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NUCLEAR DATA COVARIANCE WORKSHOP
April 22–23, 1999
Brookhaven National Laboratory

April 2000

L. C. Leal and R. W. Roussin, Editors

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Computational Physics and Engineering

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PREFACE

Donald Smith (Argonne National Laboratory) and Luiz Leal (Oak Ridge National Laboratory) organized the Nuclear Data Covariance Workshop. Dennis Cabrilla of the U. S. Department of Energy (DOE) was instrumental in developing the idea for the Workshop to help support the DOE's Nuclear Criticality Safety Program (NCSP).

The NCSP is a comprehensive program established to help assure continued safe, efficient operations with fissile materials in the United States. The major Tasks included in the NCSP are Critical Experiments, Benchmark Evaluations, Analytical Methods, Applicable Ranges of Bounding Curves and Data (AROBCAD), Information Preservation and Dissemination, Training and Qualification, and Nuclear Data. The Nuclear Data Task provides newly measured differential data and newly evaluated nuclear data for use in analyses of fissile material systems. One feature of the effort to improve the nuclear data for criticality applications is the inclusion of covariance data and sensitivity parameters that then allows the analyst to assess the uncertainty in calculated performance parameters due to uncertainties in the nuclear data. A characteristic of currently available nuclear data libraries is a lack of such covariance information. It was felt that gathering noted experts in the field would help assess the current status and offer guidance to the NCSP Nuclear Data Task on how to proceed in developing covariance information useful for criticality safety analysts.

Since many of the experts in the field are in the international community, we scheduled the Workshop to be held just prior to a meeting of the OECD Nuclear Energy Agency Working Party on Evaluation Cooperation (WPEC). Hence, the Nuclear Data Covariance Workshop, held April 22-23, 1999 at Brookhaven National Laboratory, was able to attract 28 experts from 16 institutes in 8 countries to help assess the status of nuclear data covariance information. The presentations and discussions focused on practical technical matters associated with the generation of covariance matrices, formats for covariance matrices (particularly for evaluated files), mathematical issues related to the manipulation of covariances, and applications for covariance matrices.

This publication provides a means of documenting the formal and informal presentations. The chairs of the four sessions also provided a summary of the discussions and exchange of ideas that took place. The meeting provided a rekindling of interest in this important area of work and representatives of the various international cross-section libraries were supportive of the efforts being made in the NCSP to provide evaluated data files with comprehensive covariance information. It is recommended that Workshops of this kind be planned for the future and the additional activities related to nuclear data covariances be included in the program of the NEA/NCS WPEC.

Session A
Generation of Covariance Matrices
Session Chair: Robert W. Roussin

Three formal presentations were given in this first session. In addition, a brief description of an MF=30 covariance file for hydrogen evaluated data was present during discussion and that write-up is included in these proceedings.

A.1 S. Tagesan, IRK Vienna, Austria, "Important Details in Generating and Manipulating Covariance Matrices"

Tagesan pointed out some pitfalls in dealing with covariances on a practical level. These "Watchouts" concerning the use of the current ENDF/B formats. His recommendations on procedures include always having a positive definite matrix, avoid using absolute covariances, and always use the same energy grid in MF=3 and MF=33. There was lively discussion on these topics and the discourse suffered from not having the designers of the formats in the room to provide background on the rationale that went into the development of the covariance formats.

A.2 D. Muir, IAEA Nuclear Data Section, Vienna, Austria, "Method of Treating Discrepant Data in the ZOTT99 Generalized Least Squares Program".

Muir presented this technique, which he called the Method of Least Distortion (MLD), as a modification to the Generalized Linear Least Squared (GLLS) solution which he has implemented in the latest version, ZOTT99, of his Zeroing in On The Truth code. If discrepant data are suspected, as a result of calculation of a large chi-0 (chi-squared per degree of freedom), the MLD process is invoked. The effect on chi-squared of temporarily increasing, in turn, each one of data variances by a factor of chi-0 is examined. An outlier is identified as one which shows the maximum leverage in reducing chi-squared. The increase in the variance for such a point is made "permanent" and the process is repeated from the first step. There was a lot of skepticism expressed to this approach. The software will be made available to the NEA DB and thus to RSICC for dissemination to the interested community.

A.3 S. Badikov, et al., IPPE, Obninsk, Russia, "An Efficient Way of the Representation of Covariance Data in ENDF-6 Format for Fast Neutron Cross Sections".

Ignatyuk presented this paper which seeks to utilize an infrequently used file 2 resonance parameter format (Adler-Adler) and file 32 for representing covariance data for the fast and high energy region.

During the discussion period, MacFarlane discussed the use of MF=30 to represent a covariance file for hydrogen elastic scattering data. MF=30 is particularly suited to evaluations produced with nuclear model codes and allows the inclusion of sensitivity profiles. Shibata has done a Mn evaluation with MF=30 which is at the NEA Data Bank. Muir reported that some recent evaluations from Russia use MF=30. Later in the meeting MacFarlane offered a demonstration on how one could use MF=30 for point data. In general, the discussion favored the use of this format for new evaluations.

There was additional discussion on how to retrofit covariance data for an earlier evaluation. It was asserted that one can't take the ENDF/B-VI covariances and use them with earlier evaluations, and there was an exchange, pro and con, on this topic.

Some important practical details in generating and manipulating covariance matrices

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Abstract

Neglecting fundamental properties of covariance matrices or physical constraints not automatically accounted for by format rules can lead to – sometimes not obviously – wrong or even meaningless results of propagated information. Some frequently encountered cases are pointed out and discussed.

1. INTRODUCTION

We have run quite a number of evaluations of nuclear reaction cross sections at the I.R.K. over the last years. Intention of such an effort is – of course – to get recommended values with (possibly) small and reliable uncertainties including information on correlations. It is therefore highly alarming when findings like negative variances, correlations of, e.g., 900% or cross section adjustments of 160% appear. Tracing back to the origins of such results revealed some non-obvious traps. Some of those stories, which can be summarized under the headline "watchout for..." will be communicated.

2. BASICS

Subject of our discussion are unbiased best estimates of physical quantities σ_i derived from experimental data by well established formalisms, based on ideas of Gauss, Markov, Aitken and others. Along with the evaluated values we get complete information on uncertainties (variances) and any existing correlations (covariances), which, as a whole, we call the "covariance matrix" (Fig.1).

E(I)	x-sect.	CORRELATION MATRIX
6.5094E+06	σ1	100
1.0000E+07	σ2	0 100
1.1000E+07	σ3	0 33 100
1.2000E+07	σ4	0 14 43 100
1.3000E+07	σ5	0 14 45 95 100
1.4500E+07	σ6	0 14 44 49 52 100
1.6000E+07	σ7	0 14 43 48 51 50 100
1.7500E+07	σ8	0 14 45 50 52 51 96 100
2.0000E+07	σ9	0 14 45 50 52 51 50 52 100

Fig. 1. Data and correlation matrix for a particular nuclear reaction

Two important facts should be kept in mind at this point:
- variances and covariances are part of the respective *evaluated* quantities, since they were derived from the distribution of the underlying experimental data
- the incident neutron energy indicated with the cross sections is of no importance to the evaluation formalism. The cross sections could be in an arbitrary irregular order, they could even belong to different reactions or could be completely different physical quantities, as long as only the relationship of experimental to evaluated data is correct.

For the whole process of evaluation or application of evaluated data it is therefore fundamental to be aware of the fact that

> We have excellent mathematical tools for the treatment of uncertainty information
>
> ***but***
>
> the mathematical procedures do not know anything about the physical meaning of the data.

Conclusion: It is our responsibility as evaluators or users to assure that the data which we feed into any processing code *do* reflect the correct physical properties. If we fail to do so, the results will be unreliable, wrong or meaningless.

3. SOME PARTICULAR "WATCHOUTs"

3.1. THE SUBJECT OF POSITIVE DEFINITENESS

If a covariance matrix was derived from experimental data with correctly determined uncertainties and correlations, the correct properties should automatically be guaranteed. Nevertheless it should be good practice to test each matrix prior to any application. The most rigorous test was presented e.g. by E. J. Szondi in his contribution to the ORNL 1992 Specialists' Meeting[1]: A correct covariance matrix must be positive definite and hence can be tested by analysis of its eigenvalues.

This test obviously was not applied in the "early days" of covariance-matrix design. Some of those ill-conditioned matrices survived in the data files and can now cause problems in the updating process. In particular, all cases where our evaluation resulted in negative variances could be traced back to "prior" covariance matrices with negative eigenvalues.

Special thorough consideration should be given to covariance matrices generated by an estimate of the influence of uncertainties of parameters used in nuclear model calculations. Since the number of parameters is generally small and the shape of the calculated excitation function is to a considerable amount determined by the underlying model assumptions, covariance matrices on the users grid exhibit rather large correlations over medium-size energy ranges. Moreover, these excitation functions can exhibit fairly small uncertainties which are justified only when the chosen model is in fact a good approximation of the physics in that particular case. An example of such a situation is given in the following Fig. 2, in which an analysis reveals a clearly non-positive definite matrix, which will most probably lead to problems in subsequent calculations.

```
ENERGY ERROR  CORRELATION [x1000]
[MEV]   [%]
 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

ANALYSIS OF THE RELATIVE COVARIANCE MATRIX
 WARNING. THE MATRIX IS NOT POSITIVE DEFINITE
 IER = 2
 EIGENVALUES
  1.5331D+02  6.0445D+00  5.4772D-01  3.3221D-02  1.7405D-02  1.4222D-02
  1.2864D-02  1.1032D-02  1.0410D-02  8.0304D-03  6.4252D-03  7.8162D-04
 -4.4204D-04 -2.3288D-03 -4.9451D-03 -7.1144D-03
 NUMBER OF POSITIVE EIGENVALUES:          12
 NUMBER OF ZERO EIGENVALUES:               0
 NUMBER OF NEGATIVE EIGENVALUES:           4
 EFFECTIVE RANK USING SINGLE PRECISION:   16
 EFFECTIVE RANK USING DOUBLE PRECISION:   16
 NUMBER OF EIGENVALUES TO 98 % OF TRACE:   2
 LOGARITHM OF THE CONDITION NUMBER:      5.5
```

Fig. 2. Analysis of a covariance matrix derived from model calculations

Finally, two more situations in which problems of non-positive-definite matrices might arise, are to be mentioned. Both are related to data representation practices within the ENDF-6 specifications[2].

1. Format specifications permit the use of different energy structures in MF3 and MF33. This was frequently used to give a rough estimate of uncertainties on a coarse grid without wasting much storage space in MF33. If subsequently a covariance matrix is calculated on the fine energy grid given in MF3 (cf. Fig. 3), a suitable modification has to be applied to the 100% correlated elements, else the matrix is not positive definite.

2. Format specifications permit the use of different numerical precision, though the data field width is still 11 characters. In many cases this feature is used to express cross section changes at excited levels with precisely known energy with maximum possible resolution of 7 or even 8 significant digits in energy, but leave the standard 5 significant digits for the energy in corresponding uncertainty groups. Even correct rounding may accidentally place points intended to be identical into different energy groups and lead to 100% correlation (Fig. 4).

MF3 energy	MF33	correlation							
1.0	1.0	100							
1.2		100	100						
1.4		100	100	100					
	1.5								
1.6		0	0	0	100				
1.8		0	0	0	100	100			
2.0	2.0	0	0	0	0	0	100		
2.2		0	0	0	0	0	100	100	
2.4		0	0	0	0	0	100	100	100
	2.5								

Fig. 3. Fully correlated ranges due to different energy structure in MF3 and MF33

Energy given in MF3	MF33	correlation on MF3 grid
2.297653+06	2.29765E+06	100
2.456789+06	2.45679E+06	100 100

Fig. 4. A covariance matrix can become not-positive-definite for seemingly negligible reasons

3.2. THE THRESHOLD PROBLEM

ENDF-6 specifications[2] define uncertainties as "associated with the energy interval between two adjacent data points", including the lower energy border of the interval (Fig.5). In order to allow interpolation between σ_1 at E_{thr} and σ_2 including the uncertainty, an uncertainty $\Delta\sigma_1 > 0$ is needed at E_{thr}. Uncertainties may be given as absolute or relative quantities, or as a combination of both. If there is an absolute component in $\Delta\sigma_1$, this implies that σ_{thr} which has to be 0.00 mb is uncertain by $\Delta\sigma_1$ and hence may be adjusted to some nonzero value, whereas a relative component will be multiplied by σ_1 and hence always will result in $\Delta\sigma_1$=0.00 preventing any adjustment.

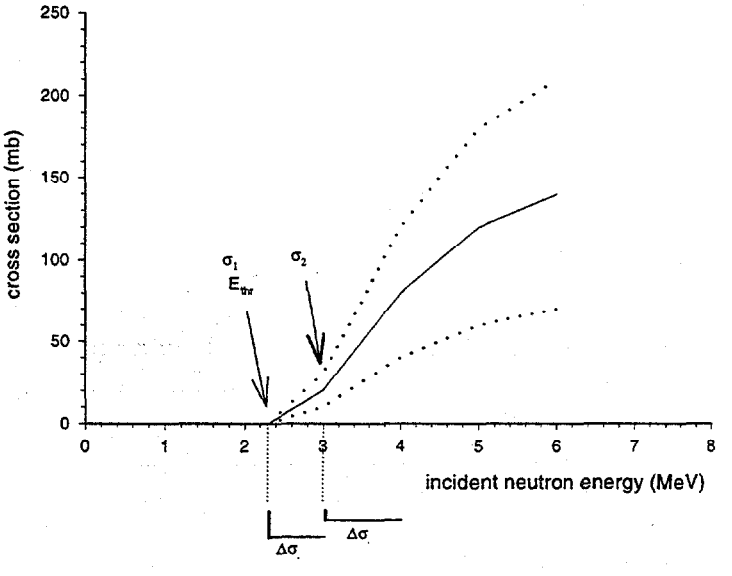

Fig. 5. Origin of threshold difficulties

The following Fig. 6 is an example of such a situation. The LB=0 subsubsection (absolute uncertainty) allows for adjustment of the threshold cross section which originally is correctly given as 0.00 mb. Since the adjustment is small, the related uncertainty which is valid for the whole interval up to σ_2 at 10 MeV, is enormous:

^{58}Ni(n,nα) from ENDF-B/VI

```
 2.805800+4 5.743800+1          0          0          0          02825 3 22
-6.398000+6-6.398000+6          0          0          1          92825 3 22
          9          2          0          0          0          02825 3 22
 6.509400+6 0.000000+0 1.000000+7 8.394700-8 1.100000+7 2.235000-52825 3 22
 1.200000+7 2.552200-4 1.300000+7 1.071200-3 1.450000+7 6.271800-32825 3 22
 1.600000+7 2.014200-2 1.750000+7 4.013900-2 2.000000+7 6.979200-22825 3 22
                                                          2825 3  0
 2.805800+4 5.743800+1          0          0          0          1282533 22
 0.000000+0 0.000000+0          0         22          0          4282533 22
 0.000000+0 0.000000+0          0     LB=  0          6          3282533 22
 1.000000-5 0.000000+0 6.509400+6 7.00000-15 2.000000+7 0.000000+0282533 22
 0.000000+0 0.000000+0          0     LB=  1          6          3282533 22
 1.000000-5 0.000000+0 6.509400+6 4.500000-2 2.000000+7 0.000000+0282533 22
 0.000000+0 0.000000+0          0     LB=  1         16          8282533 22
 1.000000-5 0.000000+0 6.509400+6 1.125000-1 1.000000+7 7.200000-2282533 22
 1.200000+7 4.050000-2 1.400000+7 4.050000-2 1.600000+7 4.050000-2282533 22
 1.800000+7 4.050000-2 2.000000+7 0.000000+0 0.000000+0 0.000000+0282533 22
 0.000000+0 0.000000+0          0     LB=  8         16          8282533 22
 1.000000-5 0.000000+0 6.509400+6 8.80890-17 1.000000+7 5.63770-17282533 22
 1.200000+7 2.93120-10 1.400000+7 9.268100-8 1.600000+7 1.825700-6282533 22
 1.800000+7 9.550800-6 2.000000+7 0.000000+0 0.000000+0 0.000000+0282533 22
                                                          282533  0
```

