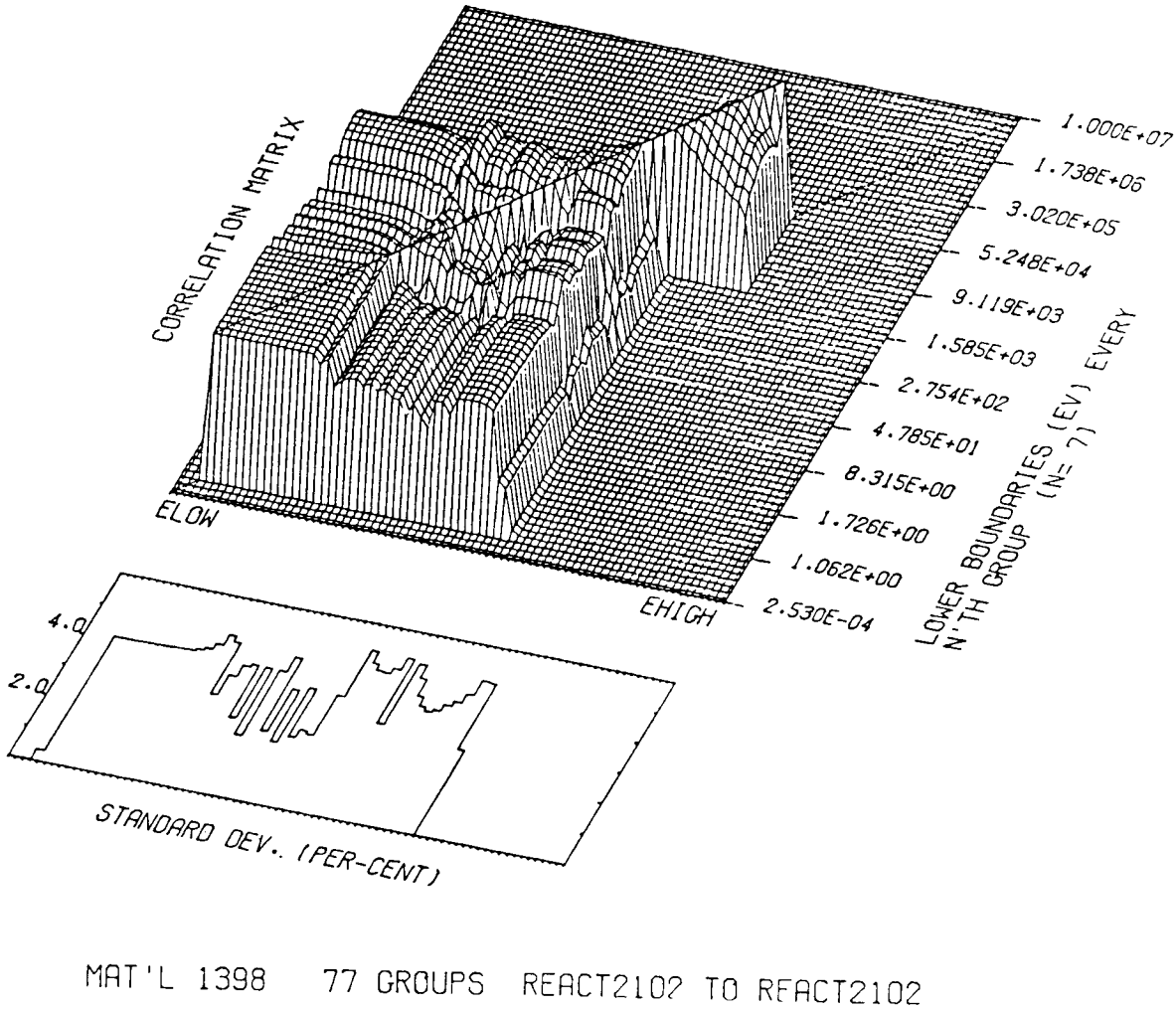

Fig. 2. Correlation matrix and standard deviation plots for ^{238}U energy self-shielding factors in the resolved and unresolved ranges.

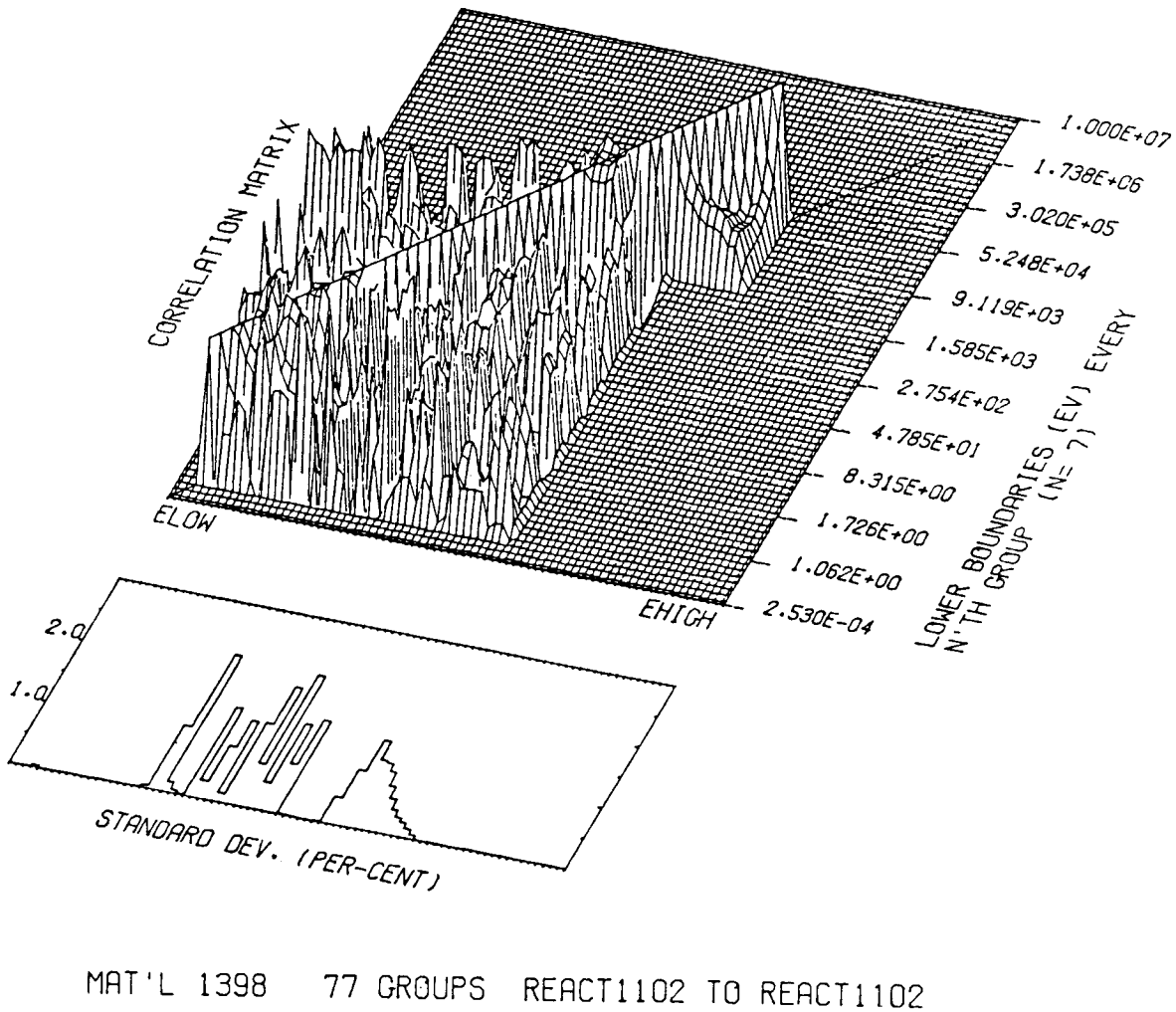

Fig. 3. Correlation matrix and standard deviation plots for ^{238}U spatial self-shielding factors in the resolved and unresolved ranges.

ranges are contained in the ENDF/B uncertainty files and can be combined with this uncertainty information.

CONCLUSIONS

The RP sensitivity methodology developed herein generally provides accurate results as compared with direct recalculations using well-known cross-section processing codes. However, several caveats are appropriate concerning the use of this methodology. It has been shown in several cases that the shielding cross sections can be a very nonlinear function of the basic parameters. For this reason, caution must be used in any undertaking that assumes a linear relationship exists between a given group cross section and its corresponding basic data parameters.

Sensitivity information of the type developed in this study can be of great value when combined with credible covariance information. However, extensions of this and/or other methodologies to cross-section models other than the single-level Breit Wigner are needed. Additionally, approximate techniques that allow the sensitivity information to be generated in a more cost-efficient manner should be pursued.

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Computer Codes for Checking, Plotting and Processing of Neutron Cross-Section Covariance Data and Their Application.

Enrico Sartori
OECD/NEA Data Bank
12 boulevard des Iles
F-92130 Issy les Moulineaux
France

and

Robert W. Roussin
ORNL/EPIC
P.O. Box 2008
Oak Ridge, TN 37831-6362
USA

Abstract

This paper presents a brief review of computer codes concerned with checking, plotting, processing and using of covariances of neutron cross-section data. It concentrates on those available from the computer code information centers of the United States and the OECD/Nuclear Energy Agency.

Emphasis will be placed also on codes using covariances for specific applications such as uncertainty analysis, data adjustment and data consistency analysis.

Recent evaluations contain neutron cross section covariance information for all isotopes of major importance for technological applications of nuclear energy. It is therefore important that the available software tools needed for taking advantage of this information are widely known as they permit the determination of better safety margins and allow the optimization of more economical designs of nuclear energy systems.

Introduction

One of the main objectives of information analysis centers is to acquire state of the art computer programs for applications in the nuclear science and technology field, to verify, publicize, and disseminate this technology to the scientific technical communities who need them.

In the form of computer programs and data libraries, the accumulated scientific knowledge is ready to be used, with the obvious constraint that the user must have the appropriate background. The availability of this technology stimulates the use of more advanced models outside research centers and comparison against approximations in use.

Cross-section covariance data have been used for uncertainty analysis in a relatively small number of research centers. The reluctance to use this most useful information is

often due to lack of understanding of its physical meaning and also to the rather complex procedures to process it to a form readily useable for uncertainty estimation.

With the provision of covariance data in the most recent evaluations such as ENDF/B-VI and JEF-2/EFF for all the important nuclides, it is essential that the tools for processing and manipulating these data are widely known. The objective of this paper is in fact to facilitate potential users to identify those codes they need for their work and which are available from information centers such as EPIC/RSIC, ESTSC and the OECD/NEA Data Bank.