FINAL THINNED DATA OF # 1 SET

I	E(I) (MeV)	X(E(I)) (barn)	STD(X(E(I))) (%)	
1	6.5094E+06	1.4482E-10	5.8135E+04	<- results are
2	1.0000E+07	8.5229E-08	1.0331E+02	nonphysical
3	1.1000E+07	2.2653E-05	2.9748E+01	
4	1.2000E+07	2.5836E-04	2.5875E+01	
5	1.3000E+07	1.0845E-03	2.4184E+01	
6	1.4500E+07	5.5426E-03	2.7806E+01	
7	1.6000E+07	2.1654E-02	1.7484E+01	
8	1.7500E+07	4.3341E-02	1.6070E+01	
9	2.0000E+07	7.5796E-02	8.0734E+00	

CORRELATION MATRIX

```
1  100
2   94 100
3    1  30 100
4    0   7  24 100
5    0   7  26  93 100
6    0   7  25  29  31 100
7    0   5  19  22  24  24 100
8    0   6  20  24  26  26  90 100
9    0   3  11  13  14  16   1   1 100
```

Fig. 6. Example of unintentional threshold adjustment

3.3. A PROBLEM AT THE UPPER END OF THE ENERGY RANGE

The difficulty is due to the definition of quantities in the ENDF-6 Formats Manual (p. 33.13):

$\{E_k, F_k\}$ $\{E_l, F_l\}$ are two arrays of pairs of numbers. Each array is referred to as an "E table".....In each E table the first member of a pair is an energy, E_n; the second member of a pair, **F_n, is a number associated with the energy interval between the two entries E_n and E_{n+1}.**

The E_k table.....must cover the complete energy range of the File 3 for the same (MAT, MT). The first energy entry in an E table must therefore be 10^{-5} eV, or the reaction threshold, and the last one 20 x 10^6 eV ....., and the **last value of F in an E table must be zero.**

We know, however, that variances and covariances are strictly related to the respective evaluated quantities, i.e., they are bound to the low-energy border, E_n, of each energy interval.

Now let Fig.7 be the result of an evaluation update for two reactions, energy E18 being the 20 MeV point of reaction 1, E30 the respective point of reaction 2.

E11	100																	
E12	-7	100																
E13	-1	2	100															
E14	-3	-11	0	100														
E15	-1	-6	0	-1	100													
E16	0	3	0	0	0	100												
E17	-3	-25	0	-5	-3	-32	100											
E18	**2**	**7**	**-3**	**1**	**0**	**-22**	**-31**	**100**										
E21	0	-3	-5	0	0	-7	12	**0**	100									
E22	0	-6	-5	-1	0	-7	10	**0**	0	100								
E23	0	-2	-5	0	0	-7	13	**0**	0	-30	100							
E24	-1	-1	-35	0	0	0	0	**0**	0	-2	0	100						
E25	0	-4	8	0	0	-22	12	**0**	0	-33	0	15	100					
E26	0	0	9	0	0	-5	0	**0**	0	-9	0	15	-34	100				
E27	0	-1	15	0	0	-6	2	**0**	0	-45	0	53	64	18	100			
E28	-3	-25	-11	-5	-3	12	-15	**3**	-2	34	-1	-53	-68	-13	-89	100		
E29	0	-2	-1	3	2	9	9	**2**	1	23	0	32	42	10	30	22	100	
E30	**1**	**1**	**3**	**2**	**1**	**5**	**7**	**0**	**0**	**11**	**0**	**18**	**25**	**7**	**13**	**9**	**41**	**100**
	E11	E12	E13	E14	E15	E16	E17	**E18**	E21	E22	E23	E24	E25	E26	E27	E28	E29	E30

Fig. 7. Resulting covariance matrix of combined evaluation of two reactions

Following commonly used procedures, the last energy entry in MF3 and MF33 will be 20 MeV and hence there will be a cross section at 20 MeV, but the related uncertainty and correlations, indicated in bold, will be dropped, because " the **last value of F in an E table must be zero".** At a first glance this may appear as a tolerable loss of information, but when the data are read back from the files, the 20 MeV column can only be extrapolated from the adjacent group and this will inevitably produce incorrect results. An extremely unfavorable example of such a situation is shown in Fig.8.

To overcome this problem, I have adopted the following solution: Always create in MF33 one extra energy entry at the upper end, i.e., beyond the last element in MF3. The last matrix column can then be kept and there are no conflicts with the ENDF-rules, as 20 MeV is a minimum requirement for the high energy end, but no limit.

DIRECT EVALUATION RESULT (correlation in %)

Energy set 1 ->									
set 2 \/	6.5	10.0	11.0	12.0	13.0	14.5	16.0	17.5	20.0 (MeV)
9.0	0	1	2	0	0	0	10	11	**18**
10.0	0	0	-4	-6	-6	-21	-3	-4	**2**
11.0	0	0	-4	-5	-6	-19	-6	-6	**6**
12.0	0	-1	-5	-5	-6	-20	-13	-11	**2**
13.0	0	-2	-11	-13	-14	-22	-59	-52	**13**
13.5	0	-1	-5	-6	-7	-9	-28	-27	**-1**
14.0	0	-3	-14	-16	-17	-17	-78	-77	**11**
14.5	0	1	3	3	3	2	23	26	**-12**
15.0	0	-4	-16	-19	-20	-20	-77	-87	**8**
16.0	0	-1	-6	-7	-8	-8	-26	-30	**-4**
17.0	0	-4	-16	-20	-21	-22	-60	-67	**-34**
18.0	0	1	5	5	5	3	18	21	**15**
19.0	0	-2	-10	-13	-14	-15	-20	-22	**-62**
20.0	**0**	**0**	**-2**	**-3**	**-3**	**-3**	**-10**	**-10**	**-10**

matrix elements indicated in bold are not written to the file

MATRIX RECONSTRUCTED, 20 MeV COLUMNS EXTRAPOLATED

Energy set 1 ->									
set 2 \/	6.5	10.0	11.0	12.0	13.0	14.5	16.0	17.5	20.0 (MeV)
9.0	0	1	2	0	0	0	10	11	**21**
10.0	0	0	-4	-6	-6	-21	-3	-4	**-9**
11.0	0	0	-4	-5	-6	-19	-6	-6	**-13**
12.0	0	-1	-5	-5	-6	-20	-13	-11	**-23**
13.0	0	-2	-11	-13	-14	-22	-59	-52	**-104**
13.5	0	-1	-5	-6	-7	-9	-28	-27	**-55**
14.0	0	-3	-14	-16	-17	-17	-78	-77	**-154**
14.5	0	1	3	3	3	2	23	26	**53**
15.0	0	-4	-16	-19	-20	-20	-77	-87	**-173**
16.0	0	-1	-6	-7	-8	-8	-26	-30	**-60**
17.0	0	-4	-16	-20	-21	-22	-60	-67	**-135**
18.0	0	1	5	5	5	3	18	21	**41**
19.0	0	-2	-10	-13	-14	-15	-20	-22	**-44**
20.0	**0**	**0**	**-2**	**-2**	**-3**	**-3**	**-4**	**-5**	**-10**

Fig. 8. Comparison of a direct evaluation result and a matrix reconstructed from the file with a cutoff at 20 MeV. The large correlations at 20 MeV are a direct consequence of the inappropriate extrapolation. In this particular case the extraordinary increase of the correlations is enhanced by a strong increase of the cross section between 17.5 MeV and 20.0 MeV.

4. CONCLUSIONS

To guarantee reliable results in evaluation updates and covariance matrix processing, all data should be checked for correct properties with respect to their physical meaning and careful usage of procedures with respect to physical constraints or limits of applicability must be continuously observed.

Among those "watchouts" are the following ones which I recommend to adopt as standard procedures:

- make sure that covariance matrices – after possible extension or reconstruction – are positive definite
- if it is necessary to quote the same energy values in different files, e.g. MF3 and MF33, use equal numerical precision to avoid artificial differences due to rounding
- do not use any absolute uncertainty contributions in places where a value has to be zero for physics reasons
- never drop any "evaluated information", seek for a possibility to keep it, in accordance with format specifications, e.g., one extra energy entry for the final matrix column.

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Treatment of Discrepant Data in the ZOTT99 Generalized Least Squares Program

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Presentation at the Covariance Workshop
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ABSTRACT

The generalized linear least squares (GLLS) program ZOTT95 has been modified recently to offer the analyst the option of applying a simple, universal and objective method, called the Method of Least Distortion (MLD), to treat discrepant data, that is, data sets for which the overall chi-squared per degree of freedom substantially exceeds unity. Discrepant data be characterized as data which are subject to additional sources of uncertainty, not recognized by the person who evaluated the nominal data uncertainties. In general, the only thing that is known about these unrecognized sources of uncertainty is that they lead to an unreasonable value of chi-squared. The MLD corrects this defect in the input data by performing a controlled and minimally-invasive set of changes to the data covariances. In view of one's total lack of knowledge of how these additional uncertainties are distributed or correlated among the data points, the modification algorithm employed in MLD aims to reach a chi-squared value of unity by changing the smallest possible number of elements of the input covariance matrix. This method, like GLLS itself, is universal, objective and computationally efficient. Some attractive features of the new method are illustrated by applying the modified code version, which we call ZOTT99, to a well-known discrepant set, namely, measurements of the ^{7}Li(n,n't) cross section above 11 MeV.

INTRODUCTION

The generalized method of linear least squares (GLLS) provides a universal, objective, and computationally efficient method of producing an optimum combination of information. It easily handles data measurements of widely varying uncertainties, and having arbitrarily large correlations, provided only that uncertainties and correlations be reasonably well estimated, and that the measured quantities be connected by linear relationships. Obviously, the covariances that quantify the quality and correlations of the data can only describe the sources of uncertainty that are known to be present to the person who has evaluated the data uncertainties. A discrepant set of measured data (meaning a data set for which the chi-squared per degree of freedom exceeds unity) is usually the result of the presence of additional, unrecognized, sources of uncertainty.

Previous authors have examined a variety of approaches to the proper handling of discrepant data. One approach, the Method of Limited Relative Weights, Ref. 1-2, is commonly used in the evaluation of nuclear structure and decay data. As discussed in Ref. 3, this method has difficulty in handling sets with chi-squared values greater than 2, which frequently are encountered in evaluation work. Another approach, pursued in Ref. 3, is to try a variety existing methods and examine the performance of each one. We felt there was a need for a more systematic approach to this problem.

To meet this need, we have modified the generalized least squares analysis program ZOTT95 to offer analysts the option of applying a simple, universal and objective method to treat discrepant data sets. This new option in the ZOTT code is based on the Method of Least Distortion (MLD). This method, like almost all other methods for treating discrepant data, modifies the input covariances in order to reduce chi-squared to its expected value of unity. Since the only thing that is known about the additional, unrecognized sources of uncertainty is that they produce too high a value of chi-squared, the MLD makes the covariance changes in a way that minimizes the number of elements of the covariance matrix that need to be altered. In this sense, the amount of "distortion" of the covariance matrix is minimized. The MLD, like the GLLS itself, is universal, objective and computationally efficient. The version of the code that implements the MLD is called ZOTT99.

The implementation of the method in ZOTT99 can be easily explained with the following flow chart:

- Compute chi-0, which is chi-squared per degree of freedom for the data set of interest.
- If chi-0 is less than unity, jump to the final step (GLLS solution).
- Otherwise, examine the effect on the chi-squared of the data set of temporarily increasing, in turn, each one of the data variances by a numerical factor equal to chi-0.
- Identify as an "outlier" the datum which shows the maximum leverage in reducing chi-squared, and make the temporary increase in the variance of this one datum permanent.
- Repeat process, starting from the first step.
- Proceed as normal, with the covariances modified in this way, to find the GLLS solution to the problem at hand, as discussed, for example in Ref. 4.

^{7}Li SAMPLE PROBLEM

In order to illustrate the attractive features of this method of treating discrepant data, we have considered a well-known case from the field of fast-neutron cross-section measurements. Two measurements of the ^{7}Li(n,n't) cross section in the 1950s using the technique of nuclear emulsions resulted in values around 50 mb at a neutron energy of 14 MeV. A large number of more modern beta-counting measurements have converged to a value of around 300 mb for this same cross section. However, in 1985 M. Swinhoe and J. Uttley published two measured values, 235 mb and 242 mb, both with an uncertainty of 11 mb (Ref. 5).

Because of the long passage time, it is not practical to learn, through re-analysis of the data or personal discussions, the reasons for the discrepancy between the early nuclear emulsion measurements and the more modern measurements (although one can create plausible explanations). The situation is rather different in the case of the modern beta-counting experiments. In spite of the technological interest in the value of the 14 MeV cross section and the expenditure of a large effort to resolve the problem, there still exists no clear explanation for the remaining 5 standard-deviation discrepancy between the Swinhoe data and the other modern measurements.

In Figs. 1 and 2, we show the results of applying ZOTT99 to the analysis of the ^{7}Li data in the energy range from 11 to 16 MeV. Note that the code, without any "steering" by the analyst, has made massive increases in the uncertainties of the early nuclear-emulsion data. Relatively strong corrections were also applied to the uncertainties of Swinhoe data. Smaller changes were applied to the data of Brown and that of Osborn. The magnitude of the changes are, in every case mentioned, near the minimum necessary to span the distance between the outlying datum and the final, converged, consensus value. There were essentially no other changes made to the remaining data, all of which is completely consistent with a straight-line fit in the energy region of interest.

CONCLUSION

When the experimental situation is as unclear as it is here, many data evaluators do not have the luxury of waiting for a clear resolution. They need to have access to universal and objective methods for finishing their work in producing recommend values with realistic uncertainties. ZOTT99 offers one such method. A clear advantage of the method over several other approaches is the information contained in the sub-set of the data that was already internally consistent is preserved. That is, there is no upward scaling of the uncertainties of these internally consistent data.

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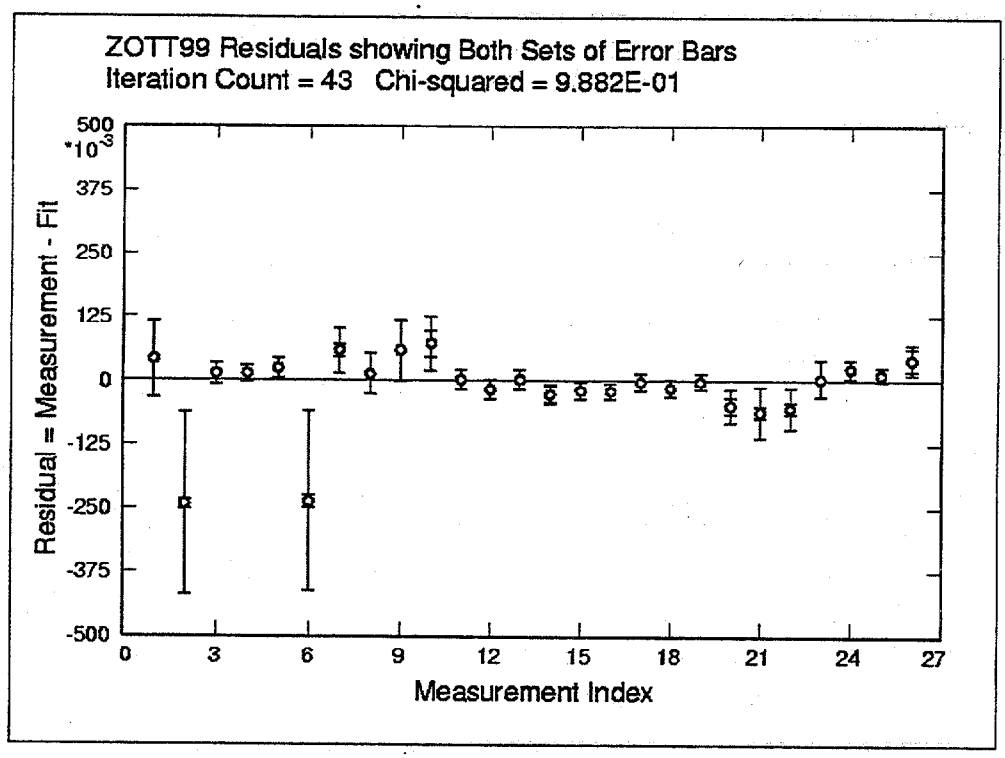

Fig. 1. Display of Original and Modified Uncertainties in the ^{7}Li Sample Problem, in Relation to the Converged Solution.

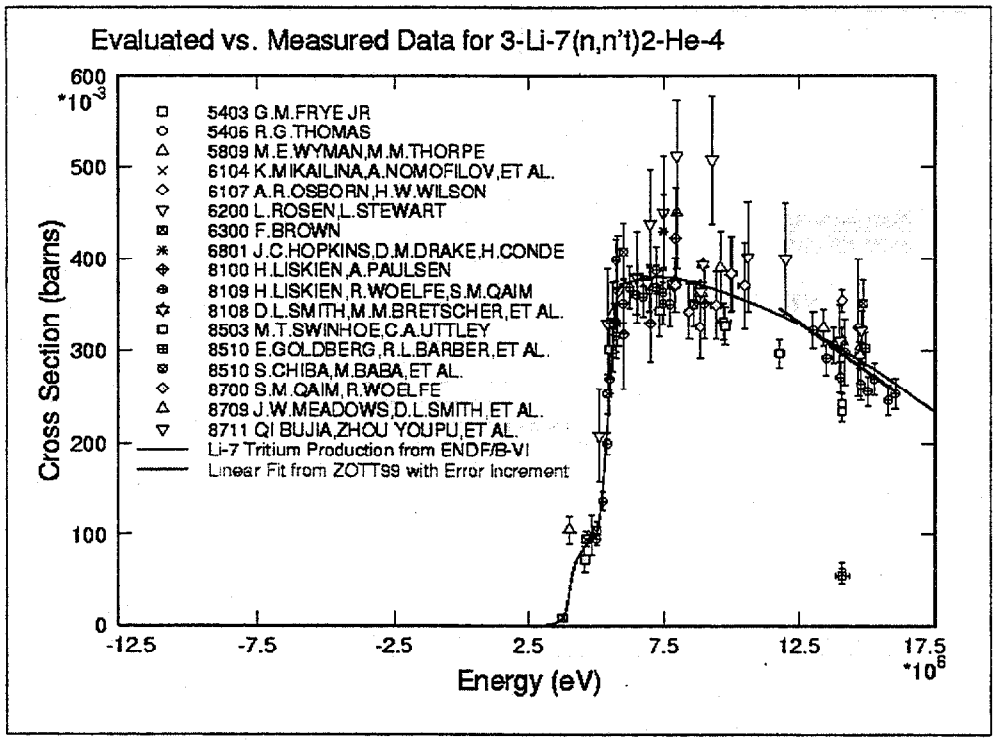

Fig. 2. ^{7}Li(n,n't) Experimental Data from EXFOR, Compared the Fit Obtained with ZOTT99, using the Method of Least Distortion (MLD) to Treat Outlying Data.

AN EFFICIENT WAY OF THE REPRESENTATION OF COVARIANCE DATA IN ENDF-6 FORMAT FOR FAST NEUTRON REACTION CROSS SECTIONS

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Abstract

An efficient way of the representation of covariance data in ENDF-6 format for fast neutron reaction cross sections is described. It is based on formal approximation of fast neutron reaction cross sections by Adler-Adler resonance formula and the representation of estimated parameters and their covariances in formats of File 2 and File 32. This approach provides drastic reduction of information volume to be stored in evaluated data files and allows to exploit existing nuclear data processing codes for getting derivative values (for example, group cross sections and their covariances for arbitrary energy grid). Due to format restrictions the method is applicable for the representation of the data for total, fission and radiative capture cross sections only. The method was successfully applied for evaluation of a few neutron fission reaction cross sections. A simplification of the calculational scheme of the generalized least squares method is also proposed. It enables to operate with large scale covariance matrices of the uncertainties of measurements.

1. INTRODUCTION

The significance of covariance evaluated data for applications was emphasized in many works (from early studies [1,2] to recent ones [3]) but this branch of nuclear data evaluation still is in an embryonic state. Actually, the existence of the covariance files in modern evaluated data libraries is rather an exception than a rule. For example, for most important fuel isotopes ^{235}U and ^{239}Pu covariance files in ENDF/B-6 library (Revisions Oct97 and Aug97) exist only for ^{235}U fission neutron yields and are absent for cross sections. But even if the covariance files would be prepared they couldn't be processed adequately due to restricted capabilities of computer codes and imperfection of the algorithms applied. In particular, none of known computer codes (NJOY [4],FIZCON [5], CHECKER [5]) processes File 30 format [6].

At present there are a few of fundamental difficulties hindering the evaluation of the covariance data and their transformation by nuclear data processing codes. One of the problems is a necessity of manipulations with large scale covariation and correlation matrices of the experimental and evaluated data. In modern studies typical value of processed data points is $10^3 - 10^5$. It requires storing 5×10^5 - 5×10^9, generally speaking, non-trivial covariations. As a consequence manipulations with the large scale matrices present a complicated problem due to computer memory restrictions and features of algorithms. It is this problem that will be addressed in present paper aimed at a simplification of 1) calculational scheme of the statistical analysis of the experimental data and 2) representation of covariance data in ENDF-6 format.

2. EQUATIONS OF THE CALCULATIONAL SCHEME

All the considerations outlined below are carried out within generalized least squares method. The object of this chapter is to get simpler structures (compared to the large-scale covariance matrices of the experimental data) in the equations of the generalized least squares method.

We start with the description of the model. The cross section measurements σ_i are assumed to be values of hypothetical "true" function distorted by additive unbiased random deviations ε_i. The minimized functional has form

$$S(\theta) = \sum_{k=1}^{M}\sum_{l=1}^{M}\sum_{i=1}^{n_k}\sum_{j=1}^{n_l} \frac{\sigma_i^k - f(E_i^k,\theta)}{e_i^k} \cdot (P^{-1})_{ij}^{kl} \cdot \frac{\sigma_j^l - f(E_j^l,\theta)}{e_j^l} \qquad (1)$$

Here • – the number of experiments, n_k – the number of cross section measurements in the k-th experiment, $n=\sum n_k$ – overall number of measurements in the experimental data base, $\boldsymbol{\sigma} = (\sigma_1^1,\ldots, \sigma_{n_1}{}^1,\ldots,\sigma_1^M,\ldots,\sigma_{n_M}{}^M)^T$ - vector of the cross sections from experimental data base, superscript • denotes a transposition, $\boldsymbol{\theta}=(\theta_1,\ldots,\theta_L)^T$ – vector of unknown parameters to be estimated, $f(E)$ – Adler-Adler resonance formula [6]:

$$f(E) = \frac{\pi}{\sqrt{E}} \sum_{r=1}^{K} \frac{\nu_r G_r + (\mu_r - E) H_r}{(\mu_r - E)^2 + \nu_r^2} \qquad (2)$$

The parameters $\{\mu_r, \nu_r, G_r, H_r\}$ form vector $\boldsymbol{\theta}$. Covariation matrix $\mathbf{V}$ of random deviations is known within factor Δ: $V_{ij}^{kl} = \Delta\, p_{ij}^{kl}\, e_i^k\, e_j^l$, e_i^k - the uncertainty of measurement $\sigma_{i_k}^k$, $\mathbf{P}=(p_{ij}^{kl})$ – correlation matrix of the random deviations, superscripts indicate number of experiment. The correlations p_{ij}^{kl} were calculated as indicated in work [7]. The matrix $\mathbf{P}$ can be presented in a block manner $\mathbf{P} = (\mathbf{P}_{kl})$, $k,l = 1,\ldots,M$. Block $\mathbf{P}_{kl}$ was approximated by a matrix with identical element

$$\overline{p_{kl}} = \left(\sum_{i=1}^{n_k}\sum_{j=1}^{n_l} p_{ij}^{kl}\right) / (n_k \cdot n_l) \qquad (3)$$

For $l=k$ the averaging is carried out over off-diagonal elements.

In routine evaluation work the symmetrical matrix $\mathbf{P}$ consists of hundreds and thousands of rows. As a consequence some operations (inversion, calculation of determinant and eigenvalues) are complicated or even impossible due to restricted computer memory and features of the matrices (often they are ill-conditioned). So a search of equivalent simpler structures would be useful.

Yacobi variables widely used in theoretical physics have unique properties. Let's make use of these properties for transformation of the quadratical form (1). Define new variables as

$$q_m^k = \sqrt{\frac{m}{m+1}}\left(\frac{1}{m}\sum_{i=1}^{m} z_i^k - z_{m+1}^k\right) \text{ for } m \le n_k - 1, \quad q_{n_k}^k = \frac{1}{\sqrt{n_k}}\sum_{i=1}^{n_k} z_i^k = \sqrt{n_k}\,\bar{z}^k \qquad (4)$$

$$\text{where } z_i^k = \cdot\frac{\sigma_i^k - f(E_i^k,\theta)}{e_i^k}$$

Correlations between new variables equal to

$$\mathrm{cov}(q_i^k, q_j^l) = (1-\overline{p_{kk}})\,\delta_{ij}\delta_{kl} + \overline{p_{kl}}\sqrt{n_k}\sqrt{n_l}\,\delta_{in_k}\delta_{jn_l} \tag{5}$$

• orrespondingly the statistical functional is

$$S = \sum_{k=1}^{M}\sum_{i=1}^{n_k-1}\frac{(q_i^k)^2}{1-p_{kk}} + \sum_{k=1}^{M}\sum_{l=1}^{M} q_{n_k}^k q_{n_l}^l (T^{-1})_{kl} / \sqrt{n_k n_l} \tag{6}$$

Here $T_{kl} = \overline{p_{kl}} + (1-\overline{p_{kk}})\delta_{kl}/n_k$. The transformation (4) of the variables is orthogonal. Keeping in mind a property of orthonogal transformation (preservation of vector's length)

$$\sum_{i=1}^{n_k}(q_i^k)^2 = \sum_{i=1}^{n_k}(z_i^k)^2 \tag{7}$$

we get final expression for the statistical functional

$$S = \sum_{k=1}^{M}\sum_{i=1}^{n_k}\frac{(z_i^k)^2}{1-p_{kk}} - \sum_{k=1}^{M}\frac{n_k(\bar{z}_k)^2}{1-p_{kk}} + \bar{\bar{z}}\cdot T^{-1}\cdot\bar{\bar{z}} \tag{8}$$

The transformations described above permits to carry out a statistical analysis for practically unrestricted number of measurements since quadratic form (1) ("two-dimensional" expression) was converted into "one-dimensional" expression (8) very similar to a sum of squares. Instead of inversion $n\times n$ matrix **P** one must operate with $M\times M$ matrix T. We omit formula for the calculation of the covariation matrix of the uncertainties of the "resonance" parameters as it has conventional form.

3. REPRESENTATION OF THE COVARIANCE DATA IN ENDF-6 FORMAT

The main difficulties in processing of the covariance data result from their cumbersome and inadequate form of representation in ENDF-6 format [6]. For example, the structure itself of LB=5 sub-subsection format in File 33 [6] is a source of numerous erroneous covariance matrices got after transformation from original File 33 energy grid to finer one. An inclusion of artificial LB=8 sub-subsection does not solve this problem. The development of File 30 [6] format was a step in right direction. This format provided a natural, flexible and universal form of representation of the covariance data. However the use of File 30 format results in difficulties of other type. The covariances files prepared in File 30 format are extremely cumbersome. Besides at present there are no codes processing File 30 format.

Meanwhile ENDF-6 format has **non-evident** opportunities for effective and adequate representation of the evaluated total, fission and radiative capture cross sections and their covariances in the range from thermal to high neutron energies. Resonance formulae (single- and multi-level Breit-Wigner, Adler-Adler [6]) are well known and applied for parametrization of neutron cross sections in resolved resonance region. In this energy region the parameters of resonance formulae have direct physical meanings. Formally (without physical interpretation of the parameters) all the resonance formulae can be used for fitting of the cross sections above resolved resonance region also. However only one of them - Adler-Adler formula – is especially convenient for fitting cross sections at intermediate and high energies. Other formulae (single- and multi-level Breit-Wigner) contain parameters (neutron widths) dependent on energy. Additional positive factor is the structure of ENDF-6 format. It has various opportunities for the representation of the resonance parameters and their covariances. In particular, the MT=151 section of Files 2 and 32 was reserved for storing appropriate information.

The fitting of the cross sections above resolved resonance region by Adler-Adler formula and representation of the "resonance" parameters and their covariances in ENDF-6 format has obvious advantages: 1) natural form of representation of the covariance data, it facilitates generation group cross sections for any energy grid and permits to avoid ambiguities inherent to representation of covariances in LB=5 and LB=8 sub-subsections of File 33; 2) drastic reduction of the information to be stored in the evaluated data files; 3) wide opportunities for transformation into other types of nuclear data with existing processing systems (NJOY [4], GRUCON [8]). Note also following important point. Original Adler-Adler formalism implies the use of the same resonance widths and energies in expressions for partial and total cross sections while ENDF-6 format admits applying different resonance widths and energies. Present carryover makes the procedure of the cross section parametrization more flexible.

At the same time there is an important restriction for the method described. According to ENDF-6 format and features of Adler-Adler formalism the respective formulae may be used for parametrization of total, fission and radiative capture cross sections only.

4. AN EXAMPLE

As an illustrative example we chose the evaluation of the ^{241}Am neutron fission cross section in the energy range 100 keV – 20 MeV. The fission cross sections of minor actinides are of special importance for the development of nuclear waste transmutation strategies.

The evaluation procedure included 3 stages. At the first stage an experimental data base was compiled after search of information in the EXFOR library and recent publications. The data base contains the results of 13 experiments. All the experiments of interest can be separated into 2 groups: 1) comprehensive relative measurements (*Nobles 55* [9], *Kuprijanov 78* [10], *Knitter 79* [11], *Hage 81* [12], *Behrens 81* [13], *Dabbs 83* [14], *Vorotnikov 86* [15]) covering wide range of neutron energy, 2) single measurements near 14.5 MeV (*Protopopov 60* [16], *Kazarinova 60* [17], *Fomushkin 67* [18], *Cance 81* [19], *Iyer 79* [20], *Khan 80* [21]).