Need for Uncertainty Analysis Tools

Uncertainty analysis in nuclear engineering is essential to determine the confidence one can place into results from design calculations and simulation of operating facilities.

There are several sources of uncertainty including those due to model simplification, discretization of variables, numerical algorithms, and finally all those related to model input data; these comprise both physical constants describing the phenomena underlying the physical processes such as interaction cross-sections and others related to composition and geometrical dimensions of materials specific to a problem.

Over the years a number of computational tools have been developed to assess the different uncertainties. Here we concentrate mainly on those relative to data uncertainties.

Uncertainty analysis consists of several phases in this context:

— the data evaluation process requiring least square methods for estimating expectation values for cross-sections and their covariances, verification of their physical and mathematical properties and checking of their format before including them into the data files.

— the processing of the group cross sections and covariance matrices into a multigroup form and their graphical display.

— the sensitivity and uncertainty analysis relative to specific target quantities characterizing the system performance.

— finally a consistency analysis of the data and improvement through adjustment.

Least Square Fitting Codes

Rigorous evaluation procedures require the use of least square methods for estimating expectation values and their covariances. The models describing the relationship between the measured quantities and the parameters being derived are used in this procedure (i.e., nuclear models, resonance parameter formalism, etc.).

A priori knowledge and the expertise of the evaluator can enter the evaluation process in a more or less rigorous way. Some least square routines implement constrained regularization algorithms consistent with a-priori knowledge. The use of Bayes' theorem provides a means of updating evaluations to include new available knowledge and to calculate the corresponding covariance matrix.

A list of these codes is provided in Annex A; it does not however, include nuclear model codes with fitting capabilities. Such a list can be obtained from the authors.

Examples of codes for determining resonance parameters and their covariance matrices are FANAC, FANAL, REFIT, and SIOB. The list includes also several general purpose least square fitting procedures that can be adapted to nuclear data evaluation needs.

Verification and Processing Codes

New nuclear data evaluations have recently been released worldwide which contain covariance data for the most important nuclides needed for technological applications; these are ENDF/B-VI, JEF-2, EFF and IRDF-90 for dosimetry reactions. As compared to ten years ago the availability of cross-section covariance data has increased considerably. Flexible formats have also been introduced to facilitate the storage of this data for easy retrieval and processing. The covariance processing modules have evolved following these new developments.

Before covariance data are released for general distribution in an evaluation they need to undergo some checking: first the format used is checked whether it conforms to the one adopted, then the mathematical properties of the matrices need to be analyzed. One check looks at whether the matrix is positive definite, whether some eigenvalues are negative, and whether correlation coefficients exceed unity.

The NNDC in Brookhaven has developed over the years a series of checking codes for ENDF format evaluations. These have been extensively used to verify new evaluations (CHECKR, FIZCON, PSYCHE). The part concerning covariance matrix checks still needs to be completed.

Several subroutines were developed to check mathematical properties of covariance matrices; examples are ACORNS, MATXTST, and LAMBDA in the ZZ-VITAMIN-J/COVA package (see Annex A).

It is recommended that the checks carried out by these routines should be implemented in the NNDC evaluated data checking codes.

The most widely used code for processing evaluated covariance data into a multigroup form is NJOY-91. Two modules carry out this task: ERRORR does the actual processing into a multigroup form, an option permits either to produce matrices for all inelastic levels or to group them according to specifications provided by the user. COVR includes convenient format transformation and data compression to the compact BOXR format. It also displays processed multigroup covariance data. This visual representation is important to gain insight into the characteristics of the matrices. Other processing codes exist: PUFF-2 and UNC 32/33. The versions of these two as distributed by the information centers have not been updated to process ENDF-6 format data.

Group-Averaged Covariance Data

Rigorous processing of covariance data into group averaged form requires the use of the corresponding cross section and also a good approximation of the actual neutron flux. Resonance self shielding in the cross sections may also affect the averaging. Ideally

group cross sections sets should be produced consistently together with the corresponding covariance matrix. The NJOY-91/ERRORR is at present the best procedure for preserving consistency.

There exist sets of ready made relative covariance matrices in group averaged form. Some of these were prepared to facilitate the task for those not wishing to embark into the full data processing. These covariance matrix libraries have proven to be of value in a number of applications, such as fusion blanket/shield studies, PWR dosimetry, and oil well logging. It is expected though that these will be superseded by newer ones in the near future with the processing of the most advanced evaluations.

Perturbation Methods, Sensitivity and Uncertainty Analysis

Sensitivity analysis and perturbation theory are of particular importance to model developers for identifying those processes and parameters requiring particular attention. They are a guide to model simplification. Sensitivity analysis codes have been developed rather early as compared to general uncertainty analysis codes because they are very useful also without covariance data as they give important insight into the model characteristics. Annex A lists a number of sensitivity analysis and perturbation codes which are widely used. Most of them are specific to reactor analysis and radiation shielding applications. SWANLAKE, FORSS, and SENSIT were developed for one-dimensional transport; through interface routines two-dimensional direct and adjoint angular flux moments can be made acceptable for these codes. SUSD on the other hand has been designed to carry out two-dimensional sensitivity analyses.

The general purpose tool GRESS deserves particular attention. It expands computer codes capabilities to include sensitivity analysis, thus avoiding the burden of developing specific sensitivity codes. It has been used successfully for a number of applications such as neutron transport, nuclear models and migration of radioisotopes in the geosphere. The input is flexible to allow users to specify which sensitivities they wish to obtain. The application to nuclear model codes seems to be most promising as it allows with the use of model parameters covariances to provide a compact form for storing cross-section uncertainties. It allows also for adjustment of model parameters rather than cross sections.

Multigroup sensitivity profiles have been generated for a variety of benchmark experiments (SENPRO library). These include profiles for fast and thermal reactors as well as shielding benchmarks and are therefore very useful for validating new cross-section evaluations against these experiments and finally to carry out consistency analyses and adjustments.

Four codes are capable of carrying out a full uncertainty analysis; these are ALVIN, LEPRICON, SENSIT, and SUSD. ALVIN is specialized in consistency analysis and adjustments. Consistency analysis aims at avoiding unphysical changes introduced through adjustment. LEPRICON quantifies the uncertainties in the fluence of a PWR pressure vessel, needed for estimating its embrittlement. These uncertainties are then reduced through adjustment with measurements in the in-vessel dosimetry capsules. SENSIT can treat in addition to uncertainties of standard multigroup cross section sets, those of secondary energy distribution (SED). SUSD, in addition to this treats also uncertainties in the angular distributions (SAD) of scattered neutrons. SENSIT and SUSD are therefore suitable also for uncertainty analysis for fusion shield and blanket studies. Data

adjustment, in addition to be useful for reducing uncertainties, also provides feedback on possible deficiencies in the evaluated nuclear data files. Additional codes used in adjustment procedures are AMARA (Legrangian multipliers), ZOTT (partitioned least squares), and unfolding codes such as FERRET, LSL-M2, STAY-SL, etc(See Annex A).

Availability of Codes and Data Sets

Programs and covariance data listed in the Annex were contributed by organizations from several countries. The largest contribution was made by the United States. Authors and their establishments can be identified in the list of references.

The distribution of this information is subject to a cooperative arrangement between the U.S. Department of Energy and OECD/NEA for the NEA member countries. Arrangements with IAEA provide a mechanism for distributing codes and data to most other countries.

Copies of computer program packages can be obtained from
EPIC/RSIC
P.O. Box 2008
Oak Ridge, TN 37831-6362 USA
or
ESTSC/OSTI
P.O. Box 1020
Oak Ridge, TN 37831-1020
USA
or
OECD/NEA Data Bank
12 boulevard de Iles
92139 Issy-les-Moulineaux
France

ANNEX A

Index to Computer Programs for Studies in Sensitivity, Uncertainty and Adjustment Analysis of Nuclear Data and Reactor Parameters

available from

EPIC/RSIC, ESTSC and OECD/NEA DB, (September 1992)

Group Averaged Covariance Data and Sensitivities

Program-name(s)	Description	Ident.*
ZZ COVERX	multigroup covariance library for reactor applications	DLC-0044 [57]
ZZ COVFILS	n cross-section & covariances for sensitivity analysis	DLC-0138 [1]
ZZ DOSCOV	24 group covariance data library from ENDF/B-V for dosimetry calculation	DLC-0090 [2]
ZZ SENPRO/45C	multigroup sensitivity library for fast reactors, thermal reactors	DLC-0045 [3]
ZZ VITAMIN J/COVA	covariance matrix data library for uncertainty analysis	NEA 1264 [4]

Covariance Data Processing, Verification, Manipulation and Plotting

Program-name(s)	Description	Ident.*
ACORNS	covariance & correlation matrix diagonalization	IAEA0975 [5]
MATXTST	basic operations for covariance matrices	USCD1159 [6]
NJOY-91	general ENDF/B format data processing system for reactor design problems	PSR-0171 [7]
PUFF-2	multigroup covariance matrices from ENDF/B-V error files	PSR-0157 [8]
UNC32/33	covariance matrices from ENDF/B-V resonance parameter uncertainties	NEA 1139 [9]
ZZ VITAMIN J/COVA	covariance matrix data library for uncertainty analysis	NEA 1264 [4]

ANNEX A (Cont.)

Perturbation Method, Sensitivity Analysis

Program-name(s)	Description	Ident.*
ABLEIT-TRANS	isotope concentration & sensitivities on cross-section data	NEA 0912 [10]
ALVIN	differential & integral data comparison & sensitivity analysis	NESC0815 [11]
ASOP	shield calculation 1-d discrete ordinates transport	CCC-0126 [12]
BALTORO	coupled n-γ transport perturbation from MORSE, ANISN calculation	IAEA0937 [13]
BOLD/VENTURE-4	reactor analysis system with sensitivity & burnup	CCC-0459 [14]
CATENA	modular system for 1-d multigroup n diffusion calculation with perturbation	NEA 0714 [15]
FORSS	sensitivity and uncertainty analysis in n transport	CCC-334 [56]
GAPER-1D	1-d multigroup 1st order perturbation transport theory for reactivity coefficient	NESC0606 [16]
GENP-2	program system for integral reactor perturbation	NEA 0605 [17]
GRESS	FORTRAN precompiler with differentiation enhancement	PSR-0231 [18]
NEUPAC	experimental n spectra unfolding with sensitivities	NEA 0823 [19]
PERT-4	1st order perturbation for reactivity coefficient in 2-d x-y r-z r-θ geometry	NESC0304 [20]
SAGEP	sensitivity analysis of reactor parameters to cross-section variation	NEA 1037 [21]
SENSIT	integral response sensitivity from n x-sec, γ cross-section errors	CCC-0405 [22]
SENSIT MUSIG COMSEN	sensitivity test analysis	NESC9438 [23]
SUSD	sensitivity & uncertainty in n transport & detector response	NEA 1151 [24]
SWANLAKE	cross-section sensitivity analysis for 1-d discrete ordinate calculation	CCC-0204 [25]
TPTRIA	reactivity for 2-d triangular geometry by transport perturbation theory	NEA 1155 [26]
VARI-1D	1-d diffusion, variational theory & 1st order perturbation sensitivity analysis	NESC0625 [27]
ZZ SENPRO/45C	multigroup sensitivity library for fast reactors, thermal reactors	DLC-0045 [3]

ANNEX A (Cont.)