At the second step all the experiments were critically reviewed. A few of them were rejected due to large difference (more than 3σ) from the main bulk of the experimental data (*Nobles 55*, *Kazarinova 60*, *Khan 80*) or too large uncertainties of the measurements (*Iyer* 79, Vorotnikov *86*). All the results of measurements were renormalized to new values of reference cross sections and decay constants. In addition special correction was applied to the data of *Behrens 81* [13]. As noted in [22] the results of fission cross section measurements carried out by Behrens et al. with the threshold cross section method are systematically shifted relative to other measurements. Besides for the isotopes ^{237}Np and ^{243}Am there is a considerable disagreement [22] between differential cross sections as given by Behrens et al. averaged over ^{252}Cf fission neutron spectrum and results of integral measurements. A probable source of inconsistency is an error in determination of ratio of the number of nuclei in the samples. For this reason the experimental data *Behrens 81* [13] were corrected according to procedure described in work [22].

At the third stage a statistical analysis of the measurements from adopted experimental data base was carried out in correspondence with the scheme outlined in Section 2. The results of the evaluation are given in Figures 1,2 and Tables 1,2. In Figures 1 and 2 our evaluated curve is shown compared to the experimental data and ENDF/B-6 evaluation. On the whole both evaluations agree with each other and the experimental data. Above 8 MeV our evaluation is systematically lower than ENDF/B-6 one. This discrepancy is explained by the difference in methods applied for getting evaluations (the ENDF/B-6 evaluation is a result of theoretical calculations). The evaluated ^{241}Am fission cross section is presented by Adler-Adler resonance formula (2) in the energy range from 100 keV to 20 MeV. The expression includes 4 "resonances". The parameters are given in Table 1. The "resonance" parameters and covariances of their uncertainties were also formatted within MT=151 section of File 2 and File 32. The correlations of uncertainties of the parameters are given in

Table 2. Unlike results of the resonance analysis (where strong correlations between parameters ν_r and G_r, H_r and μ_r are observable) in this case we don't see any considerable correlations. As seen from Table 2 the correlations of the uncertainties don't show any trend. This result agree with statement emphasized above: the parameters of the Adler-Adler resonance formula applied for fitting cross sections above resolved resonance region haven't any physical meanings.

5. CONCLUSIONS

1. The opportunity of a) the application of Adler-Adler resonance formula for fitting of fast neutron reaction cross section and b) the representation of the "resonance" parameters and their covariances in ENDF-6 format (MT=151 section of Files 2 and 32) has been demonstrated. At least for three cross sections (total, fission and radiative capture) the Adler-Adler resonance formula gives an instrument for universal parametrization of the cross sections from thermal to high neutron energies. The representation of the "resonance" parameters and their covariances in ENDF-6 format provides a drastic reduction of information volume to be stored in evaluated data files (compared to the conventional way of storage in Files 3 and 33). The reduction will be even more impressive after removal of shortcomings inherent to format of File 32 (for Adler-Adler formalism).

2. Within the generalized least squares method a simplification of the calculational scheme is proposed. In particular the transformation of minimized functional enables to carry out the statistical analysis of practically unrestricted number of measurements.

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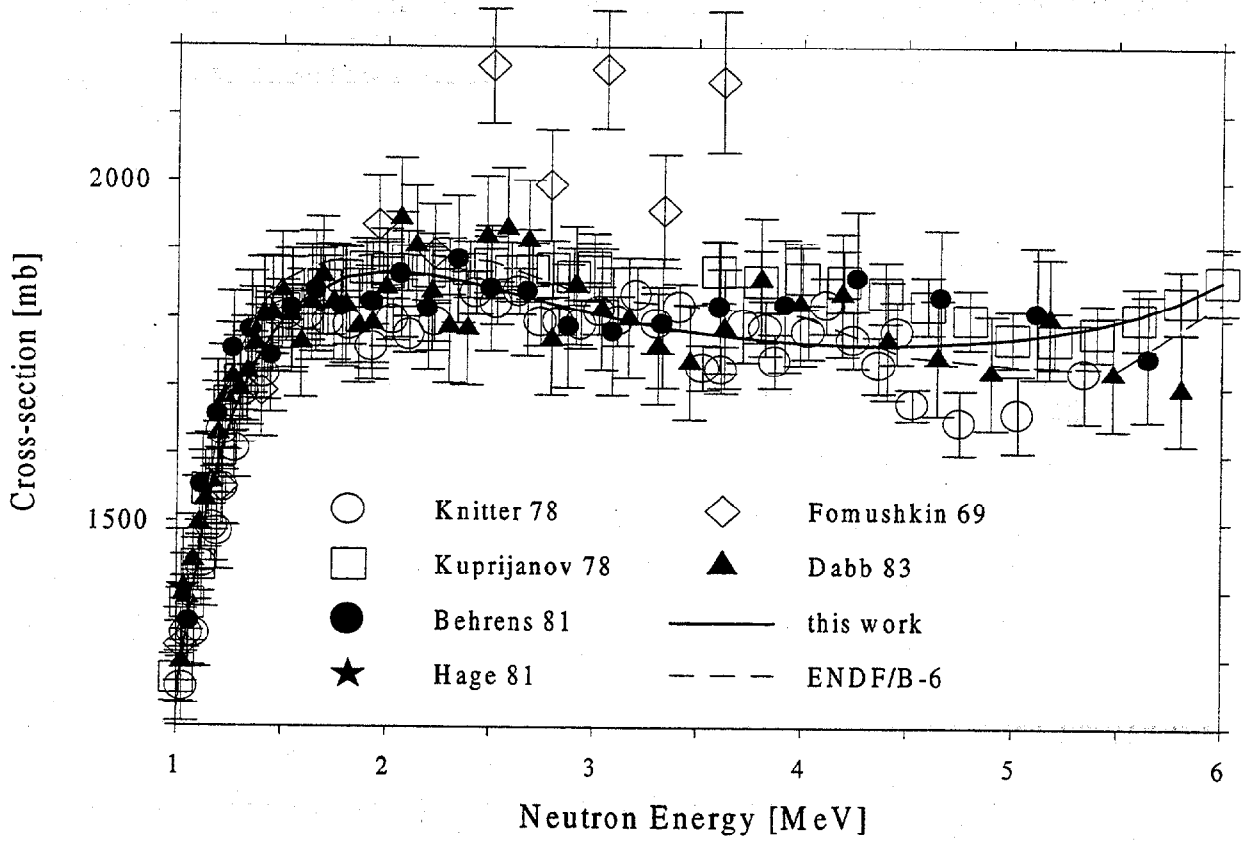

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Fig.1. The evaluated ^{241}Am(n,f) reaction cross section compared to the experimental data and the ENDF/B-6 evaluation in the energy range 1 – 6 MeV.

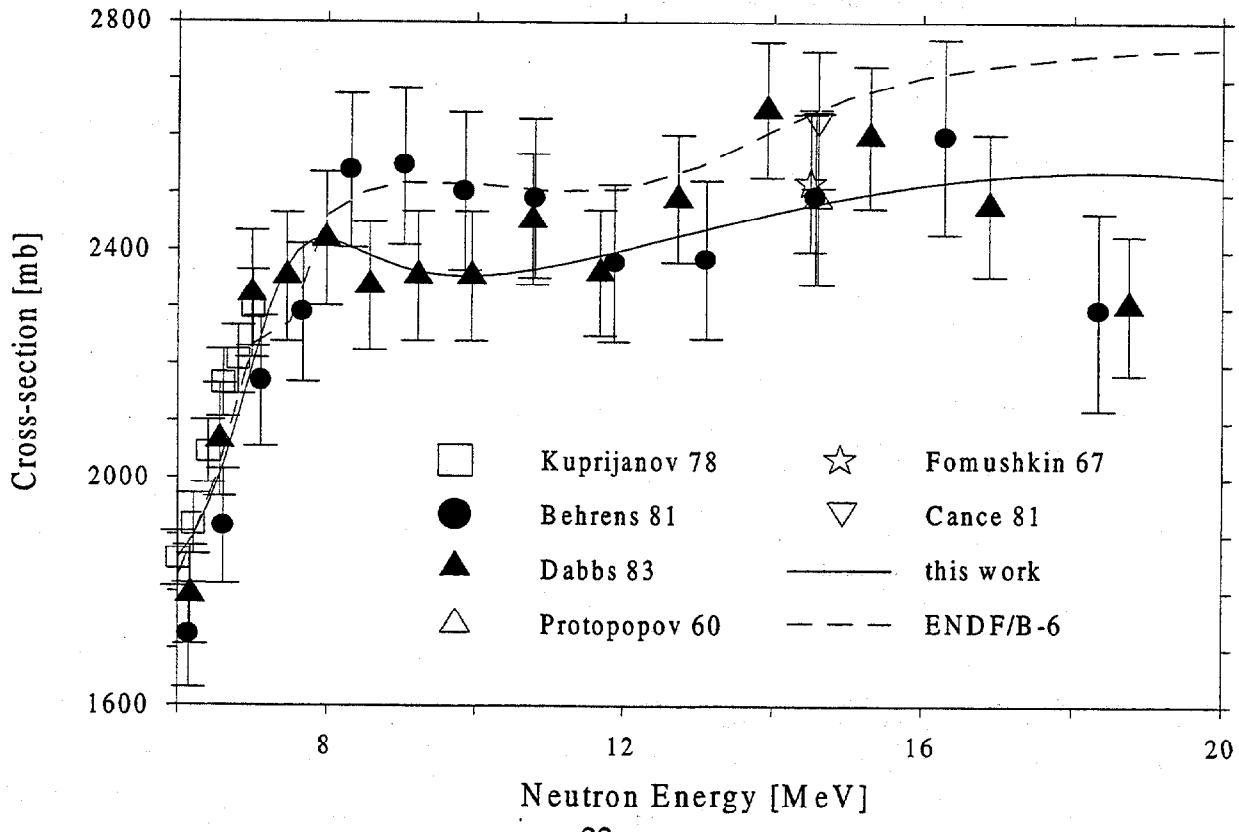

Fig.2. The evaluated ^{241}Am(n,f) reaction cross section compared to the experimental data and the ENDF/B-6 evaluation in the energy range 6 – 20 MeV.

Table 1. The parameters of the Adler-Adler formula (2) for representation of the evaluated ^{241}Am(n,f) reaction cross section in the energy range 100 keV – 20 MeV.

r	μ_r	ν_r	G_r	H_r
1	1.33711E+7	2.49968E+7	6.83180E+10	-9.94233E+10
2	8.20920E+5	1.21767E+6	-2.35967E+ 8	-4.88687E+ 8
3	7.14540E+6	1.14693E+6	2.40444E+ 8	-4.22780E+ 8
4	8.00862E+5	3.54737E+5	-5.16893+ 7	-7.13229E+ 7

Table 2. Correlation matrix of the "resonance" parameters of the Adler-Adler formula (2) for the representation of the evaluated ^{241}Am(n,f) reaction cross section.

	μ_1	ν_1	G_1	H_1	μ_2	ν_2	G_2	H_2	μ_3	ν_3	G_3	H_3	μ_4	ν_4	G_4	H_4
μ_1	1															
ν_1	-0.57	1														
G_1	-0.27	0.94	1													
H_1	0.61	0.99	-0.93	1												
μ_2	-0.33	0.01	-0.11	-0.05	1											
ν_2	0.86	-0.74	-0.53	0.77	-0.36	1										
G_2	-0.71	0.36	0.15	-0.41	0.81	-0.80	1									
H_2	-0.86	0.85	0.66	-0.88	0.13	-0.94	0.62	1								
μ_3	0.70	-0.44	-0.25	0.47	0.01	0.54	-0.29	-0.63	1							
ν_3	-0.16	0.52	0.54	-0.49	-0.24	-0.11	-0.18	0.25	-0.23	1						
G_3	0.79	-0.39	-0.16	0.43	-0.08	0.62	-0.41	-0.67	0.95	-0.12	1					
H_3	0.32	-0.69	-0.67	0.66	0.25	0.26	0.10	-0.43	0.31	-0.91	0.21	1				
μ_4	0.16	-0.25	-0.23	0.25	0.59	0.32	0.14	-0.34	0.21	-0.12	0.21	0.18	1			
ν_4	0.64	-0.44	-0.27	0.48	-0.72	0.78	-0.83	-0.59	0.30	0.02	0.38	0.06	-0.07	1		
G_4	-0.44	0.21	0.08	-0.25	0.94	-0.47	0.79	0.29	-0.12	-0.10	-0.19	0.07	0.56	-0.85	1	
H_4	-0.67	0.57	0.41	-0.60	0.14	-0.88	0.59	0.76	-0.42	0.07	-0.49	-0.20	-0.64	-0.70	0.25	1

An MF30 Covariance File for n+H

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April 20, 1999

The MF30 Format is Ideal

The File-30 format is ideal for representing the covariances of n+H because...

- The EDA R-matrix code used to do the evaluation automatically produces a full covariance matrix for the parameters of the model,
- The code also provides sensitivities derived analytically from the model,
- The methods behind MF=30 provide a complete, accurate, and smooth representation of the covariances.

A Preliminary File

A simplified preliminary MF30 for n+H was prepared using sensitivities from 0.5 to 20 MeV. Only elastic scattering was represented, for now (the capture channel will be added soon).

The model uses 33 parameters.