Uncertainty Analysis

Program-name(s)	Description	Ident.*
ALVIN	differential & integral data comparison & sensitivity analysis	NESC0815 [11]
FORSS	sensitivity and uncertainty analysis in n transport	CCC-334 [56]
LEPRICON	PWR vessel dose analysis with DORT & ANISN programs	PSR-0277 [28]
SENSIT	integral response sensitivity from n x-sec, γ cross-section errors	CCC-0405 [22]
SUSD	sensitivity & uncertainty in n transport & detector response	NEA 1151 [24]

Data Adjustment and Consistency Analysis

Program-name(s)	Description	Ident.*
ALVIN	differential & integral data comparison & sensitivity analysis	NESC0815 [11]
AMARA	correlation of nuclear data to integral experiment by Lagrange multipliers	NEA 0403 [29]
FORSS	sensitivity and uncertainty analysis in n transport	CCC-334 [56]
LEPRICON	PWR vessel dose analysis with DORT & ANISN programs	PSR-0277 [28]
LSL-M2	n spectra logarithmic adjustment for dosimetry applications	PSR-0233 [30]
ZOTT	data correlation using partitioned least-squares	PSR-0272 [31]

ANNEX A (Cont.)

Least-Square Fitting, Data Unfolding

Program-name(s)	Description	Ident.*
ANYOLS	least square fit by stepwise regression	NESC9977 [32]
BRGLM	interactive linear regression analysis by least square fit	NESC9804 [33]
CONTIN-2	experimental data fit by constrained regularization	NEA 0696 [34]
CRYSTAL-BALL	n spectra calculation from activation experiment with error estimate	CCC-0233 [35]
DANTE	activation analysis n spectra unfolding by covariance matrix method	NEA 0694 [36]
DEM4-26	least square fit for IBM PC by Deming method	NESC9681 [37]
FANAC	resonance parameters by multilevel shape analysis of n capture yield data	NEA 0530 [38]
FANAL	resonance parameters by multilevel shape analysis of n transmission data	NEA 0529 [39]
FATAL	general experiment fitting by nonlinear regression method	NEA 0732 [40]
FC LSEI WNNLS	least-square fitting algorithms using B-splines	NESC0909 [41]
FERD-PC	interactive multichannel n & γ spectrum matrix unfolding	PSR-0273 [42]
FERRET	least square fit to nuclear data & reactor physics problems	PSR-0145 [43]
GLUCS	experimental reaction cross-section evaluation for ENDF/B-V	PSR-0192 [44]
GRAPH	data processing, statistical analysis, correlations & graphics	NESC0624 [45]
LSL-M2	n spectra logarithmic adjustment for dosimetry applications	PSR-0233 [30]
MINPACK-1	subroutine library for nonlinear equations system	NESC0888 [46]
NEUPAC	experimental n spectra unfolding with sensitivities	NEA 0823 [19]
PLOTNFIT.4TH	data plotting & curve fitting by polynomials	NESC1130 [47]
RADAK	multichannel analyser n spectra & γ spectra unfolding	NEA 0487 [48]
RDMM	flux spectra from in-pile fast n activation experiment	NEA 0168 [49]
REFIT	multilevel resonance parameters least square fit of n transmission & capture data	NEA 0914 [50]
SAMMY	mutlilevel R-matrix fits to neutron data using Bayes' equations	PSR-0158 [58]
SAND-2	n flux spectra from multiple foil activation experiments	CCC-0112 [51]
SIOB	least square fit of n transmission data using multilevel Breit-Wigner	PSR-0139 [52]
STAY-SL	dosimetry unfolding with activation, dosimetry, flux error calculation	PSR-0113 [53]
TENDANCES	search for tendencies by least square fit method	NEA 1112 [54]
VMCON	minimization of nonlinear function with constraints	NESC0922 [55]
ZOTT	data correlation using partitioned least-squares	PSR-0272 [31]

* CCC-,DLC- and PSR- identifies computer programs packaged by EPIC/RSIC;
NESC identifies those packaged by NESC and now distributed by ESTSC;
NEA, IAEA and USCD identifies those packaged by NEA-DB

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INTERNAL CONSISTENCY OF THE COVARIANCE INFORMATION IN THE INTERNATIONAL REACTOR DOSIMETRY FILE IRDF-90

E. J. Szondi
Institute of Nuclear Techniques of the Technical University
H-1521 Budapest, Hungary

Paper for presentation at the NEANSC Specialists' Meeting
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A B S T R A C T

The most recent cross section set of the Nuclear Data Section of the International Atomic Energy Agency is the International Reactor Dosimetry File (IRDF-90), compiled in ENDF-6 format. A new version of the library was distributed for testing among selected laboratories in June 1992.

This paper reports the results of the test on the data of the files MF=33 of the library. The data for each reaction were analyzed in the energy grid applied in the covariance file to detect the possible sources of bugs appearing in the data processing by the users.

Special attention was paid to the investigation of the cross-covariance information between the pairs of reactions.

The information content of the covariance files has been studied performing the complete factor analysis known from the mathematical statistics.

Keywords: A CODES; CROSS SECTIONS; GROUP CONSTANTS; MULTIGROUP; NEUTRON; X CODES

INTRODUCTION

The most recent neutron dosimetry cross section set of the Nuclear Data Section of the International Atomic Energy Agency (IAEA NDS) is the 1990 issue of the International Reactor Dosimetry File (IRDF-90) [1,2]. The library has been compiled in ENDF-6 format [3]. The covariance information on the cross sections of the library is given, as well. In frame of the continuous update of the data set, new dosimetry reactions were added to the library in June 1992, and a few laboratories were asked to investigate the quality of the file.

The majority of the reaction cross sections contained in the library is newly evaluated at different laboratories and/or the data were converted into the new (ENDF-6) format. The list of evaluators is shown in Table 1. As a consequence of the use of many sources of the data and of the conversion procedure, discrepancies are present in the test version of the library. The aim of this analysis is to point out the improper or erroneous sections of the covariance information in the library, and to make easier the correction of the discrepancies. The investigation of the compatibility of the cross sections eg using them to evaluate benchmark quality measured data (eg [4,5]) lies out of the scope of this study.

THE CONTENTS OF THE CROSS SECTION LIBRARY IRDF-90

It was decided in the REAL-88 project of the IAEA NDS that the update (IRDF-90) of the old reactor dosimetry library IRDF-85 would be available in two forms: the "point" version with the point cross section data and interpolation rules, and the "group" version to make the user's cross section procedure more convenient.

Till now, only the "group" version is available. The list of the dosimetry reactions in the June 1992 test version is given in Table 2. (Other cross sections are also present, without covariance data, see: Table 3.) The "group" form means, that the sum of the cross section data available in the files MF=2 (resonance parameter data) and MF=3 (neutron cross sections) are converted into histogram form and are stored in the new file MF=3. This histogram is given in the rather fine energy grid called "SAND II extended structure" originated from the old neutron spectrum unfolding code SAND II [6].

Table 1

Target	MAT	Evaluator(s)	Date of the Eval.	Distr.	Note
3-Li- 6	325	LANL	Apr.89	Feb.91	
5-B - 10	525	LANL	Nov.89	Feb.91	
9-F - 19	925	IRK	Jun.80	Feb.91	
11-Na- 23	1123	CNDC	Apr.90	Apr.90	
12-Mg- 24	1225	IRK	Apr.90	Feb.91	
13-Al- 27	1325	IRK	Apr.90	Feb.91	ENDF/B-VI
15-P - 31	1525	IRK	Jun.80	Feb.91	
16-S - 32	1625	US	89	Feb.91	ENDF/B-VI
21-Sc- 45	2126	CNDC	Feb.91	?	
22-Ti- 46	2225	US	89	Feb.91	ENDF/B-VI
22-Ti- 47	2228	ANL	Jan.77	Feb.91	ENDF/B-VI
22-Ti- 48	2231	ANL	Jan.77	Feb.91	ENDF/B-VI
23-V - 0	2300	ANL,LLNL,&c	Jun.88	Feb.91	ENDF/B-VI
24-Cr- 0	2400	ECN	85	Mar.85	dpa,IRDF85
24-Cr- 52	2431	IRK	Apr.90	Feb.91	
25-Mn- 55	2525	JAERI,ORNL	Mar.88	Feb.91	ENDF/B-VI
26-Fe- 0	2600	ECN	79	Jan.82	dpa,IRDF85
26-Fe- 54	2625	ORNL	Nov.89	Feb.91	
26-Fe- 56	2631	ORNL	Mar.89	Feb.91	
26-Fe- 58	2637	ORNL	Nov.89	Sep.91	
27-Co- 59	2725	ANL,IRK	Apr.90	Feb.91	ENDF/B-VI
28-Ni- 0	2800	ECN	85	Mar.85	dpa,IRDF85
28-Ni- 58	2825	ORNL,IRK	Apr.90	Feb.91	ENDF/B-VI
28-Ni- 60	2831	ORNL	Oct.89	Feb.91	
29-Cu- 63	2925	ORNL,IRK	Nov.89	Feb.91	ENDF/B-VI
29-Cu- 65	2931	ORNL	Nov.89	Feb.91	
30-Zn- 64	3025	IRK	Apr.90	Feb.91	
39-Y - 89	3925	ANL,LLNL	Jan.86	Feb.91	ENDF/B-VI
40-Zr- 90	4025	IRK	Apr.90	Feb.91	
41-Nb- 93	4125	IRK,ANL,LLL	Jul.91	Aug.91	ENDF/B-VI
45-Rh-103	4525	IRK	Jun.80	Feb.91	
47-Ag-109	4731	CNDC	Jun.91	?	
48-Cd- 0	4800	BNL	May.74	Feb.91	ENDF/B-VI
49-In-115	4931	ANL,CNDC	Jan.90	Feb.91	
53-I -127	5325	CNDC,CIAE	Jun.91	?	
64-Gd- 0	6400	NDS	Aug.90	Sep.90	
79-Au-197	7925	LANL,IRK	Apr.90	Feb.91	ENDF/B-VI
90-Th-232	9040	BNL,ANL,&c	Dec.77	Feb.91	ENDF/B-VI
92-U -235	9228	ORNL,LANL	Apr.89	Feb.91	ENDF/B-VI
92-U -238	9237	ORNL,LANL,&c	Nov.89	Feb.91	ENDF/B-VI
93-Np-237	9337	HEDL,SRL,INEL,ANC,LASL	Apr.78	Mar.84	
94-Pu-239	9437	LANL	Apr.89	Feb.91	ENDF/B-VI