Samples pages from the file follow.

```
1.001000+3 9.991700-1          0          0          0         33 12530  1  546
0.000000+0 0.000000+0          0          0        231          0 12530  1  547
0.000000+0 0.000000+0          1          3          2         16 12530  1  548
0.000000+0 0.000000+0          1          3          0          0 12530  1  549
0.000000+0 0.000000+0          1          0          0          0 12530  1  550
0.000000+0 0.000000+0          1          4          2        603 12530  1  551
0.000000+0 0.000000+0          1          4          0          0 12530  1  552
0.000000+0 0.000000+0          1          0          0          0 12530  1  553
0.000000+0 0.000000+0          0          0          0          0 12530  1  554
0.000000+0 0.000000+0          2          3          2         16 12530  1  555
0.000000+0 0.000000+0          2          3          0          0 12530  1  556
0.000000+0 0.000000+0          2          0          0          0 12530  1  557
0.000000+0 0.000000+0          2          4          2        603 12530  1  558
0.000000+0 0.000000+0          2          4          0          0 12530  1  559
0.000000+0 0.000000+0          2          0          0          0 12530  1  560
0.000000+0 0.000000+0          0          0          0          0 12530  1  561
0.000000+0 0.000000+0          3          3          2         16 12530  1  562
0.000000+0 0.000000+0          3          3          0          0 12530  1  563
0.000000+0 0.000000+0          3          0          0          0 12530  1  564
0.000000+0 0.000000+0          3          4          2        603 12530  1  565
0.000000+0 0.000000+0          3          4          0          0 12530  1  566
0.000000+0 0.000000+0          3          0          0          0 12530  1  567
0.000000+0 0.000000+0          0          0          0          0 12530  1  568
0.000000+0 0.000000+0          4          3          2         16 12530  1  569
0.000000+0 0.000000+0          4          3          0          0 12530  1  570
0.000000+0 0.000000+0          4          0          0          0 12530  1  571
0.000000+0 0.000000+0          4          4          2        603 12530  1  572
0.000000+0 0.000000+0          4          4          0          0 12530  1  573
0.000000+0 0.000000+0          4          0          0          0 12530  1  574
0.000000+0 0.000000+0          0          0          0          0 12530  1  575
0.000000+0 0.000000+0          5          3          2         16 12530  1  576
0.000000+0 0.000000+0          5          3          0          0 12530  1  577
0.000000+0 0.000000+0          5          0          0          0 12530  1  578
0.000000+0 0.000000+0          5          4          2        603 12530  1  579
0.000000+0 0.000000+0          5          4          0          0 12530  1  580
0.000000+0 0.000000+0          5          0          0          0 12530  1  581
0.000000+0 0.000000+0          0          0          0          0 12530  1  582
0.000000+0 0.000000+0          6          3          2         16 12530  1  583
0.000000+0 0.000000+0          6          3          0          0 12530  1  584
0.000000+0 0.000000+0          6          0          0          0 12530  1  585
0.000000+0 0.000000+0          6          4          2        603 12530  1  586
0.000000+0 0.000000+0          6          4          0          0 12530  1  587
0.000000+0 0.000000+0          6          0          0          0 12530  1  588
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0.000000+0 0.000000+0          7          0          0          0 12530  1  592
0.000000+0 0.000000+0          7          4          2        603 12530  1  593
0.000000+0 0.000000+0          7          4          0          0 12530  1  594
0.000000+0 0.000000+0          7          0          0          0 12530  1  595
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0.000000+0 0.000000+0          8          3          2         16 12530  1  597
0.000000+0 0.000000+0          8          3          0          0 12530  1  598
0.000000+0 0.000000+0          8          0          0          0 12530  1  599
0.000000+0 0.000000+0          8          4          2        603 12530  1  600
0.000000+0 0.000000+0          8          4          0          0 12530  1  601
0.000000+0 0.000000+0          8          0          0          0 12530  1  602
0.000000+0 0.000000+0          0          0          0          0 12530  1  603
0.000000+0 0.000000+0          9          3          2         16 12530  1  604
0.000000+0 0.000000+0          9          3          0          0 12530  1  605
0.000000+0 0.000000+0          9          0          0          0 12530  1  606
```

```
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 6.877722-3-2.513644-3-2.173085-3 3.610428-3-8.586360-4 3.255207-1 12530  2  783
-1.394611-6 6.974998-6-2.443943-3 3.091290-2 1.525519-2-3.862686-3 12530  2  784
-1.265266-4 2.016644-2-7.515924-4 1.198275-2-3.008286-3-1.122992-2 12530  2  785
-9.944371-3-6.918301-3-3.226807-4 5.841490-5 1.130121-3-1.869307-3 12530  2  786
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 1.605847-2-5.411435-1-4.648274-2 4.120505-2 1.492850-2 9.179682-3 12530  2  789
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 6.449992-6-3.305760-3 4.585924-2 2.271101-2-1.433530-3-1.173890-4 12530  2  791
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 3.111111-2 2.254177-2 9.902579-3 1.201057-2-2.955431-1 1.713121-5 12530  2  827
 9.612766-6 8.837220-3-2.441076-2-1.109886-2-2.842374-2-1.607902-6 12530  2  828
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-3.385225-3 6.697164-6                                             12530  2  831
 4.40348276 0.000000+0          0          0         25          9 12530  2  832
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-9.093751-3-6.197698-3 1.170334-2-8.958046-3 2.260818-5-2.342672-3 12530  2  836
 5.128593-6                                                        12530  2  837
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```

```
 1.001000+3 9.991700-1          0          0          0          2 12530 11  923
 0.000000+0 0.000000+0          0          0          1         40 12530 11  924
         40          2                                              12530 11  925
 5.000000+5-6.218500-5 1.000000+6-2.570412-4 1.500000+6-5.956546-4 12530 11  926
 2.000000+6-1.087368-3 2.500000+6-1.739871-3 3.000000+6-2.559286-3 12530 11  927
 3.500000+6-3.550246-3 4.000000+6-4.715970-3 4.500000+6-6.058334-3 12530 11  928
 5.000000+6-7.577943-3 5.500000+6-9.274194-3 6.000000+6-1.114534-2 12530 11  929
 6.500000+6-1.318857-2 7.000000+6-1.540005-2 7.500000+6-1.777498-2 12530 11  930
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 1.100000+7-3.840390-2 1.150000+7-4.182090-2 1.200000+7-4.532586-2 12530 11  933
 1.250000+7-4.890794-2 1.300000+7-5.255603-2 1.350000+7-5.625880-2 12530 11  934
 1.400000+7-6.000482-2 1.450000+7-6.378252-2 1.500000+7-6.758033-2 12530 11  935
 1.550000+7-7.138671-2 1.600000+7-7.519019-2 1.650000+7-7.897941-2 12530 11  936
 1.700000+7-8.274321-2 1.750000+7-8.647065-2 1.800000+7-9.015106-2 12530 11  937
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 2.000000+7-1.042003-1                                             12530 11  939
 0.000000+0 0.000000+0          0          0          0          0 12530 11  940
 0.000000+0 0.000000+0          0          0          0          0 12530 11  941
 0.000000+0 0.000000+0          0          0          1         40 12530 11  942
         40          2                                              12530 11  943
 0.000000+0 5.000000+5          0          0          1          0 12530 11  944
 1.674596-3                                                        12530 11  945
 0.000000+0 1.000000+6          0          0          2          0 12530 11  946
 4.184292-3 8.518170-7                                             12530 11  947
 0.000000+0 1.500000+6          0          0          3          0 12530 11  948
 6.818545-3 1.907614-6 1.430366-6                                  12530 11  949
 0.000000+0 2.000000+6          0          0          3          0 12530 11  950
 9.374113-3 3.073103-6 3.824803-6                                  12530 11  951
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 1.398200-2 4.237779-6 1.514582-5                                  12530 11  955
 0.000000+0 3.500000+6          0          0          3          0 12530 11  956
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 1.777047-2 1.009243-6 3.973542-5                                  12530 11  959
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 1.933464-2-3.364319-6 5.870817-5                                  12530 11  961
 0.000000+0 5.000000+6          0          0          3          0 12530 11  962
 2.068932-2-1.016389-5 8.302645-5                                  12530 11  963
 0.000000+0 5.500000+6          0          0          3          0 12530 11  964
 2.182103-2-1.977619-5 1.132269-4                                  12530 11  965
 0.000000+0 6.000000+6          0          0          3          0 12530 11  966
 2.273590-2-3.257670-5 1.498196-4                                  12530 11  967
 0.000000+0 6.500000+6          0          0          4          0 12530 11  968
 2.343548-2-4.888559-5 1.932232-4 1.679708-6                       12530 11  969
 0.000000+0 7.000000+6          0          0          4          0 12530 11  970
 2.392303-2-6.897818-5 2.437437-4 2.338978-6                       12530 11  971
 0.000000+0 7.500000+6          0          0          4          0 12530 11  972
 2.420051-2-9.306900-5 3.015699-4 3.183337-6                       12530 11  973
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 2.161396-2-3.260143-4 7.943828-4 1.421102-5                       12530 11  985
 0.000000+0 1.100000+7          0          0          4          0 12530 11  986
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 0.000000+0 1.150000+7          0          0          4          0 12530 11  988
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 1.605264-2-5.573232-4 1.215117-3 3.064068-5                          12530 11  993
 0.000000+0 1.300000+7          0          0          4          0 12530 11  994
 1.420929-2-6.219406-4 1.320910-3 3.637794-5                          12530 11  995
 0.000000+0 1.350000+7          0          0          4          0 12530 11  996
 1.219006-2-6.883261-4 1.423365-3 4.290106-5                          12530 11  997
 0.000000+0 1.400000+7          0          0          4          0 12530 11  998
 9.998093-3-7.559623-4 1.520398-3 5.025687-5                          12530 11  999
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 7.635816-3-8.242270-4 1.609661-3 5.851838-5                          12530 11 1001
 0.000000+0 1.500000+7          0          0          4          0 12530 11 1002
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 0.000000+0 1.800000+7          0          0          4          0 12530 11 1014
-1.346583-2-1.261560-3 1.780708-3 1.474064-4                          12530 11 1015
 0.000000+0 1.850000+7          0          0          4          0 12530 11 1016
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 0.000000+0 1.950000+7          0          0          4          0 12530 11 1020
-2.482853-2-1.382070-3 1.424731-3 2.057754-4                          12530 11 1021
 0.000000+0 2.000000+7          0          0          4          0 12530 11 1022
-2.893746-2-1.408696-3 1.221372-3 2.285720-4                          12530 11 1023
                                                                      12530  0 1024
 1.001000+3 9.991700-1          0          0          0          2 12530 12 1025
 0.000000+0 0.000000+0          0          0          1         40 12530 12 1026
         40          2                                               12530 12 1027
 5.000000+5 6.043826-5 1.000000+6 2.484135-4 1.500000+6 5.723896-4 12530 12 1028
 2.000000+6 1.038908-3 2.500000+6 1.652725-3 3.000000+6 2.416932-3 12530 12 1029
 3.500000+6 3.333079-3 4.000000+6 4.401282-3 4.500000+6 5.620333-3 12530 12 1030
 5.000000+6 6.987795-3 5.500000+6 8.500106-3 6.000000+6 1.015267-2 12530 12 1031
 6.500000+6 1.193993-2 7.000000+6 1.385550-2 7.500000+6 1.589220-2 12530 12 1032
 8.000000+6 1.804216-2 8.500000+6 2.029690-2 9.000000+6 2.264743-2 12530 12 1033
 9.500000+6 2.508427-2 1.000000+7 2.759759-2 1.050000+7 3.017723-2 12530 12 1034
 1.100000+7 3.281280-2 1.150000+7 3.549375-2 1.200000+7 3.820941-2 12530 12 1035
 1.250000+7 4.094908-2 1.300000+7 4.370207-2 1.350000+7 4.645779-2 12530 12 1036
 1.400000+7 4.920575-2 1.450000+7 5.193568-2 1.500000+7 5.463753-2 12530 12 1037
 1.550000+7 5.730152-2 1.600000+7 5.991821-2 1.650000+7 6.247852-2 12530 12 1038
 1.700000+7 6.497376-2 1.750000+7 6.739568-2 1.800000+7 6.973646-2 12530 12 1039
 1.850000+7 7.198880-2 1.900000+7 7.414588-2 1.950000+7 7.620140-2 12530 12 1040
 2.000000+7 7.814958-2                                               12530 12 1041
 0.000000+0 0.000000+0          0          0          0          0 12530 12 1042
 0.000000+0 0.000000+0          0          0          0          0 12530 12 1043
```

Summary of the Technical Discussion in the Session on Representation and Processing of Covariance Matrices

The discussion pointed out the difficulty in obtaining a consensus between various groups of users of the uncertainty files. The community of the users of the large data processing and neutron transport codes was relatively satisfied with the existing formats, whereas most of the experimentalists were disappointed with the complexity of the formats which hampers the easy reading of the uncertainties of the data.

In the course of the discussion, Bob MacFarlane gave a short overview on the work planned with the MF30 format. This new format circumvents some of the insufficiencies of the other formats and includes the capability of representing the results of R-matrix calculations.

Two independent contributions made proposals for a simplification of the formats. The contribution of Fritz Froehner, in form of a written communication, proposed a modification of the formats to allow a direct listing of (relative) standard deviations and correlation coefficients. He argued that these quantities best approach the need of users.

The second proposal, presented by Wolf Mannhart, was of a similar tendency. However, instead of introducing new formats the proposal remains within the existing formats and requires only some additional structural rules. Mannhart demonstrated in an example the complexity of the combination process of the individual sub-subsections of File 33 representing various relative and absolute components of the final covariance matrix. He proposed to simplify all that by directly quoting the final matrix in form of a single LB=5 sub-subsection representing the relative covariance matrix. The diagonal terms of such a matrix can easily be read from the file as relative variances or standard deviations (after forming the square root). The proposed procedure is sufficient as long as the matrix will not be expanded to an energy grid finer than that given in the LB=5 sub-subsection. With an additional LB=8 sub-subsection this limitation becomes obsolete. The values of the diagonal elements of the LB=8 matrix should not exceed the order of 1% of the variances of the LB=5 sub-subsection. This condition allows a neglect of the LB=8 part when using the original energy grid of the evaluation. The given proposal of representing a final covariance matrix ignores missing components of the matrix as the resonance region represented in File 32. With the introduction of an empty energy group in the LB=5 matrix this deficiency can be circumvented. Vice versa such a empty group can be used as an indicator of a partial incompleteness of the matrix. Cross-correlations between different cross sections can easily be described with the LB=6 format which substitutes the LB=5 format in such cases and allows to avoid the cumbersome procedure of handling NC subsections in the files.

A last point of discussion were obvious inconsistencies in the evaluated covariance matrices in violating fundamental mathematical rules as the positive semi-definitness of such matrices. To avoid that in future evaluations a more careful checking of the final covariance matrix by the evaluator is mandatory. This requirement indirectly supports Mannhart's proposal to quote final matrices instead of a sum of components.

From: IAEAND::MUIR "D. W. MUIR, IAEA NUCLEAR DATA" 20-NOV-1998 17:0
To: @COVAR
CC: MUIR
Subj: Covariance Processing News

Covariance Processing News, 20 November 1998

I would like to inform you of the implementation of a number of changes to NJOY97 over the past few months. These changes improve the usefulness of the code in processing data covariances with the ERRORR module and plotting the covariances in the COVR module, and they restore the previous (NJOY94) capability to produce a compressed ASCII covariance library in BOXR format in the COVR module.

Bob MacFarlane has made many improvements in the COVR module, in order to convert the graphics output to pure PostScript and to add a color option to the covariance plots (green for positive correlation, red for negative). For very detailed covariance plots, the color graphics are far superior to the older black-and-white shading option. My contribution of recent months was to track down some small problems in the implementation of the color option, and to add some minor new features, such as additional reaction names in the plot labels and some refinements of the color and black-and-white shading logic.

The revisions and improvements to the ERRORR and COVR modules are now complete, and they are included in the standard version of NJOY, which was recently upgraded to version NJOY97.45. See http://t2.lanl.gov/ for details of this new version.

In addition to the substantial improvements in ERRORR and COVR in the standard NJOY version, I have created some local variations on the standard version which perform some rather specialized additional tasks. These can be appended to Bob MacFarlane's *ident up45 in the usual NJOY update procedure. The idents have the following special purposes:

new1

Increase the container array in ERRORR to permit processing of multigroup covariances in the SAND-IIa (640-group) structure. The code runs faster with this dimensioning than the standard dimension. For more typical group structures the standard dimension of 30,000 words is fine.

new2

These very large dimensions are necessary in order to run the BOXR format library option in the SAND-IIa structure. The Windows PC version of NJOY with these dimensions is large but not impractically so (executable occupies 23 megabytes). For more typical group structures, the standard dimension of 50,000 words is fine.

new3

This is an experiment to evaluate the effect of removing all sub-subsections with LB=8 from an evaluation. In very fine-group libraries, LB=8 produces very large in-group covariances, which may or may not be realistic. The option is activated by setting the material number MATD negative.

==========
beginning of local updates to ERRORR and COVR