Table 2

Reaction	MAT.MT	Energy boundaries in the files (eV) low end MF=3		low end MF=33	high end MF=3		high end MF=33
LI6T	325.105	1.00E-4	>	1.00E-5	2.00E+7	=	2.00E+7
B10A	525.107	1.00E-4	>	1.00E-5	2.00E+7	=	2.00E+7
F192	925.016	1.09E+7	<	1.10E+7	2.00E+7	<	2.80E+7
NA23G	1123.102	1.00E-4	>	1.00E-5	2.00E+7	=	2.00E+7
MG24P	1225.103	3.20E+6	<	4.60E+6	2.00E+7	<	2.10E+7
AL27P	1325.103	1.08E+6	<	1.90E+6	2.00E+7	=	2.00E+7
AL27A	1325.107	5.00E+6	<	5.40E+6	2.00E+7	<	2.10E+7
P31P	1525.103	1.20E+6	<	1.50E+6	2.00E+7	=	2.00E+7
SC45G	2126.102	1.00E-4	>	1.00E-5	2.00E+7	=	2.00E+7
TI46P	2225.103	1.60E+6	<	2.40E+6	2.00E+7	=	2.00E+7
TI47NP	2228.028	1.06E+7	<	1.07E+7	2.00E+7	=	2.00E+7
TI47P	2228.103	6.90E+5	<	8.00E+5	2.00E+7	=	2.00E+7
TI48NP	2231.028	1.16E+7	<	1.17E+7	2.00E+7	=	2.00E+7
TI48P	2231.103	3.20E+6	>	4.00E+6	2.00E+7	=	2.00E+7
V0A	2300.107	2.00E+6	<	2.10E+6	2.00E+7	=	2.00E+7
CR522	2431.016	1.22E+7	<	1.24E+7	2.00E+7	=	2.00E+7
MN552	2525.016	1.04E+7	<	1.04E+7*	2.00E+7	=	2.00E+7
MN55G	2525.102	1.00E-4	>	1.00E-5	2.00E+7	=	2.00E+7
FE54P	2625.103	6.90E+5	>	5.00E+5	2.00E+7	=	2.00E+7
FE56P	2631.103	2.60E+6	<	3.00E+6	2.00E+7	=	2.00E+7
FE58G	2637.102	1.00E-4	>	1.00E-5	2.00E+7	=	2.00E+7
CO592	2725.016	1.06E+7	<	1.08E+7	2.00E+7	<	2.30E+7
CO59G	2725.102	1.00E-4	>	1.00E-5	2.00E+7	=	2.00E+7
CO59A	2725.107	3.90E+6	>	1.00E-5	2.00E+7	=	2.00E+7
NI582	2825.016	1.24E+7	<	1.28E+7	2.00E+7	=	2.00E+7
NI58P	2825.103	5.00E+5	=	5.00E+5	2.00E+7	=	2.00E+7
NI60P	2831.103	2.00E+6	<	3.00E+6	2.00E+7	=	2.00E+7
CU632	2925.016	1.06E+7	<	1.12E+7	2.00E+7	=	2.00E+7
CU63G	2925.102	1.00E-4	>	1.00E-5	2.00E+7	=	2.00E+7
CU63A	2925.107	1.70E+6	<	2.50E+6	2.00E+7	=	2.00E+7
CU652	2931.016	1.00E+7	<	1.05E+7	2.00E+7	=	2.00E+7
ZN64P	3025.103	5.00E+5	<	9.90E+5	2.00E+7	=	2.00E+7
Y892	3925.016	1.16E+7	=	1.16E+7	2.00E+7	=	2.00E+7
ZR902	4025.016	1.21E+7	<	1.22E+7	2.00E+7	=	2.00E+7
NB932	4125.016	8.90E+6	<	8.92E+6	2.00E+7	=	2.00E+7
NB93N	4125.051	3.00E+4	=	3.00E+4	2.00E+7	<	2.10E+7
NB93G	4125.102	1.00E-4	>	1.00E-5	2.00E+7	=	2.00E+7
RH103N	4525.051	4.00E+4	<	1.00E+5	2.00E+7	=	2.00E+7
IN115N	4931.051	3.20E+5	>	1.00E-5	2.00E+7	=	2.00E+7
IN115G	4931.102	1.00E-4	>	1.00E-5	2.00E+7	=	2.00E+7

(turn over)

Continuation of Table 2

Reaction	MAT.MT	Energy boundaries in the files (eV) low end MF=3		low end MF=33	high end MF=3		high end MF=33
AU1972	7925.016	8.10E+6	<	8.25E+6	2.00E+7	<	3.00E+7
AU197G	7925.102**						
TH232F	9040.018	5.00E+5	<	6.00E+5	2.00E+7	=	2.00E+7
TH232G	9040.102	1.00E-4	>	1.00E-5	2.00E+7	=	2.00E+7
U235F	9228.018	1.00E-4	>	1.00E-5	2.00E+7	=	2.00E+7
U238F	9237.018	1.00E-4	<	9.50E+5	2.00E+7	=	2.00E+7
U238G	9237.102	1.00E-4	>	1.00E-5	2.00E+7	<	2.30E+6
NP237F	9337.018	1.00E-4	<	1.00E+1	2.00E+7	=	2.00E+7
PU239F	9437.018	1.00E-4	>	1.00E-5	2.00E+7	=	2.00E+7

* MF=33: 1.041E+07 eV.
** MF=3: continuous from 1.00E-4 to 2.00E+7 eV;
MF=33: two parts from 1.00E-5 to 2.90E+6 eV
and from 4.00E+6 to 2.00E+7 eV.

Table 3

Reaction	MAT.MT	Note
CR0-D	2400.900	dpa
FE0-D	2600.900	dpa
FE0-D	2600.901	dpa
FE0-D	2800.900	dpa
CD0TOT	4800.001	cover, total xsec
CD0G	4800.102	
GD0TOT	6400.001	cover, total xsec
GD0G	6400.102	

This energy grid consists of 640 energy groups, and covers the energy range of the thermal, fast, and fusion reactors, from 0.0001 eV to 20 MeV. Each decade between 0.0001 eV and 1 MeV contains 45 groups, roughly equidistant in the lethargy scale. The step above 1 MeV is 0.1 MeV.

The pre-processing of the cross sections means that the "group" version of the IRDF-90 should not contain the resonance parameters (file MF=2). The user's processing is controlled by the value of the parameter LRP given in the file MF=1 (general information). Due to the philosophy mentioned above, only the values 0 and 2 have meaning. In spite of this rule, other values are also present related to certain materials, see: Table 4.

Table 4

Material	MAT	D i a g n o s t i c s
11-Na- 23	1123	LRP=1 but no file MF=2 is present
23-V - 0	2300	LRP=1 but no file MF=2 is present
28-Ni- 58	2825	LRP=1 but the file MF=2 corresponds to LRP=0
28-Ni- 60	2831	LRP=1 but no file MF=2 is present
29-Cu- 65	2931	LRP=1 but no file MF=2 is present
39-Y - 90	3925	LRP=1 but no file MF=2 is present
49-In-115	4931	LRP=-1, not allowed for incident neutrons

As an intermediate solution of this problem, the user must assume that the value of the LRP has no importance.

The definition of the parameter LRP in Section 1.1 and the general description of the covariances of the resonance parameters in Section 32.1 of Ref [3] can be interpreted in the following way: if the file MF=2 has to be used in the cross section calculation in the user's energy grid, then the file MF=32 (covariances of the resonance parameters) has to be processed, as well. Therefore, during the analysis, the processing of the file (present in the library) MAT=2126, MF=32, MT=151 (21-Sc-45) was skipped, as LRP=2 was given in file MF=1.

One has to take into consideration, that processing of the file MF=32 is only possible, if a proper code like UNC32 [7] is available.

On the other side, the structure of the uncertainty information of the source libraries (Table 1) has not been changed, ie the files MF=32 and the files MF=33 (covariances of the cross sections) have been simply copied into the IRDF-90. As the contents of the file MF=2 has been combined with the data in the file MF=3, analogous treatment of the covariance matrix of the file MF=32 is necessary, ie this matrix has to be added to the covariance matrix of the smooth cross section (file MF=33).

Due to the copying, the lower and upper energy limits of the files MF=3 and MF=33 differ in certain cases, as it is shown in Table 2. If the energy range in the files MF=33 is broader than the ones in the MF=3, the inconsistency does not disturb the data processing. The deviation in the opposite direction (the covariance matrix "starts" above the threshold energy of the reaction cross section) makes wrong the calculation of the covariance matrix in the user's structure. The form of error depends on the actual values and on the code used. Eg the old code UNC33 [7] may result several thousands of % relative standard deviation, while the new code X333 [8] issues an error message.

The small differences in the lower energies may be originated from the conversion of the point cross section data into the group data and they can be eliminated with systematic modification of the lower energies in the files MF=33. If the differences are large (eg TI46P), then a new evaluation of the file MF=33 is needed.

ANALYSIS OF THE COVARIANCE MATRICES

Generation of the covariance matrices

In frame of testing the covariance matrices the data for each reaction in the library were analyzed in the energy grid applied in the covariance file to detect the possible sources of bugs appearing in the data processing by the users. (Eg: if one of the user's energy groups covers the whole gap in the covariance matrix, mentioned in the previous paragraph, the calculation procedure will skip this gap and a meaningless value will be resulted in as the "relative covariance matrix element" of the pertinent cross section, possible without any error message.)

The generation of the cross section covariance matrix in the user's structure was done using the code X333. This code requires a weighting spectrum; the spectrum PS1 of the REAL-84 project [9,10] of IAEA NDS was selected for this set. (The benchmark spectrum PS1 refers to the simulated surveillance capsule position at the Pool Side Facility of the Oak Ridge research reactor. However, due to the special energy grid, the shape of the weighting spectrum affects only the output values, and does not affect the structure of the output covariance matrix.)

Several reaction cross sections cannot be processed due to critical errors in the library. These are listed in Table 5.