```
==========

*ident new1
*/ errorr -- 2nov98
*/   increase storage to permit processing of sand-iia 640 groups
*d errorr.128
      common/estore/a(120000)
*d errorr.154
      namax=120000
*d errorr.2192
      common/estore/a(120000)
*ident new2
*/ covr -- 2nov98
*/   increase storage to permit processing of sand-iia 640 groups
*/   note change to both iamax and ntics3
*d covr.100
      common/storec/a(880000)
*d covr.131
      data iamax/880000/, niad/15/, ipr/1/, ntics3/1200/
*d covr.1070
      common/storec/a(880000)
*ident new3
*/ errorr -- 2nov98
*/   add a new feature to optionally suppress lb=8
*d errorr.126
      common/mode/imode,isupp
*i errorr.198
c     use a negative value of matd to suppress lb=8 by 10.**(-10)
      isupp=0
      if (matd.lt.0) then
         isupp=-10
         matd=-matd
      endif
*d errorr.1070
      common/mode/imode,isupp
*d errorr.1317
      a(icov+jh-1)=a(icov+jh-1)+a(loci+5+k2)*xcv*10.**isupp
*d errorr.1789
      common/mode/imode,isupp
```

Representation and Processing of Covariance Matrices for Resonance Parameters

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Abstract

The number of elements in a resonance-parameter covariance matrix can be exceedingly large; archival storage of such a matrix may be prohibitively expensive. A variety of formats have been proposed for ASCII storage of resonance-parameter covariance matrices; each format implicitly assumes that the matrix is to be abbreviated in some fashion. In this paper, the consequences of such abbreviations are explored by examining the behavior of multigroup cross sections (and, in particular, of the associated covariance matrix) when calculated using various approximations to the resonance-parameter covariance matrix.

1. INTRODUCTION

It has long been implicitly assumed that ASCII storage of a resonance-parameter covariance matrix would require the matrix to be abbreviated in one form or another. The reason is obvious: there are two many numbers to store all of them. For example, ^{235}U has 3193 resonances with five parameters per resonance, for a total of 15965 resonance parameters. The number of elements in the triangular half of the associated covariance matrix is then (15965×15966)/2 = 127,448,595 elements, a very large number. ASCII storage of this entire array, using six real numbers per line (as is conventional in ENDF formats, for example), would require 21,241,433 lines.

The current ENDF format for File 32 and File 33 is based on a premise which is neither proven nor well-defined: "In the resonance region, the covariances of the partial cross sections are often characterized by a) 'long-range' components which affect the covariances over many resonances, and b) 'short-range' components affecting the covariances of the different partial cross sections in the neighborhood of individual resonances. The former often can best be represented in File 33, while the latter can be given in File 32." (Section 32.1 of ENDF-102.[1])

This author suspects that the availability of resonance covariance information in ENDF files will increase directly with the ease of generation of such information. Abbreviation of the covariance matrix via "a cookbook prescription" would be significantly easier than the subjective-interpretation procedure required by the current ENDF format, and conceivably, also be less susceptible to evaluator error.

In the next section, one possible scheme for abbreviating resonance-parameter covariance matrices is introduced. This scheme involves two free parameters; in subsequent sections the effects of using different values for those two parameters are examined, by studying changes in the

uncertainties and correlation coefficients for multigroup cross sections obtained by averaging over the theoretical energy-differential cross sections.

2. APPROXIMATING THE COVARIANCE MATRIX

Several authors have proposed formats for introducing resonance-parameter covariance information into ENDF. Fröhner[2] may have been the first to suggest that the covariance matrix ought to be stored as uncertainties plus correlation matrix, as the information is far more intelligible to mere humans in this form. Muir[3] suggested mapping the correlation coefficients to integers; he also designed a format for reporting these integers, making use of assumed trends within the matrix. This author[4,5] proposed a variation on Muir's scheme, since examination of several "real" covariance matrices did not find evidence of these trends.

The approximation to be discussed in this report is a generalization of the author's earlier proposal.[5] We begin by defining notation, which is chosen to be consistent with that used in the SAMMY manual,[6] and hence differs somewhat from that used in the oral presentation of this report.

Let P represent the resonance parameters, and M represent the corresponding covariance matrix. The uncertainty on parameter P_i is given by the square root of the diagonal matrix element; that is,

$$\Delta P_i = \sqrt{M_{ii}} \ .$$

The correlation coefficient between parameter number i and parameter number j is the covariance matrix element divided by the two uncertainties:

$$c_{ij} = \frac{M_{ij}}{\Delta P_i \, \Delta P_j} \ .$$

Note that values for c fall between the limits ± 1, while values for M have very different ranges.

In the approximation to be studied here, a many-to-one mapping (c to K, where K is an integer of N digits, and N is to be determined) is defined as follows:

(a) Drop small correlations; i.e., for $|c| < small$ then set $c = 0$.
(b) Map all points c within a specified range to a single integer K; for example, if $0.4 \le c < 0.6$, set $K = 7$.
(c) The "user" program then interprets that integer as the mid-point in that range; *e.g.*, $K = 7$ becomes $c' = 0.5$.

Figure 1 shows this mapping schematically for the example described above, using a 1-digit mapping ($N = 1$) with $small = 0.2$. The top line shows the (continuous) values for c, the dotted lines indicated which values are mapped to the integers shown at the bottom. Points marked with "o" on the bottom dashed line are the values which the "user" program will then assign to all correlation coefficients in the original range.

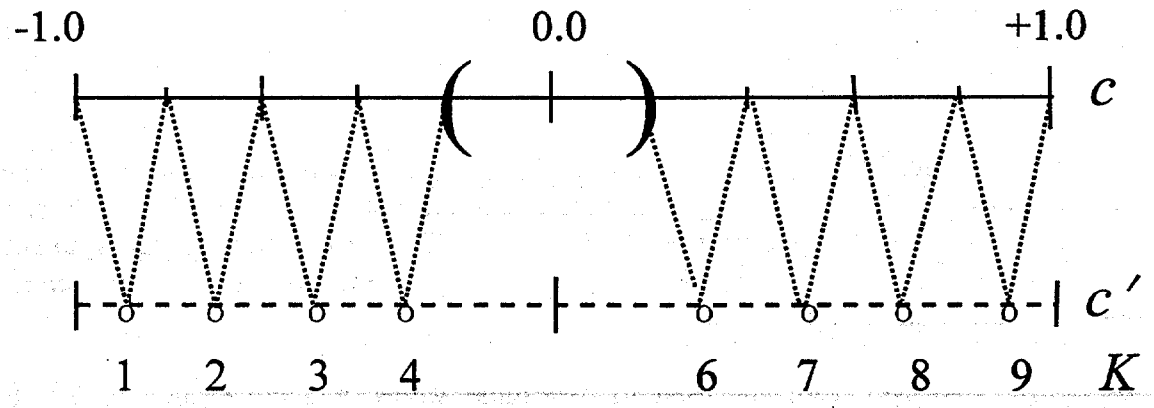

Fig. 1. One-digit mapping from correlation coefficient c to integer K, then back to correlation coefficient c', dropping coefficients smaller than 0.2.

It should be noted that the single-digit mapping shown in Fig.1 is not likely to be used in practice, since this is an extreme approximation; nevertheless $N = 1$ was chosen for the figure because it is most easily illustrated. Also note that the real-to-integer mappings described here assume uniform spacings of $(10^N - 2) / 2$ integer values covering the range from $small \le c \le 1$, and the same number of values covering the range $-1 \le c \le -small$. A uniform mapping was chosen for convenience only, but there may be virtue in using, for example, a mapping which is sparse for lower values of c and dense at higher values. This possibility merits further inspection.

Use of any such integer mapping requires, in addition to the mapped integers themselves, an indexing system to identify the particular element of the covariance matrix for which the value is given. The system currently employed by SAMMY for reporting correlation coefficient c_{ij} is to give i in the first five columns on a line in the ASCII file, and j in the second five columns. The next column is left blank, and the remaining columns of the line (up to column 66) contain the integer value K for correlation coefficient c_{ij}, $c_{i(j+1)}$, $c_{i(j+2)}$, etc., using N columns for each N-digit integer; thus there may be only one coefficient on a line, or there may be many. For an example, see the next section of this report.

3. TESTING THE APPROXIMATION

Before choosing any one particular abbreviation over another, it is necessary to understand the consequences of such abbreviations. In particular, we need to understand whether an abbreviated covariance matrix can contain the same information as the complete covariance matrix. To this end, we will calculate certain quantities which depend upon the covariance matrix, and then track how

those quantities change as the parameters of the abbreviation are changed. This should provide at least a zeroth-order test of the validity of the abbreviated resonance-parameter covariance matrix.

3.1 RESONANCE PARAMETER SET

The test case for this study was ^{235}U in the energy range from 4.5 to 50 eV, chosen for a variety of reasons: ^{235}U is intrinsically an important and interesting nuclide. ^{235}U contains a large number of closely-spaced resonances. The parameter set is large enough to be meaningful yet small enough to be manageable; manageability is not an unimportant criterion, as a large number of computer runs are required for these tests.

A initial SAMMY run was used to determine values and covariance matrix from a simultaneous fit to transmission (3021 data points), capture (1976), and fission (1976) data. For all resonances from 0 to 50 eV, all five resonance-parameters (energy, capture width, neutron width, and two fission widths) were varied, for a total of 590 parameters. For resonances at higher energies, the parameter values were assumed to be "exact," and thus are not included in the covariance matrix.

Table 1 shows a small portion of the covariance matrix for this example. There are a total of 173,755 off-diagonal elements in the entire (triangular portion of the) correlation matrix. In the SAMMY.LPT file, this translates into 7982 lines (since lines with all zero's are not printed), or 130 pages. Table 2 shows a similar portion of the same matrix in the concise format described earlier, with *small* = 0.1 and $N = 2$. For this abbreviation, there are 5250 off-diagonal elements in the triangular portion of the correlation matrix, or 1065 lines in the ASCII file (plus 100 lines for uncertainties), for a total of 20 pages.

3.2 MULTIGROUP CROSS SECTIONS

The general definition of the flux-weighted multigroup cross section is

$$\bar{\sigma}_{x,i} = \int_{E_i}^{E_{i+1}} \sigma_x(E)\ \Phi(E)\ dE \Bigg/ \int_{E_i}^{E_{i+1}} \Phi(E)\ dE$$

in which subscript x indicates the particular type of cross section (e.g. capture, fission, total) and the flux $\Phi(E)$ is the energy-dependent neutron flux. Since this flux is not known, the Bondarenko[7] narrow-resonance scheme is often used:

$$\bar{\sigma}_{x,i} = \int_{E_i}^{E_{i+1}} \frac{\sigma_x(E)\ C(E)}{\sigma_t(E) + \sigma_0}\ dE \Bigg/ \int_{E_i}^{E_{i+1}} \frac{C(E)}{\sigma_t(E) + \sigma_0}\ dE$$

in which σ_t is the total cross section, σ_0 is an energy-independent constant, and $C(E)$ is a smooth function of energy. The limit in which C is constant and σ_0 is effectively infinite,

Table 1. Resonance parameter covariance matrix in SAMMY format (uncertainties plus correlation matrix).

```
   STD.DEV.   (REL.)   CORRELATION*100
. . .
                      556 557 558 559 560 561 562 563 564 565 566 567 568 569 570
557  1.672      .044   12 100
558 1.3713E-02 .027   25  47 100
559  4.291      .049   26  70  71 100
560 4.5826E-02 .100   -3   1   1  -1 100
561 5.1775E-03 .000   -1  11  12  13   0 100
562  2.803      .069   -6  -1   0   0   0   4 100
563 4.7201E-03 .037   -5  -1  11   5   0  -4  29 100
564  4.680      .071   -9  -1   5   3   0  -5  61  47 100
565 0.1322      .100    0   0  -1   0   0   1   1   1  -1 100
566 5.4157E-03 .000   -5   4   9   8   0  17   1  -2  -5   0 100
567  2.106      .058   -3  -2   4   2   0   3  -2   2   2   0   5 100
568 3.2413E-02 .061  -11   1   5   5   0  27   0   8   0  -1  69  20 100
569  8.738      .050  -10  -2   1  -1   0   9  -3   8   4   0 -13  39  29 100
571 4.2264E-03 .000   -3   0   7   5   0  10   2   6   4   0  65  38  51  32   0
572  2.048      .040    3  -2  -6  -5   0 -11  -1  -1   4   0 -38 -40 -36  23   0
573 2.9526E-02 .041   10   0  -5  -4   0 -25  -2  -7   0   1 -75 -18 -93 -19   0
574  5.454      .040    1  -2  -5  -3   0 -10  -2   2   6   0 -40  20 -24  57   0
576 1.7554E-03 .000    0   0   1   1   0   0   0  -1  -1   0  -4  -4   0   1  -1
577  2.260      .047    0   0   0   0   0   0  -1  -1   0   0   1   0   1  -2   0
. . .
```

Table 2. Resonance parameter uncertainties plus correlations in concise format as described in the text, with *small* = 0.01 and *N* = 1.