Table 5

Reaction	MAT.MT	D i a g n o s t i c s
S32P	1625.103	Invalid combination of NT=34 and NE=2926
NB93N	4125.051	Correlation coefficients >1.00
AG109G	4731.102	MF1=0 missing (the given MF1 lies out of range)
IN1152	4931.016	NL=0
I1272	5325.016	NL=0
AU197G	7925.102	Gap in the data in the file MF=33

The cross-covariance submatrix between two reaction cross sections is of great importance in the neutron spectrum adjustment calculations. The available sets of the IRDF-90 are shown in Table 6. It can be seen, that for most of the cross covariance data the pairs of the reactions in the library are not present at all. The referred AU197G cross section is lacking, as well. (File MF=33 refers to MAT1=7926, while the IRDF-90 contains the evaluation of MAT=7925.) Furthermore, there is a reference in the file MF=33 of the reaction U238F (9237.018) to the reaction U238G (9237.102) but the inverse reference is lacking. It means, that the user's cross-covariance matrix may be incomplete, even if only the reactions listed in Table 6 are used, depending on the strategy of the covariance matrix generation.

The algorithm of the analysis

The output covariance matrices generated by the code X333 have been normalized calculating the related correlation matrices. As a small sample, the TH232F data are shown here:

Gr	Lower energy (eV)	Cross section (b)	Rel. std (%)	100*correlation matrix									
1	6.0E+05	5.791E-05	32.25	100									
2	8.0E+05	2.786E-04	12.65	4	100								
3	9.0E+05	1.013E-03	10.77	5	12	100							
4	1.0E+06	2.522E-03	8.06	6	16	18	100						
5	1.2E+06	2.386E-02	7.21	7	18	21	28	100					
6	1.4E+06	8.171E-02	5.66	9	22	26	35	39	100				
7	1.6E+06	1.141E-01	7.21	7	18	21	28	31	39	100			
8	3.0E+06	1.399E-01	5.66	9	22	26	35	39	50	39	100		
9	4.0E+06	1.428E-01	7.21	7	18	21	28	31	39	31	39	100	
10	6.0E+06	3.006E-01	10.77	5	12	14	18	21	26	21	26	21	100

It is necessary to note, that it may happen, that certain figures in Tables 7 and 8 are not completely correct, as the cross section processing code X333 has been extended to treat new format elements introduced by the tested version of the IRDF-90, and the result of all the modifications has not been completely tested yet. Nevertheless, the probable errors do not affect the general conclusions.

Table 6

Reaction	MAT.MT	MAT1.MT1			
LI6T	325.105	525.107	525.800	525.801	7926.102
		9228.018	9237.018	9237.102	9437.018
B10A	525.107	325.700	525.800	525.801	7926.102
		9228.018	9237.018	9237.102	9437.018
AU197G	7925.102	325.700	525.107	525.800	525.801
		9228.018	9237.018	9237.102	9437.018
U235F	9228.018	325.700	525.107	525.800	525.801
		7926.102	9237.018	9237.102	9437.018
U238F	9237.018	325.700	525.107	525.800	525.801
		7926.102	9228.018	9237.102	9437.018
U238G	9237.102	325.700	525.107	525.800	525.801
		7926.102	9228.018	9437.018	
PU239F	9437.018	325.700	525.107	525.800	525.801
		7926.102	9228.018	9237.018	9237.102

The methodology of the "factor analysis" known from the mathematical statistics (eg [11]) was used to investigate the information content of the correlation matrices. This procedure consists of the following steps:

1) transformation of the **R** correlation matrix into the normal form of product of the **V** eigenvectors and **E** eigenvalues:

$$\mathbf{R} = \mathbf{V}\,\mathbf{E}\,\mathbf{V}'$$

2) substitution the diagonalmatrix of the eigenvalues with two diagonalmatrices of the square roots of the eigenvalues:

$$\mathbf{R} = (\,\mathbf{V}\ \mathrm{sqrt}(\mathbf{E})\,)\,(\,\mathrm{sqrt}(\mathbf{E})\ \mathbf{V}'\,)$$

or

$$\mathbf{R} = \mathbf{W}\,\mathbf{W}'$$

3) orthogonal transformation ("varimax" rotation) of **W** into the directions of the **V** eigenvectors (in this case the variance of the coordinates is maximal), to separate the "factors" that are responsible for the correlations. (The coordinates are called as "factor loading", ie the contribution to the total correlation of the pertinent "factor". The interpretation of the "factors" can be obtained with deep and detailed physical analysis.)

The "rotated factor vectors" can be used to reconstruct the correlation matrix. The main advantage of the use of them is that each vector is related to a single eigenvalue, therefore the "factor" of the largest eigenvalue has the greatest importance as a common reason of the correlations, &c. If one selects less terms than the total number of the eigenvalues (ie the size of the correlation matrix), the limited set of those will show the most important characteristics of the correlations.

The calculations have been done using the code ACORNS [12]. Its output contains the ordered eigenvalues and some values characterizing the correlation matrix. These are listed in Table 7 under the subtitles:

- >0 number of the positive eigenvalues
- 0 number of the eigenvalues that will be lost during the calculations due to the rounding errors (they may be either positive or negative)
- <0 number of the negative eigenvalues
- 98% number of the ordered eigenvalues (the first one is the largest) the sum of which is greater or equal to the 98 % of the trace of the correlation matrix (ie size); a part of 98 % of the information content is hold by them.

A correlation matrix must be "positive definite", ie all of the eigenvalues must be positive. It can be seen from the data in the Table 7, that 8 correlation matrices do not fulfill this requirement: their negative eigenvalues significantly differ from the range of the rounding errors. Neither these, nor the further 12 ones of the group "0" can be used in the adjustment of cross sections, since the inversion of them will lead to unpredictable results.

Table 7

Reaction	MAT.MT	Characteristics of the covariance matrix								
		No. of eigenvalues					Shape	Cond. numb.	Rel. std (%)	
		Size	>0	0	<0	98%			min.	max.
LI6T	325.105	38	18	17	3	13	chb.	17.9	0.14	20.00
F192	925.016	20	16	4	0	14	chb.	17.0	1.19	21.52
NA23G	1123.102	5	5	0	0	5	diag.	0.0	2.00	25.00
MG24P	1225.103	44	44	0	0	42	chb-b.	1.4	0.46	32.65
AL27A	1325.107	48	48	0	0	46	band	1.3	0.29	11.58
P31P	1525.103	33	28	0	5	21	chb-b.	4.6	1.79	20.49
SC45G	2126.102	19	13	6	0	10	chb.	17.4	0.74	22.36
TI46P	2225.103	22	22	0	0	21	chb.	1.1	6.70	14.18

(turn over)

Continuation of Table 7

Reaction	MAT.MT	Characteristics of the covariance matrix								
		No. of eigenvalues					Shape	Cond. numb.	Rel. std (%)	
		Size	>0	0	<0	98%			min.	max.
TI47NP	2228.028	1	1	0	0	1	scalar	N/A	30.00	30.00
TI47P	2228.103	40	40	0	0	38	band	1.6	5.98	11.75
TI48NP	2231.028	1	1	0	0	1	scalar	N/A	30.00	30.00
TI48P	2231.103	31	24	7	0	22	chb-b.	18.3	4.78	13.43
V0A	2300.107	12	12	0	0	12	diag.	0.0	3.00	15.00
CR522	2431.016	14	11	3	0	10	chb.	17.2	2.21	20.08
MN552	2525.016	2	2	0	0	2	diag.	0.0	10.00	15.00
MN55G	2525.102	13	13	0	0	12	band	1.2	4.47	67.56
FE54P	2625.103	49	43	3	3	39	chb.	17.6	3.06	18.33
FE56P	2631.103	45	45	0	0	43	chb.	1.2	1.83	22.73
CO592	2725.016	16	16	0	0	16	chb-b.	1.0	0.79	41.53
CO59G	2725.102	14	14	0	0	14	band	0.6	0.67	20.25
CO59A	2725.107	34	33	0	1	25	band	2.1	1.30	20.80
NI582	2825.016	16	16	0	0	16	chb.	1.1	1.36	17.63
NI58P	2825.103	41	39	0	2	35	chb.	4.5	4.55	22.65
NI60P	2831.103	6	6	0	0	6	diag.	0.0	9.96	28.46
CU632	2925.016	17	14	3	0	14	chb.	17.0	0.93	20.40
CU63G	2925.102	23	23	0	0	16	chb.	2.3	4.12	20.89
CU63A	2925.107	47	45	2	0	40	chb.	18.2	5.33	24.81
CU652	2931.016	29	22	5	2	20	chb.	17.3	2.24	14.95
ZN64P	3025.103	32	32	0	0	31	chb-b.	1.5	2.32	24.15
Y892	3925.016	10	10	0	0	10	diag.	0.0	5.00	25.00
ZR902	4025.016	20	20	0	0	19	chb-b.	1.3	0.83	10.77
NB932	4125.016	18	18	0	0	16	chb-b.	1.5	0.88	102.57
NB93N	4125.051	31	21	3	7	14	chb-b.	17.1	2.66	17.80
NB93G	4125.102	16	16	0	0	16	diag.	0.0	10.00	63.32
RH103N	4525.051	32	26	0	6	17	chb.	4.4	2.97	30.77
IN115N	4931.051	30	30	0	0	27	band	1.8	2.30	27.90
IN115G	4931.102	6	6	0	0	6	diag.	0.0	6.00	15.00
AU1972	7925.016	22	22	0	0	19	chb.	1.7	1.29	48.74
AU197G	7925.102						chb.			
lower part:		27	14	13	0	13		18.3	0.14	1.55
upper part:		7	2	5	0	2		16.9	22.36	25.00
TH232F	9040.018	10	10	0	0	10	band	0.8	5.66	32.25
TH232G	9040.102	4	4	0	0	4	chb.	0.1	1.41	20.62
U235F	9228.018	33	22	11	0	20	band	17.9	0.19	0.90
U238F	9237.018	12	9	3	0	9	band	17.3	0.59	1.06
U238G	9237.102	25	14	11	0	12	chb-b.	17.9	0.35	2.05
NP237F	9337.018	3	3	0	0	3	diag.	0.0	10.00	30.00
PU239F	9437.018	32	21	11	0	19	band	18.3	0.25	1.08

The values in the column "Cond. numb." are the necessary numbers of the decimal digits to process these matrices. Using single precision (REAL*4 variables), the number of the available digits is about 6. The reaction covariance matrices characterized with larger values are "ill conditioned" ones.