```
. . .
1.03127E-02 12.623    0.12054    2.51460E-03 1.6719    1.37128E-02
 4.2912    4.58261E-025.17749E-03 2.8030    4.72012E-03 4.6804
0.13221    5.41568E-03 2.1060    3.24127E-02 8.7380    4.96678E-02
4.22637E-03 2.0479    2.95259E-02 5.4541    1.66682E-021.75540E-03
 2.2599    1.41951E-027.45269E-03 2.4510    5.06119E-02 3.9055
3.55928E-03 6.2884     6.5015    1.20957E-03 2.1486    9.82355E-03
0.75787    4.51497E-02
. . .
  557   30 49
  557  201 51                                                    49
  557  233 525151  51          52495255384056  49  4949
  557  273 4949            51    49
  557  509 51            51  49  4951            49        49
  557  536 52515252    49  51  5649  495234383749  56
  558   24 51        5248
  558  153 4949            51  49  4951    51
  558  191 51                51        49        52515252  52
  558  218 5253            48  49    52  5253    515251    515746
  558  245 58823512413946  4949  51    51    5152  52
  558  273 4949      4949  51  4949
  558  421 51              51                              51
  558  448 51                51          51          49
  558  481 51        51  51        49    48  4749            49
  558  511 49        51  5251    515251  51  49    5151  52495253
  558  538 5556  5147  52        465235434949496274
. . .
```

$$\bar{\sigma}_{x,i} = \int_{E_i}^{E_{i+1}} \sigma_x(E)\, dE \Big/ \int_{E_i}^{E_{i+1}} dE \,,$$

is the form used in the calculations for this study.

To generate the covariance matrix for the group cross sections, we first take small increments

$$\delta \bar{\sigma}_{x,i} = \sum_k \frac{\partial \bar{\sigma}_{x,i}}{\partial P_k} \delta P_k \,,$$

where P represents the resonance parameters. The covariance matrix is then found by taking expectation values

$$C_{i,j} = < \delta \bar{\sigma}_{x,i} \, \delta \bar{\sigma}_{x,j} > = \sum_{k,k'} \frac{\partial \bar{\sigma}_{x,i}}{\partial P_k} < \delta P_k \, \delta P_{k'} > \frac{\partial \bar{\sigma}_{x,j}}{\partial P_{k'}} = \sum_{k,k'} \frac{\partial \bar{\sigma}_{x,i}}{\partial P_k} M_{k,k'} \frac{\partial \bar{\sigma}_{x,j}}{\partial P_{k'}} \,,$$

in which

$$M_{k,k'} = < \delta P_k \, \delta P_{k'} >$$

is the (known) covariance matrix for the resonance parameters.

4. RESULTS

Average total, fission, and capture cross sections were calculated for those nine members of the 199-group (Vitamin B) cross section library[8] which lie completely within the energy range 5 to 50 eV. Uncertainties and correlation matrix for those group cross sections were also calculated, using first the exact resonance-parameter covariance matrix and then various abbreviations thereto. Comparisons were made of the results of those calculations.

Table 3 shows comparisons of the uncertainties for the average total cross sections when the exact resonance-parameter covariance matrix is used, and when small values of correlation coefficients are dropped (with *small* ranging from 0.01 to 0.99). As can be seen from the table, uncertainties change only slightly for *small* = 0.01, change moderately for *small* = 0.04, and change substantially for *small* = 0.40; for the "usual" case (dropping all off-diagonal correlation coefficients, equivalent to *small* = 0.99), uncertainties on the average cross sections bear little resemblance to the correct values. (Fortunately, but perhaps fortuitously, they are conservatively larger rather than smaller.)

Similar information is given in Table 4, but here a 2-digit mapping is used in addition to dropping correlations smaller than *small*. The interesting result here is that the integer mapping, even to as few as 2 digits, appears to produce as small (or smaller) an effect on the uncertainties for the group averages as does dropping small correlations. Hence a two-digit mapping should be adequate for most purposes.

Table 3. Changes to the multigroup total cross section uncertainties when using the real*8 representation of correlation matrix, dropping small correlations for resonance parameters.

				Uncertainty when corr is >...						
	Emin	Emax	value	exact	>0.01	>0.02	>0.03	>0.04	>0.40	>0.99
1	5.043	6.476	87.58	0.26	0.26	0.26	0.26	0.27	0.38	0.53
2	6.476	8.315	39.66	0.13	0.13	0.13	0.14	0.15	0.22	0.23
3	8.315	10.677	143.54	0.24	0.25	0.26	0.28	0.28	0.45	0.73
4	10.677	13.710	127.10	0.22	0.23	0.23	0.24	0.24	0.32	0.46
5	13.710	17.604	60.56	0.14	0.13	0.15	0.16	0.17	0.29	0.48
6	17.604	22.603	121.36	0.20	0.21	0.21	0.22	0.22	0.30	0.46
7	22.603	29.023	73.30	0.14	0.15	0.16	0.16	0.16	0.29	0.42
8	29.023	37.266	105.52	0.27	0.28	0.27	0.27	0.26	0.29	1.18
9	37.266	47.851	62.39	0.12	0.13	0.13	0.14	0.15	0.23	0.35

Ratio of uncertainties to "exact" value

	Emin	Emax	>0.01	>0.02	>0.03	>0.04	>0.40	>0.99
1	5.043	6.476	1.0	1.0	1.0	1.0	1.5	2.1
2	6.476	8.315	1.0	1.0	1.1	1.1	1.7	1.8
3	8.315	10.677	1.0	1.1	1.1	1.2	1.9	3.0
4	10.677	13.710	1.0	1.0	1.1	1.1	1.4	2.1
5	13.710	17.604	1.0	1.1	1.1	1.2	2.1	3.4
6	17.604	22.603	1.0	1.1	1.1	1.1	1.5	2.3
7	22.603	29.023	1.0	1.1	1.1	1.1	2.1	3.0
8	29.023	37.266	1.0	1.0	1.0	1.0	1.1	4.3
9	37.266	47.851	1.0	1.0	1.1	1.2	1.9	2.8

Table 4. Changes to the multigroup total cross section uncertainties when using 2-digit mapping of correlation matrix and dropping small correlations for resonance parameters.

				Uncertainty when corr is >...				
	Emin	Emax	value	exact	>0.01	>0.02	>0.03	>0.04
1	5.043	6.476	87.58	0.26	0.26	0.25	0.27	0.26
2	6.476	8.315	39.66	0.13	0.13	0.13	0.14	0.15
3	8.315	10.677	143.54	0.24	0.25	0.25	0.28	0.27
4	10.677	13.710	127.10	0.22	0.23	0.23	0.24	0.24
5	13.710	17.604	60.56	0.14	0.14	0.14	0.15	0.16
6	17.604	22.603	121.36	0.20	0.20	0.21	0.22	0.22
7	22.603	29.023	73.30	0.14	0.14	0.16	0.16	0.16
8	29.023	37.266	105.52	0.27	0.28	0.26	0.26	0.26
9	37.266	47.851	62.39	0.12	0.13	0.13	0.14	0.14

Ratio of uncertainties to "exact" value

	Emin	Emax	>0.01	>0.02	>0.03	>0.04
1	5.043	6.476	1.0	1.0	1.0	1.0
2	6.476	8.315	1.0	1.0	1.1	1.1
3	8.315	10.677	1.0	1.0	1.1	1.1
4	10.677	13.710	1.0	1.0	1.1	1.1
5	13.710	17.604	1.0	1.0	1.1	1.2
6	17.604	22.603	1.0	1.0	1.1	1.1
7	22.603	29.023	1.0	1.1	1.1	1.1
8	29.023	37.266	1.0	0.9	0.9	1.0
9	37.266	47.851	1.0	1.0	1.1	1.2

The correlation matrices corresponding to the first three cases of Table 3 and two cases of Table 4 are shown in Table 5. Note that the general results described above hold true here as well: Dropping resonance-parameter correlations less than 1% has a modest effect, the effect increases as larger correlations are dropped. The effects from the two-digit mapping are as small as the effect of dropping correlations smaller than 1%.

Tests were also run with 3-, 4-, and 11-digit mappings, but the requirements for additional storage space for these cannot be justified in terms of information gained. Table 6 indicates the storage requirements for the various mappings.

Tests results with capture and fission cross sections are similar to those from the total cross sections, and will not be shown here.

5. CONCLUSIONS AND RECOMMENDATIONS

If the resonance-parameter covariance matrix is to be communicated from SAMMY (or other analysis codes which generate this information) to other codes via ASCII files, some abbreviation is necessary. In this study we have seen that, at least for some applications, it may be adequate to (1) convert from covariance matrix to uncertainty plus correlation matrix, (2) drop correlations smaller than 1 %, and (3) represent other correlations by a 2-digit mapping. Further study is needed to ensure that such abbreviations are adequate for other applications as well. In addition, investigation should be made into the mathematical properties of the abbreviations, to determine whether they obey the positive-definite requirements for covariance matrices.

Table 6. Number of rows required in an ASCII file to report the abbreviated covariance matrix, when the abbreviation uses $|c| \le$ *small* and an *N*-digit mapping. The final row (labeled "#") gives the number of non-zero correlation coefficients for each value of *small*.

N \ *small*	0	0.01	0.02	0.03	0.04	0.40	0.99
11	28960	8509	4724	3149	2362	214	0
4		4694	2786	1908	1462		
3		3765	2306	1600	1254		
2		2890	1765	1345	1065		
#	173755	21231	10977	7173	5250	294	0

Table 5. Changes to the correlation matrix for the group average total cross section when dropping small correlations for resonance parameters. The first case is exact, the second and third drop small correlations but otherwise use exact values, the fourth and fifth use the two-digit mapping.

```
### Correlation matrix for "exact" representation
  1  0.257233     100
  2  0.129223      19 100
  3  0.243501       6  15 100
  4  0.224939       6  13   7 100
  5  0.138666      11  23  11  12 100
  6  0.202932       6  14   6   7  12 100
  7  0.143338       8  17   7   8  14   9 100
  8  0.272453       3   6   5   5   7   4   3 100
  9  0.124235       8  19   8   9  16  10  13  10 100

### Correlation matrix for |c|>0.01 with no mapping
  1  0.256447     100
  2  0.130852      19 100
  3  0.246180       8  16 100
  4  0.229061       8  13  10 100
  5  0.134845      12  23   7  11 100
  6  0.205806       7  13   6   6  10 100
  7  0.147624       8  16   6   9  14  12 100
  8  0.279022       6   7   3   5  10   4   5 100
  9  0.125663       8  17   4   9  13  10  13  10 100

### Correlation matrix for |c|>0.02 with no mapping
  1  0.256268     100
  2  0.134963      21 100
  3  0.258970       6  18 100
  4  0.233165       6  12  14 100
  5  0.146268      17  30  12  15 100
  6  0.214572       8  16   9  11  24 100
  7  0.155602      11  20  11   8  27  16 100
  8  0.274365       6   4   6   8  12  10   6 100
  9  0.130191       6  15   5   8  18  14  20  12 100

### Correlation matrix for |c|>0.01 with 2-digit integer mapping
  1  0.262813     100
  2  0.130865      18 100
  3  0.254181      12  19 100
  4  0.226823       8  13   9 100
  5  0.136988      13  21  17   9 100
  6  0.201926       8  12   8   5   9 100
  7  0.142912       9  17  12  11  14  10 100
  8  0.277877       6   8   3   5  15   1  -3 100
  9  0.125644       9  17   7  11  12   8  14   2 100