The output of the ACORNS contains the "rotated factor vectors". The data of the reaction TH232F are shown here:

	Ordered eigenvalues								
Group No.	3.223	0.982	0.891	0.860	0.837	0.732	0.690	0.690	0.594	0.500
	Coordinates of the rotated factor vectors									
1	.0238	.9976	.0140	.0180	.0180	.0203	.0238	.0238	.0295	.0295
2	.0639	.0146	.9847	.0436	.0436	.0573	.0639	.0639	.0734	.0734
3	.0755	.0190	.0443	.9788	.0515	.0640	.0755	.0755	.0886	.0886
4	.1048	.0224	.0612	.0674	.0674	.9604	.1048	.1048	.1252	.1252
5	.1182	.0272	.0706	.0821	.0821	.1083	.1182	.9488	.1430	.1430
6	.1604	.0377	.0907	.1078	.1078	.1451	.1604	.1604	.2027	.9098
7	.9488	.0272	.0706	.0821	.0821	.1083	.1182	.1182	.1430	.1430
8	.1604	.0377	.0907	.1078	.1078	.1452	.1604	.1604	.9098	.2027
9	.1182	.0272	.0706	.0821	.0821	.1083	.9488	.1182	.1430	.1430
10	.0755	.0190	.0443	.0515	.9788	.0640	.0755	.0755	.0886	.0886

It can be seen, that the correlations are decreasing with the distance between the pertinent energy groups (cf the values eg in the column 3.223 and the rows 7-6, 7-8, 7-5, 7-9, or in the column 0.500 and the rows 6-5, 6-7, &c). This structure is similar to a "band" matrix.

On the basis of the output set of the ACORNS, the reaction cross section correlation matrices of the IRDF-90 are characterized in Table 7 by short notations:

- band: like a band matrix
- chb.: the matrix consists of fields like a chess-board
- chb-b.: combination of the band and chess-board structure
- diag.: diagonal matrix

At the present time, no theoretical requirements on the structure of the cross section correlation matrices are known. Nevertheless, a diagonal matrix cannot be correct, as the cross sections on the both sides of any point in the energy grid cannot be uncorrelated.

The last two columns of Table 7 show the extreme values of the standard deviations. Making the usual assumption, the ±3 std limits have to be taken into account. Therefore special attention has to be paid to the analysis of the largest uncertainty figures, listed in Table 8.

Table 8

Reaction	MAT.MT	Max. std. (%)	Energy region (eV)
MG24P	1225.103	32.65	4.60E+6 .. 5.20E+6
TI47NP	2228.028	30.00	1.07E+7 .. 2.00E+7
TI48NP	2231.028	30.00	1.17E+7 .. 2.00E+7
MN55G	2525.102	67.56	2.00E+3 .. 6.00E+4
CO592	2725.016	41.53	1.00E+7 .. 1.10E+7
NB932	4125.016	102.57	8.92E+6 .. 9.25E+6
NB93G	4125.102	63.32	1.50E+7 .. 2.00E+7
RH103N	4525.051	30.77	1.00E+5 .. 3.00E+5
AU1972	7925.016	48.74	8.25E+6 .. 8.50E+6
TH232F	9040.018	32.25	6.00E+5 .. 8.00E+5
NP237F	9337.018	30.00	1.00E+1 .. 1.00E+5

CONCLUSIONS

The tables show that too much format errors are present in the test version of IRDF-90. At the same time, the information content of this cross section library is also not completely correct. Before the release of the new version of IRDF-90 the shortcomings should be removed. The release should be fast not to delay the distribution of the Nuclear Metrology File NMF-90 of the IAEA NDS [13].

The tools to this work are available: the last tests of the program package X333 are going on, and the package will be part of NMF-90. The package ACORNS is distributed through the Radiation Shielding Information Center at ORNL.

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EXPERIENCES WITH CROSS SECTION PROCESSING CODES FOR UNCERTAINTIES

H. J. Nolthenius
Netherlands Energy Research Foundation ECN
NL 1755 ZG Petten, The Netherlands

and

E. J. Szondi
Institute of Nuclear Techniques of the
Technical University of Budapest
H-1521 Budapest, Hungary

ABSTRACT

A neutron spectrum adjustment procedure requires among others on its input the cross-sections for the reactions of interest with their covariance matrices in the user's energy group structure. The most recent data set, a test version of the International Reactor Dosimetry File (IRDF-90) of the Nuclear Data Section of the International Atomic Energy Agency was compiled in the ENDF-6 format. Computer codes have been developed in order to convert the uncertainty of the IRDF-90 library data into the user's energy grid. Experiences with two conversion codes and some data for this test version of the IRDF-90 library are given.

1 INTRODUCTION

A number of international intercomparisons for the application of neutron spectrum adjustment procedures, organized by the IAEA, was made in the REAL exercises. In these comparisons the output of neutron spectrum adjustment methods by various laboratories were analyzed and the quality of the input data was considered (eg.[1]).

Some of the conclusions of the exercises were that the best results could be achieved by the generalized least-squares method which requires that all data are accompanied by uncertainty data, and that the quality of the cross-section and their uncertainty information should be improved. The latter point was elaborated by the Nuclear Data Section of the IAEA. A new version of the International Reactor Dosimetry File was composed and distributed for testing. An older preliminary version of the IRDF-90 (version V.1) had been tested earlier [2]. An important conclusion of this test was that this preliminary library was not yet suitable for the REAL benchnark exercise due to missing reaction cross-sections and uncertainty data. For that reason an extended test version of the IRDF-90 has been made by the Nuclear Data Section of the IAEA. This version (received in June 1992) was applied for the calculations described here.

The IRDF-90 library which we received was the so called "group" version in the ENDF/B-6 format. For this "group" version of the IRDF-90, the original "point" cross-section data of the file MF=3 were converted into a histogram (group averaged) format with help of the codes GROUPIE and LINEAR. The 640 groups of SAND II are used as the fine-group structure in the histogram format. The uncertainty data of the cross-section information in the original files have the format MF=33 for the "point" data and occasionally MF=32 for the resonance parameters. Uncertainty information in the IRDF-90 has only the MF=33 format. A MF=32 part of the original file will be converted to a MF=33 format before insertion in the IRDF-90.

2 CONVERSION PROGRAMS

Due to the change in format of the IRDF-90 library (ENDF/B-6) with respect to the IRDF-85 (ENDF/B-5) the conversion program UNC33 [3] which was applied for the calculation of the cross-section uncertainty values from the IRDF-85 had to be modified. The principle of the conversion in the UNC33 program is that the response-weighted covariance matrix is calculated in the group structure of the user.

The two conversion codes applied for this purpose are reorganized, and extended follow-ups of the original program UNC33 and they are running on PC's. The program UNC33 was written for the CDC CYBER mainframe computer at ECN, Petten, [3,4] and it was then adjusted to the IBM System/370 computer at the Budapest Technical University in the frame of IAEA's REAL-84 project [1]. The latter version was used as base for developing the FORTRAN77/PC version X333. Independently another version UNC33M was written by Matzke [6]. Both conversion programs (UNC33M and X333) are parts of packages of programs developed for the neutron metrology task applying the generalized least-squares method.

These packages will be part of the " Reference data file for neutron spectrum adjustment and related radiation damage calculations " which is outlined in [5]. These packages are not yet published in the open literature. During the conversion of the UNC33 program to the PC a number of changes were needed and the two versions of the conversion program available now are different in respect of input and internal organization. The extensions required due to the change from ENDF/B-5 to the ENDF/B-6 format were incorporated in the programs. These extensions refer to new formats for so called Sub-subsections in the ENDF/B-6 format with partial uncertainty data. The input of both programs is rather simple so that the conversion can be done on a routine base without too much effort for data treatment. In the following part some details of the conversion programs are given.

Both of the packages use the FORTRAN77 programming language and they were translated with the Microsoft FORTRAN version 5 or 5.1 for the calculations presented here.

2.1 THE MIEKE PACKAGE

The package is written by Matzke at PTB [6]. It comprises besides the generalized least-squares method also programs for the unfolding of counting results with Bonner spheres and it contains a Monte Carlo method which unfolds without input spectrum information. Also a number of utility programs is included eg. one for displaying cross-section data and neutron spectra. For the conversion of the uncertainty data of the IRDF-90 file the program UNC33M is available. This last mentioned program needs the following input files.

- The IRDF-90 library in the SAND II 640 group format.
- A (help) library in the Sand II format which can be made with the utility program MCROBI (present in the package). The input for this program is the IRDF-90 and a file with the relation between the MAT identification in the IRDF-90 and the names of the cross-section in the new library.
- The weighting fluence rate spectrum in the 640 group structure.
- The user's group structure for which the uncertainty matrix has to be calculated.
- The reactions for which the uncertainty matrix has to be calculated.

Of course other cross-section libraries in the ENDF/B-6 "groups" format can be treated as well.
For reactions which have uncertainty data for the resonance parameters in file MF=32 an extra file with preprocessed data can be added to the UNC33M program.

2.2 THE BME+ECN PACKAGE

This package is mainly written at the Technical University of Budapest. It is also intended to perform the generalized least-squares method for neutron metrology tasks and it contains a number of programs for this purpose. The uncertainty conversion is done with the program X333. The input for the program consists of three files ie.:

- The IRDF-90 library in the SAND II 640 group format.
- The weighting fluence rate spectrum in the 640 group structure.
- The reactions of interest and the user's group structure for which the uncertainty matrix is required.

In case that a library of the type IRDF-90 contains irregularities in the format then it is advisable to make first a run with the checking program FORCE (included in the package) to prevent a number of stops of the conversion program for incorrect library data.

3 RESULTS AND EXPERIENCES

Computations were made with the two programs and the test version of the IRDF-90 for various user group structures.
In the execution of tasks with the same input data the X333 program is remarkably faster than the UNC33M program. This is mainly due to the reading of the IRDF-90 as a " direct access" file.

For a few reactions the format of the uncertainty information was not correct in this test version of the IRDF-90 (ie. S32P, Ti48P and Ag109G). For the latter two reactions "unauthorized" corrections of the library were performed so that the format was accepted in the conversion programs. Results for these corrected reactions are listed in the tables also.

Table 1 shows some results of calculations performed with the codes UNC33M and X333 in a user's group structure of 27 groups covering the energy region from 100 eV to 15 MeV. The weighting spectrum used in these calculations was a typical MTR spectrum in 640 groups. The column " Remarks" gives some information on the results. The + sign indicates that the two conversion codes gave identical results for the uncertainty matrices in the users' structure. The minus sign indicates discrepancies between the results of the codes. The number in the column " Remarks " for reactions which did not give identical results, indicates which types of Sub-subsections are present in the IRDF-90 library. It was observed that the LB=4 representation in the IRDF-90 Sub-subsection was not read and analysed by the X333 program. For that reason all data sets with this type of uncertainty contribution show differences in the output of the two programs.

It was also observed that the output of the two conversion programs for the Sub-subsection with LB=8 representation are different. In general these differences are small due to the relative small uncertainty contribution of the LB=8 Sub-subsection. A few reactions yield very large uncertainties for the uncertainty part LB=8. Some calculations with simplified libraries with just the Sub-subsection for LB=8 indicated that the output of X333 is not correct.
If the code NX is given in the column "remarks" no data were available for the uncertainty in the output of the X333 program. Tables 2 shows a conversion program output for a covariance matrix. For this reaction both programs gave the same results. Table 3 gives an example of an output matrix calculated with UNC33M for a reaction with large uncertainties due to the LB=8 Sub-subsection.

In table 4 the uncertainties of the reactions of the test library IRDF-90 are listed in a three-groups users' structure. For most reactions reasonable uncertainty data are derived but a few reactions show unexpectedly large values. ie. Mn55G, Fe58G, Nb93G and In115G which gave relatively (too) large uncertainties for the thermal and the intermediate groups. Some reactions give also large uncertainties in the fast neutron group ie. Ti47NP, Ti48NP, Ni60P, Nb932 and Mn552. This might partly be due to the high threshold and the large uncertainty values present near the threshold in the high-energy tail of the fission spectrum.

4 CONCLUSION AND REMARKS

When the work for this contribution was started we had the opinion that both conversion programs worked correctly. Due to the comparison of the output of the two codes bugs were found, they will be corrected as soon as possible so that two conversion codes are available for conversions.
This test version of the IRDF-90 contains still some format irregularities which are described in another contribution to this meeting [7].
The calculated results derived for this test version of the IRDF-90 show that the uncertainty values of a few reactions are still (too) large for metrology purposes. Especially for this point work has to be done so that the usual metrology reactions will have the same weight in adjustment calculations.
This test version of the new IRDF-90 is much more useful for practical applications in neutron metrology work than the first version.

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Table 1 Comments on the performance of the two conversion codes

N	Reaction	MAT	MT		Remarks *)	
1	LI6T	325	105	+		
2	B10A	525	107	+		
3	F192	925	16	+		
4	NA23G	1123	102	+		
5	MG24P	1225	103	+		
6	AL27P	1325	103	-	4 8	
7	AL27A	1325	107	+		
8	P31P	1525	103	+		
9	SC45G	2126	102	-	1 1 8	
10	TI46P	2225	103	-	5 4 1 8	NX
11	TI47NP	2228	28	+		
12	TI47P	2228	103	-	5 8	
13	TI48NP	2231	28	+		
14	TI48P	2231	103	-	5 4 1 8	
15	V0A	2300	107	+		
16	CR522	2431	16		5	
17	MN552	2525	16	+		
18	MN55G	2525	102	-	1 1 8	
19	FE54P	2625	103	-	5 4 1 8	
20	FE56P	2631	103	-	5 4 1 8	
21	FE58G	2637	102	-	0 1 1 8	
22	CO592	2725	16	+		
23	CO59G	2725	102	+		
24	CO59A	2725	107	+		
25	NI582	2825	16	+		
26	NI58P	2825	103	-	5 4 1 8	
27	NI60P	2831	103	-	1 8	
28	CU632	2925	16	+		
29	CU63G	2925	102	-	1 1 8	
30	CU63A	2925	107	-	5 4 1 8	
31	CU652	2931	16	-	5 4 1 8	NX
32	ZN64P	3025	103	+		
33	Y892	3925	16	+		
34	ZR902	4025	16	+		
35	NB932	4125	16	-	5	
36	NB93N	4125	51	+		
37	NB93G	4125	102	+		

*) Remarks

+ Identical results for UNC33M and X333

- Different results for UNC33M and X333
  The numbers indicate the various types of Sub-subsections or the reaction

NX Means no reliable results with X333

Table 1 (continued)

No	Reaction	MAT	MT		Remarks *)	
38	RH103N	4525	51	+		
39	AG109G	4731	102	-	1 1	NX
40	IN1152	4931	16	-	5	NX
41	IN115N	4931	51	+		
42	IN115G	4931	102	+		
43	I1272	5325	16	-	5	NX
44	AU1972	7925	16	+		
45	AU197G	7925	102	+		
46	TH232F	9040	18	+		
47	TH232G	9040	102	+		
48	U235F	9228	18	+		
49	U238F	9237	18	+		
50	U238G	9237	102	-	5	
51	NP237F	9337	18	-	1	
52	PU239F	9437	18	+		

*) Remarks

+ Identical results for UNC33M and X333

- Different results for UNC33M and X333
  The numbers indicate the various types of Sub-subsections for the reaction

NX Means no reliable results with X333

Table 2 Example of output of conversion program for reaction LI6T

REACTION: LI6T MAT= 325 MT= 105

****

GROUP NO	REL.S %	ENERGY EV																												
1	.14	1.000E-04	100																											
2	.14	2.150E-01	100	100																										
3	.14	4.650E-01	100	100	100																									
4	.14	1.000E+00	100	100	100	100																								
5	.14	2.150E+00	100	100	100	100	100																							
6	.14	4.650E+00	100	100	100	100	100	100																						
7	.14	1.000E+01	100	100	100	100	100	100	100																					
8	.14	2.150E+01	100	100	100	100	100	100	100	100																				
9	.14	4.650E+01	100	100	100	100	100	100	100	100	100																			
10	.14	1.000E+02	100	100	100	100	100	100	100	100	100	100																		
11	.14	2.150E+02	100	100	100	100	100	100	100	100	100	100	100																	
12	.14	4.650E+02	100	100	100	100	100	100	100	100	100	100	100	100																
13	.14	1.000E+03	99	99	99	99	99	99	99	99	99	100	100	100	100															
14	.14	2.150E+03	99	99	99	99	99	99	99	99	99	100	100	100	100	100														
15	.14	4.650E+03	99	99	99	99	99	99	99	99	99	99	99	99	100	100	100													
16	.14	1.000E+04	92	92	92	92	92	92	92	92	92	93	93	93	96	96	97	100												
17	.16	2.150E+04	79	79	79	79	79	79	79	79	79	79	79	80	85	85	86	96	100											
18	.23	4.650E+04	42	42	42	42	42	42	42	42	42	43	43	44	50	50	53	71	88	100										
19	.31	1.000E+05	14	14	14	14	14	14	14	14	14	14	14	15	20	20	22	37	54	80	100									
20	.22	2.000E+05	10	10	10	10	10	10	10	10	10	10	10	10	11	11	12	14	17	25	51	100								
21	.29	4.000E+05	15	15	15	15	15	15	15	15	15	15	15	15	16	16	16	17	17	12	12	41	100							
22	.39	8.000E+05	7	7	7	7	7	7	7	7	7	7	7	8	9	9	10	16	21	25	17	10	65	100						
23	.50	1.400E+06	3	3	3	3	3	3	3	3	3	3	3	3	3	3	4	4	5	7	8	6	20	64	100					
24	4.05	2.500E+06	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	3	6	100				
25	10.00	4.000E+06	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	29	100			
26	11.23	6.500E+06	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	15	59	100		
27	14.82	1.050E+07	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	6	42	100	

Table 3 Example of output of conversion program for reaction FE58G

```
************************************************
REACTION: FE58G      MAT=2637  MT= 102
************************************************
```

GROUP NO	REL.S %	ENERGY EV																											
1	46.44	1.000E-04	100																										
2	116.56	2.150E-01	0	100																									
3	116.80	4.650E-01	0	0	100																								
4	116.72	1.000E+00	0	0	0	100																							
5	116.15	2.150E+00	0	0	0	0	100																						
6	116.37	4.650E+00	0	0	0	0	0	100																					
7	116.24	1.000E+01	0	0	0	0	0	0	100																				
8	115.56	2.150E+01	0	0	0	0	0	0	0	100																			
9	115.39	4.650E+01	0	0	0	0	0	0	0	0	100																		
10	7.84	1.000E+02	4	2	2	2	2	2	2	3	3	100																	
11	6.38	2.150E+02	5	2	2	2	2	2	2	2	2	82	100																
12	10.50	4.650E+02	3	1	1	2	2	2	2	3	3	86	61	100															
13	18.55	1.000E+03	0	0	0	0	0	0	1	1	2	46	20	59	100														
14	40.50	2.150E+03	0	0	0	0	0	0	0	0	1	14	0	22	26	100													
15	20.87	4.650E+03	0	0	0	0	0	0	0	0	0	4	0	6	20	52	100												
16	20.59	1.000E+04	0	0	0	0	0	0	0	0	0	2	0	4	18	52	98	100											
17	21.09	2.150E+04	0	0	0	0	0	0	0	0	0	8	0	13	26	54	97	98	100										
18	28.99	4.650E+04	0	0	0	0	0	0	0	0	0	9	0	14	16	10	11	10	12	100									
19	24.16	1.000E+05	0	0	0	0	0	0	0	1	1	15	0	24	25	12	8	7	10	60	100								
20	27.91	2.000E+05	0	0	0	0	0	0	1	1	2	31	1	49	45	21	10	7	15	15	46	100							
21	29.52	4.000E+05	0	0	0	0	0	1	1	1	2	34	1	53	49	22	10	8	16	16	26	48	100						
22	31.37	8.000E+05	0	0	0	0	0	1	1	1	2	36	1	56	51	23	10	7	17	16	27	51	64	100					
23	32.98	1.400E+06	0	0	0	0	0	1	1	1	2	38	1	60	52	24	9	6	16	16	27	53	57	91	100				
24	61.19	2.500E+06	0	0	0	0	0	1	1	1	2	41	1	64	53	24	7	4	15	15	27	55	60	63	84	100			
25	86.66	4.000E+06	0	0	0	0	0	1	1	2	2	46	1	71	59	27	8	5	16	17	29	60	66	70	76	82	100		
26	99.84	6.500E+06	0	0	0	0	1	1	1	2	2	47	1	74	61	28	8	5	17	17	30	62	68	72	78	84	93	100	
27	97.43	1.050E+07	0	0	0	0	0	1	1	2	2	46	1	72	60	27	8	5	16	17	30	61	67	71	76	82	91	94	100

Table 4 Standard deviation (in %) and correlations for three neutron spectra (Maxwell, 1/E and Watt) calculated with UNC33M for test version of IRDF-90

Maxwell = (thermal Maxwellian) number (1)
1/E = 1/E in intermediate region number (2)
Watt = U235 fission spectrum number (3)

		Standard deviation for spectrum			Correlation coefficient between spectra numbers		
		Maxw	1/E	Watt	(1)-(2)	(1)-(3)	(2)-(3)
1	LI6T	.14	.14	1.22	100	1	1
2	B10A	.16	.16	13.19	100	0	0
3	F192			2.37			
4	NA23G	2.00	3.25	18.93	39	0	2
5	MG24P			2.27			
6	AL27P		3.33				
7	AL27A		1.37				
8	P31P		3.59				
9	SC45G	6.35	7.42	12.80	1	1	0
10	TI46P			2.96			
11	TI47NP			30.00			
12	TI47P		8.32	4.32		39	
13	TI48NP			30.00			
14	TI48P			3.64			
15	V0A			3.40			
16	CR522			2.69			
17	MN552			9.12			
18	MN55G	12.38	7.97	11.68	15	0	2
19	FE54P		10.97	2.19		16	
20	FE56P			2.21			
21	FE58G	44.21	16.34	37.61	2	0	5
22	CO592			2.82			
23	CO59G	.66	.77	8.57	95	0	0
24	CO59A			2.76			
25	NI582			2.94			
26	NI58P		13.40	2.47		10	
27	NI60P			10.26			
28	CU632			1.76			
29	CU63G	4.11	3.90	7.66	77	0	12
30	CU63A			2.84			
31	CU652			2.36			
32	ZN64P		2.99	4.80		55	
33	Y892			4.38			
34	ZR902			1.60			
35	NB932			15.72			
36	NB93N		7.45	3.02		41	
37	NB93G	10.00	9.49	8.15	100	0	0
38	RH103N		5.43	3.02		86	
39	AG109G	5.10	6.91	10.81	71	45	34
40	IN1152			3.59			
41	IN115N		2.56	2.18		78	
42	IN115G	6.00	5.98	6.89	100	0	0
43	I1272			2.54			
44	AU1972			4.24			
45	AU197G	.14	.17	1.07	83	1	1
46	TH232F		6.94	5.18		44	
47	TH232G	4.34	10.94	20.62	2	0	11
48	U235F	.19	.27	.35	59	13	25
49	U238F	.00	.26	.54	0	0	58
50	U238G	.35	.37	1.22	89	9	15
51	NP237F	.00	9.53	9.34	0	0	97
52	PU239F	.25	.26	.43	90	22	36

REPORT OF WORKING GROUP A
GENERATION OF COVARIANCES TO MEET USER NEEDS: HANDLING STUBBORNLY DISCREPANT DATA

Members of the Working Group:
C.Y.Fu,
D.C.Larson
Y.Kanda
W.Mannhart
V.Pronyaev
N.Rabotnov
S.Chiba,
R.W.Peelle
C.Bastian
Z.Zhao
D.L.Smith
N.Larson
H.Vonach, Moderator

(A) Needs for Covariances

Our needs for covariances are basically twofold.

(1) Rough uncertainty information for the whole body of evaluated nuclear data that is for all types of cross-sections, angular distribution, secondary energy distribution, etc.

(2) Detailed covariance data, as accurate as possible for a rather limited number of important materials and cross-section types.

Uncertainty information of type one is needed for a quick estimate of the influence of data uncertainties on any nuclear response that might become of technological interest. Such estimates will in many cases show that nuclear data uncertainties are not important or at least reduce the problem from many materials and cross-sections to a few important ones. For this purpose it will be sufficient to have "qualitative" covariance information, that is essentially reasonably safe estimates of the maximum cross-section uncertainties in a very crude bin structure (e.g., a short MF33LB1 sub-subsection) and corresponding information for other data types.

On the other hand there exists a rather small number of materials and special reaction types, where evaluated nuclear data as accurate as possible are needed, because data uncertainties for such materials result in costly safety margins in fission and fusion reactor technology. Such materials are especially the major actinides, the structural materials, materials considered as neutron multipliers and tritium breeders in fusion reactors and materials used for cross-section standards and dosimetry reactions.

For such materials it will be essential that the evaluations really provide the best information which can be extracted from the existing experimental data base and theoretical knowledge. Therefore, in most cases it will be necessary to combine all information quantitatively by generalized least-squares techniques (as for example, successfully completed in the ENDF/B-VI standards evaluation) and covariances are then obtained automatically as a result of such evaluations based on advanced statistical methods.

(B) Further development of the methods used to generate covariance information.

In order to achieve the needed covariance information it will be necessary to further improve our evaluation methodology. The most urgent tasks seem to be the following:

(1) More work is needed on the problem how to perform accurate quantitative evaluations, which involve combining our knowledge of both accurate measurements and model calculations; at present the construction of covariance information of calculated cross-sections has only been done in a very qualitative way. One way to future progress is certainly the approach presented by D. Muir to consider the model calculations as a fitting problem.

(2) It would be highly desirable if the "qualitative" methods, used for example at ORNL and IRK could be formalized in ways so as to allow mass-production of such covariances with limited resources. A document on this subject, giving also simplified instructions on the actual production of ENDF/B-VI formatted covariance files should be produced and made available to all evaluators.

(3) There should be new formats for specifying the uncertainties of coupled energy-angle distributions of secondary particles and the total and energy-differential gamma-production cross-sections. Detail of these formats should be created according to the recommendations of working group B.

(C) Handling of discrepant data: Concerning the handling of inconsistencies the following procedures are recommended:

If inconsistencies within the data base remain after the conventional checks (e.g., for renormalization to new cross-section standards or check which systematic errors were included in the authors' estimate) the following steps should be taken.

1) Identify or eliminate the source of the discrepancy
2) If this is not possible it will be necessary to either reject specific data, increase the uncertainties for specific data or increase the uncertainties of all data in order to achieve a Chi-square value per degree of freedom of about unity.

The decision which of those two possibilities is preferable depends on the specific case and has to be made by the evaluator. In any case all renormalizations of cross-sections, and/or uncertainties and rejections of specific data have to be documented in the evaluations.

3) Discrepancies do exist not only between different experimental data, but also between data and model calculations. In many cases data contradicting well-founded calculations have proved to be incorrect. Thus, in cases where only one data set exists, which contradicts theoretical expectations, the evaluator has to consider this also as a discrepancy to be handled as described before.

(D) Procedures used for linearization within least-squares analysis

All contemporary least-squares methods are based upon linearization of the relationships between measured quantitites and those parameters to be evaluated. Experience has indicated that anomalous evaluated results may emerge from such analyses if the linearization is carried out in an inconsistent manner. Attention needs to be paid to this issue in the determination of the actual covariance and design matrix elements introduced into least-squares analysis codes employed for data fitting or evaluation exercises.

RECOMMENDATIONS OF WORKING GROUP B
COVARIANCE FILE FORMATS AND PROCESSING

D.W. Muir, Chairman
E. Sartori
D. Hetrick
S. Ganesan
S. Chiba
S. Tagesen

1) There are unmet needs for evaluated covariance for many materials. Even for the structural materials, which received considerable attention in preparing ENDF/B-6, covariances are still needed for the emission properties. The covariance application areas discussed in the 1986 Rome meeting remain valid. They include

a) fission reactor core physics;
b) fission reaction fuel cycle;
c) pressure vessel damage and surveillance;
d) fusion neutronics; and
e) fusion dosimetry.

Other emerging needs were identified in health physics (e.g., Hiroshima/Nagasaki analysis) and geophysics (oil well logging).

2) Participants emphasized the need for formatted files describing uncertainty in secondary angle- and energy-distributions. Both the existing File-30 format and the File-36 format proposed by H. Vonach were felt to be very suitable for use in particular evaluation situations. It was recommended that the ENDF processing codes be updated soon to handle these new formats, as well as the recent changes to the other ENDF covariance files.

3) Participants expressed concern over the problems implied for covariance evaluation and processing caused by the large number of isotopic (as opposed to elemental) evaluations in the newer evaluated files.

4) Both as an aid to users and as a mechanism for additional file checking, participants recommended that each new covariance evaluation be processed at the relevant data center in order to extract summary information (e.g., standard deviations at a few energies for important reactions) and that this summary information be placed as free text in "File 1".

MINUTES OF SECOND MEETING OF THE SUBGROUP 2 (GENERATION OF COVARIANCE FILES FOR Fe-56 AND NATURAL Fe) OF THE NSC - WORKING GROUP ON EVALUATION COOPERATION

The second meeting of this working group was held in the afternoon of October 9th 1992 at the Oak Ridge National Laboratory.

List of Attendees:

H. Vonach, coordinator	IRK
C.Y. Fu	ORNL
S. Ganesan	IAEA
D. Hetrick	ORNL
Y. Kanda	ORNL
N. Larson	ORNL
W. Mannhart	PTB
S. Tagesen	IRK

Prof. Vonach summarized the work that has been performed within the working group since the last meeting (May 1991) as follows.

1) A new evaluation of all important cross-sections of iron has been performed at IRK, Vienna [1]. This evaluation used the EFF evaluation [2] and its covariances [3] as a starting point and combined this theory-based evaluation with the complete existing experimental data base using the Bayesian Code GLUCS [4]. In this way the uncertainties could be reduced on average by factors of 2-3 for most cross-sections.

2) Using the accurate evaluated cross-sections from [1], a detailed comparison was made with both EFF and ENDF/B VI. By this comparison it is confirmed that the covariances derived for EFF 2 and ENDF/B VI by rather qualitative methods give reliable uncertainty estimates. This work is also described in [1].

3) A complete covariance matrix covering all resonance parameters of ^{56}Fe has been derived by N. Larson et al. [4] within her analysis of the resonance data of ^{56}Fe. This information is available on request, although not yet in form of a MF32 file.

4) Further work has been done by Prof. Kanda on the determination of covariances for calculated cross-sections by the method of adjustment of the model parameters (e.g. level density parameters) to the experimental data by means of least-squares methods [5,6]. Up to now, however, the quality of the fits is not sufficient to give a good description of the experimental data, thus practical application of the method for generation of covariances is not yet possible [6]. A more extended set of parameters to be varied will probably improve the situation.

5) A proposal for a new format MF36 for uncertainties of secondary coupled-energy-angle distributions for particles and photons has been made by H. Vonach [7] and presented at the NSC-Specialists' Meeting on Generation and Processing of Covariances at Oak Ridge , October 1992. The proposal has been recommended by the participants of that meeting and will be submitted to the chairman of the CSWG format committee for adoption as ENDF/B format.

As a basis for further work Prof. Vonach pointed out that a rather complete experimental data base (180 data sets for 10 types of cross-sections with complete covariance matrices for each data set) is now available at the Radiuminstitut Vienna as a result of the evaluation work described in ref. 1. This data base is available on request and may be used for testing new advanced evaluation methods.

Dr. Zhao, Bejing, expressed strong interest in applying his evaluation method [8] to this ^{56}Fe data base, which will be sent to him by the IRK.

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