### Correlation matrix for |c|>0.02 with 2-digit integer mapping
  1  0.252963     100
  2  0.134652      19 100
  3  0.251358       0  15 100
  4  0.234649       4  12  11 100
  5  0.142890      18  34  14  14 100
  6  0.212502       7  16  10  11  25 100
  7  0.157785       8  18  11   9  27  15 100
  8  0.258328       5   5   4   9  14  10  -1 100
  9  0.129757       4  16   5   7  22  15  18  12 100
```

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PROCESSING AND USE OF COVARIANCE MATRICES FOR APPLICATIONS IN FISSION AND FUSION

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Abstract

This paper describes the calculational tools developed for the sensitivity and uncertainty analysis. The computer code system was prepared which includes the SUSD3D cross-section sensitivity and uncertainty package, and the cross-section covariance matrix library VITAMIN-J/COVA. VITAMIN-J/COVA includes also a code for the extrapolation of the matrices from one energy group structure to another, and a code to test the mathematical properties of the matrices. Next some examples of practical application of this code system in the fields of fission and fusion are shown. Major uncertainties of the transport calculation are considered, with an emphasis on those related to the cross section data. The role of the covariance matrices is discussed.

1. INTRODUCTION

Cross-sections are among the major sources of uncertainties. All steps used in the preparation of cross-section data (the evaluation, as well as the processing) include their proper uncertainties. Measurements include intrinsic uncertainties, and all contemporary nuclear models are inherently approximate. The quality of nuclear reaction models and parameters can be assessed by comparing their production with experimentally obtained results, or by inter-comparison of their predictions.

Error estimations related to the evaluation of the cross-sections are added to the evaluated data files in the form of covariance matrices. Covariance matrices are usually derived from Bayesian analyses or(/and) the scatter among data sets. Alternatively if the cross-sections are obtained as a sum, or difference of other reaction types, the covariance matrices are derived from the corresponding covariances. Where no measurements are available the uncertainty information is deduced from the calculation uncertainties.

Specific error components are either correlated or un-correlated. Correlation between various observations influence substantially the final estimations of the uncertainties and should be taken into account where available.

Estimation of these errors is usually nontrivial and subjective procedure. In particular this is true for systematic errors representing the deviations from the true values which, contrary to the statistical errors, cannot be assessed by repetition of the particular procedure. The procedure of uncertainty assessment requires therefore detailed examination and documentation of the experimental procedure. Participation of the experimentalists in the uncertainty evaluation is indispensable. The feedback information from the end-user of the data, providing the evaluator with the experience from the use of the covariances in practice, is also substantial and beneficial for both the user and the evaluator.

Covariance matrices proved to be very useful basically in two kinds of radiation transport analysis:

- Uncertainty analysis, usually combined with sensitivity calculations, provide valuable information about the physical process involved, in particular about the importance of different calculational parameters and the accuracy of the calculation.
- Adjustment analysis: The uncertainties can be reduced through data adjustment, which can also provide feedback on possible deficiencies in the evaluated nuclear data files. The basic idea of the adjustment procedure is to change the values of the basic parameters within assumed uncertainties, so that the calculated results agree, within experimental errors, with the measured values. In this way a parameter possessing larger uncertainty is allowed to change more than one in which the uncertainty is small. The least square method is generally adopted. Therefore data adjustment requires, besides the sensitivity analysis of the integral results to the nuclear data, also an evaluation of the uncertainties in the nuclear data and the correlations among them, as well as a covariance matrix of the measured integral data. Insofar as the set of data used for adjustment are well consistent with each other, the expected uncertainties in the adjusted parameters would be substantially smaller than those in the unadjusted library. Examples of codes used for adjustment are AMARA (using Lagrangian multipliers) and ZOTT [1] (using partitioned least squares, logarithmic adjustment option available). Examples of unfolding codes are FERRET, STAY-SL, LSL-M2. The above codes are available through RSICC and NEA Data Bank.

Both uncertainty and adjustment analyses proved to be very useful in many domains of application, ranging from nuclear research and power reactors (e.g. PW reactor pressure vessel surveillance), to fusion (blanket design), integral benchmark pre- and post-analysis, accelerator, and medical problems.

Several calculational tools were developed for the uncertainty and adjustment in the past. The starting and very crucial part is the determination of the covariance matrices of the basic data (like cross-sections, response functions, fission spectrum etc.), which requires quite a good sense of judgement and usually a lot of time. Without any reliable information on the covariance matrices the uncertainty analyses are, of course, not meaningful, although methods for investigating the sensitivity of transport calculations to uncertainties in the basic cross-section are known since quite a long time.

For typical reactor application quality covariance information for all relevant types of cross-sections is required for major actinides, important structural materials, and dosimetry reactions. Other materials are important for specific applications (like Be for fusion). Although the availability of cross-section covariance data is being rapidly improved, there are still many gaps waiting to be filled. In particular the problem of covariance representation for secondary angular (SAD) and energy (SED) distributions of scattered neutrons is not completely resolved.

The various types of covariance data are stored in different ENDF/B formats (Files):

- File-31 stores the covariances of the average number of neutrons per fission ($\nu(E)$);
- File-32 describes the uncertainty in the shape and area of individual resonances;
- File-33 contains covariances corresponding to File-3 energy-dependent cross-sections;
- File-34 is used for SAD covariances (corresponding to File-4 data);
- File-35 is used for SED covariance matrices (corresponding to File-5 data);
- File-30 is a very promising approach, both flexible and compact. The uncertainties of relatively small set of key parameters are stored together with the derivatives of the

nuclear data with respect to the parameters. At present no data exist in this format, but the possibilities of using this format for SAD and SED uncertainties was pointed out [2];
- File-36 format was proposed as an alternative format for uncertainties of secondary coupled energy-angle distributions [3];
- File-40 includes covariances for production of radioactive nuclei.

ENDF/B-VI evaluation contains relatively complete File 33 covariance information. Most important structural materials covariance data are included in EFF-2.4 evaluation as well. EFF-2.4 evaluation contains in addition File-34 covariances for elastic scattering on iron, chromium and nickel [4]. For Fe the terms P-1 to P-6, and for Cr and Ni the terms P-1 to P-3 are given. No data is available yet for uncertainties in SED (File-35). SAD and SED uncertainties are less important for fission reactor shielding, but must be considered in fusion studies and for other neutron sources at high energy. International Reactor Dosimetry File (IRDF-90) [5] contains very complete covariance information for neutron dosimetry cross-sections.

NJOY [6] is the most widely used code for processing evaluated covariance data into multigroup form. ERRORR can process File-31, 32 and 33 covariances, the COVR module is used for transformation of data to the compact BOXR format, and for graphical display of the multigroup covariance data.

Examples of already processed multigroup neutron cross-section covariance matrix libraries are COVFILS [7], COVFILS-2 [8] and ZZ-VITAMIN-J/COVA [9].

An overview of the data files and computer codes for processing of cross-section covariance data can be found in [10].

2. SENSITIVITY AND UNCERTAINTY CODE SYSTEM

A calculational system was developed at first intended primarily for the sensitivity and uncertainty analysis of the fission reactors, but was found general enough to be used subsequently in other fields, like fusion, and different integral benchmark analysis. Fusion analysis is usually much more sensitive to the secondary energy and angular distributions than most fission type problems and requires different approaches. The system consists of the covariance matrix library, covariance matrix processing codes and a computer code for 1-, 2-, and 3-dimensional sensitivity and uncertainty analysis.

2.1. ZZ-VITAMIN-J/COVA

The multigroup relative neutron cross-section covariance data library was developed and is available from the NEA Data Bank (Code package NEA 1264). The objective was to promote and facilitate the use of covariance matrices. The package includes:

- Multigroup neutron cross-section covariance matrix library: Some older JEF-1, ENDF/B-IV, and ENDF/B-V data are included in version NEA 1264/03, and EFF-2 covariances in /04 version (ZZ-VITA.-J/COVA/EFF package). Detector response function covariance matrices are included as well: NEA 1264/03 containes data from IRDF-85, and NEA 1264/04 those from IRDF-90.2. EFF-3 version of the library is in preparation. Highly compressed BOXER format [6] is used to store the matrices which were previously tested for their mathematical properties.

- Interpolation procedure called ANGELO to collapse or extrapolate the multigroup covariance data from the original to a user defined energy group structure. Due to the absence of cross-section and flux weighting the interpolations to group structures which differ significantly from the original should be avoided (especially if the number of groups is reduced considerably). Still, the procedure tends to be conservative. The interpolation procedure was found to give reliable results if the number of groups changed for up to a factor of 4. In this range the procedure can be therefore considered as an adequate and easy-to-use alternative to more rigorous methods, like ERRORR module of NJOY.
- Program to verify some mathematical properties and physical consistency of the data and the interpolation procedure, in particular the positive definiteness of the multigroup covariance matrices. The trace and the number of positive, negative, and zero eigenvalues is calculated and the matrix is classified on this basis. The correlation matrix is tested to determine if any element exceeds unity. This quality verification is highly recommended before using the covariance information to data consistency analysis with integral experiments and to data adjustment.

2.2. File 34 Multigroup Processing

A computer code (provisionally called ERRORR34) for the processing of the File 34 covariance matrices, which are available in the EFF-2.4 evaluation in ENDF/B-6 format, was developed within the European Fusion File (EFF) project of the European Community [11]. These processed multigroup SAD covariance matrices can be subsequently used by the SUSD3D code described below. Group-collapse strategy similar to the one used in NJOY [njoy] was adopted. The code is an extension of ERRORR module of NJOY, and is prepared in the UPD format modifications.

An example of a File-34 covariance matrix for Fe, processed by the ERRORR34 code, is presented in Figure 1.

2.3. SUSD3D Sensitivity and Uncertainty Code Package

A computer code package for one-, two- and three-dimensional cross-section sensitivity and uncertainty analysis has been developed. The starting point was the SUSD code [12], [13] developed more than 10 years ago by Furuta and co-workers, but several major modifications and updates were introduced [11]. The code calculates sensitivity coefficients using the first order perturbation theory. Variances and standard deviations of detector responses or design parameters can be obtained using cross-section covariance matrices.

SUSD3D calculates the relative variance in the response due to the uncertainties in the cross-sections, and due to the uncertainties in the response functions, as well as those due to the fission yield and fission spectrum for the analysis of a multiplying medium.

Different background cross-section values can be used for the sensitivity calculations, and the self-shielding effect can be evaluated in this way.

The main advantage of SUSD3D over similar codes (like SWANLAKE, SENSIT) is, apart from some user friendly options, its much more sophisticated treatment of the sensitivities and uncertainties of secondary neutron angular and energy distributions (SAD/SED), which makes it in particular suitable also for fusion neutronics and shielding analysis. SUSD3D code can treat the complete covariance matrices in secondary angular distribution (file MF=34), as provided by the ERRORR34 code. The File33 covariance matrices also required

for the uncertainty analysis can be either processed by NJOY or taken from the ZZ-VITAMIN-J/COVA library (i.e. processed by ANGELO code).

The present version of the code calculates the sensitivity coefficients from the direct and adjoint angular flux files obtained by discrete ordinates (S_N) codes ANISN or DORT, or from flux moment files obtained by DORT, TORT [14], TWODANT and THREEDANT [15] transport codes. Use of angular moment files instead of the bulky angular flux files produced by the transport codes reduces considerably the size of the files required, as well as the CPU time, whereas at the same time the accuracy of the calculation is preserved. In particular the advantages of this approach are appreciated in the 3-dimensional sensitivity and uncertainty analysis, which would otherwise require prohibitively large computer space.

The system was extended to 3-dimensional analysis since we expect that the 3D effects can be substantial in some sensitivity calculations. In the past the analysis of more complex and 3D geometry was generally reserved for Monte Carlo methods. Now with the development of some powerful 3D discrete ordinates codes, like TORT [14], THREEDANT [15], the delimitation between the two methods is less clear than before. The sensitivity methods based on discrete ordinates and Monte Carlo can be now considered as complementary, presenting each same advantages and deficiencies. Discrete ordinates based methods could be preferred due to their CPU time advantages and relative simplicity of use for the problems which can be modelled efficiently by the available geometry options, whereas the sensitivity/uncertainty analysis of the very complex geometry would be still reserved for Monte Carlo based methods.

3. EXAMPLES OF PRACTICAL APPLICATIONS

The quality and availability of covariance data as well as calculational tools improved over last years and the sensitivity and uncertainty analysis proved very useful in many domains of neutronics calculations, like nuclear reactor safety, installation cost reduction, improved design and such analysis influence directly the decision-making process. Examples of successful use of uncertainty analysis can be found in fission reactor core physics and fuel cycle analysis, PW reactor pressure vessel surveillance, fusion blanket studies, integral experiment pre- and post-analysis, health physics, oil well logging, etc. In all these cases the accuracy of the numerical results is crucial and determines the safety margins attributed to the calculated values and in this way the design and the cost of the project.

Examples of the application of the computer code package described above include:

- PWR Pressure Vessel (PV) Surveillance
- ASPIS Iron Benchmark
- VENUS-3 Benchmark
- FNG Bulk Shield Benchmark

The system was first applied to the 900 MWe EDF type PW reactors with the objective to validate the methodology used in the pressure vessel surveillance programme [16-18]. The irradiation induced degradation of reactor components, in particular of the pressure vessel material, is one of the major factors limiting the life of the nuclear installation. In addition to the neutron fluence values at the most critical locations in the reactor, it is essential to know their accuracy. Vague knowledge about the accuracy of the neutron fluence would require larger design and operational margins, and in this way effect operational conditions, the life

of the power plant, and the cost of the electricity produced. The sensitivity and uncertainty analysis was therefore started in 1990 as an integral part of the PV surveillance programme. The objective was, similarly to the LEPRICON project [19], to quantify the uncertainties in the PWR capsule and pressure vessel fluence, and to reduce these uncertainties through adjustment of measured and calculated reaction rates in the surveillance capsules.

A characteristic of the French nuclear installations which is very favourable for the uncertainty analysis, is their high degree of standardisation. Two main types of PWRs are CPY 900 MWe and P4 1300 MWe reactors produced by a single manufacturer in France - EDF. Loading schemes are very standardised, although higher diversification was introduced in the last years due to implementation of some new loading schemes (LLLP, MOX, extended fuel cycle).

The pressure vessel (PV) surveillance programme benefits in this way from the availability of large number of experimental results from surveillance capsules irradiated in reactors of similar types. This presents an important advantage that the dispersion of experimental results is very low and that some errors (the non-systematic errors) are greatly reduced.

The contributions of the uncertainties in the cross-sections, response functions, fission spectrum, density and material compositions were studied using SUSD3D and flux moments calculated by TWODANT. The adjustment analysis was carried out to improve important nuclear data, such as the iron cross-sections, fission spectrum, response functions, neutron source strength. The adjustment factors determined in this way were found to be realistic and consistent with some recent evaluations. ZOTT code [1] was used for the adjustment. The SAD/SED effects were judged negligible in this case and were not considered in the study.

The basic data uncertainties available from different sources were compared. The cross-section covariance data from the ENDF/B-VI evaluated files were found to yield for about 30 to 40 % lower uncertainties in the reaction rates in the capsule with respect to the ENDF/B-IV and /B-V data. This is mostly due to the improved inelastic Fe cross-sections. The comparison of ENDF/B-V and /B-VI based uncertainties in the calculated reactor rates and fast flux in the surveillance capsules of a PWR (CPY 900 MWe) is given in Table 1.

The analysis and the results are presented in detail in [16-18].

The recommended way to determine the state-of-the-art of the nuclear data files, as well as the calculational procedure is to test them against some well defined benchmark experiments. These experiments present the advantage that the uncertainties other than those due to the basic data (e.g. cross-sections) are considerably reduced. Observed C/E values provide information on the quality of the covariance information. Complete description of several benchmark experiments for fission, fusion, and accelerator application is included in the SINBAD (Shielding Integral Benchmark Experiment Database) [20].

To make an independent test of the PWR-PV results the ASPIS-Iron benchmark experiment was examined using the same procedure. In ASPIS-Iron experiment the neutron transport through more than 1 m thick iron slab was studied. This benchmark is therefore a severe test of the iron cross-section data. The results of these analyses are presented in detail in [17] and [21].

VENUS-3 benchmark experiment was studied in the scope of the OECD-NEA Nuclear Science Committee "Task Force on Computing Radiation Dose and Modelling of Radiation-induced Degradation of Reactor Components" and the SINBAD project [20]. Due to its 3-D complexity VENUS-3 sensitivity and uncertainty analysis was performed using 3-dimensional option of SUSD3D code. Direct and adjoint transport calculations were

performed by TORT code, using variable mash option. The sensitivity analysis provide information on the representativity of the experiment with respect to the real reactor environment. The uncertainties of the calculated reaction rates was found consistent with the actually observed spread of C/E values, although showing a general tendency of overestimation. The results are presented in [22].

FNG 14 MeV neutron bulk shield experiment was performed at ENEA Frascati. The benchmark represents the mock-up of the ITER inboard blanket and vacuum vessel. The corresponding sensitivity and uncertainty analysis is presented in [23], [24]. The direct and adjoint flux moments were calculated using DORT code and FENDL-1 and –2 cross-section and covariance matrix data. Large differences between uncertainty estimations based on EFF and ENDF/B-VI cross-section covariance matrices was found, EFF-3 based uncertainties being by about a factor of ~3 lower than those based on ENDF/B-VI, and by a factor of ~2 lower than those based on EFF-2. Comparing the uncertainty predictions with the observed C/E values ENDF/B-VI covariances seem to be on the conservative side, whereas the EFF-3 values could be already slightly low to explain some discrepancies.

The analysis confirmed that the secondary angular distribution (SAD) uncertainties are important in this typically fusion problem. Using EFF-3 covariance data it follows that the contribution of SAD uncertainties are by a factor 2 to 3 superior to the "normal" (i.e. File-33) cross-section uncertainties for the elastic scattering on iron.

A sensitivity and uncertainty analysis of another fusion benchmark experiment, FNG streaming experiment, and a comparative analysis between discrete ordinates and M/C approaches to the sensitivity analysis are underway.

4. CONCLUSIONS

A computer code package for the cross-section sensitivity and uncertainty analysis, based on discrete ordinates transport analysis, was developed. The system was successfully used in several fission and fusion type applications.

The intention of this paper is also to inform the evaluators on how the available covariance matrices are used in practice, on what are the pressing needs for new evaluations, as well as to encourage the future processing and use of the covariance data.

Covariance data from various evaluations was used in the analyses, from ENDF/B-IV, /B-V, /B-VI, to EFF-2 and EFF-3 data. Important differences were observed between the evaluations.

Major improvements in the quality of the covariance information were made over the last years. Reduced uncertainties in Iron data reflect mainly the improved inelastic cross-sections (in particular with respect to the older ENDF/B-IV and /B-V evaluations). On the other hand the problem of covariance representation for the secondary angular and energy distributions of scattered neutrons is not yet completely resolved.

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Table 1. Uncertainties (in %) in the calculated neutron fast flux and detector responses in the surveillance capsules of a PWR (CPY 900 MWe) under standard operational conditions. The comparison of estimations based on ENDF/B-V and /B-VI evaluations is presented.

Source of Covariance matrix	$\Phi > 1$ MeV	$^{54}Fe(n,p)$	$^{58}Ni(n,p)$	$^{63}Cu(n,\alpha)$	$^{237}Np(n,f)$	$^{238}U(n,f)$
ENDF/B-VI	5.8	6.7	6.5	11.7	4.0	6.3
ENDF/B-V	10.8	12.3	10.1	12.2	7.1	11.2

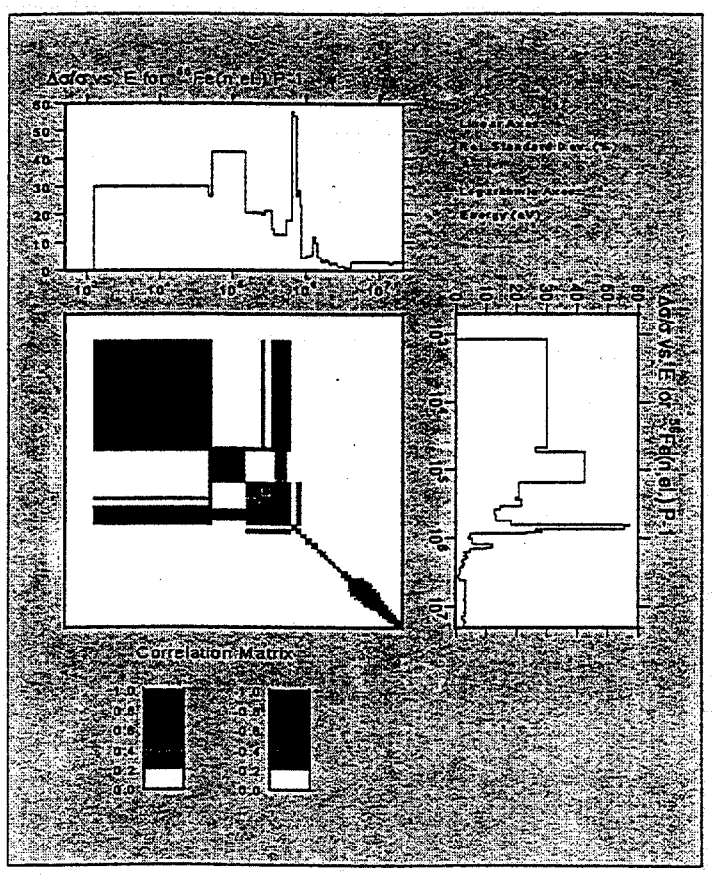

Figure 1. Secondary angular distribution (SAD -File34) covariance matrix for EFF-2.4 Fe-56 cross-sections processed by ERRORR34 code. The term P-1 is shown (Vitamin-J 175 energy group structure).

Reflexions on Uncertainty Files
(15 April 1999)

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1. Representation of Uncertainties in Evaluated Data Files.

Evaluated nuclear data files provide input for reactor calculations and other computations in science and technology. The output accuracy depends on the accuracy of the input and can be assessed by the usual methods of (linear) error propagation if the evaluated data x_j are accompanied in the file by standard (1 σ) errors Δx_j and correlation coefficients ρ_{jk}, or by variances and covariances,

$$\text{var } x_j \equiv (\Delta x_j)^2, \qquad \text{cov } (x_j, x_k) \equiv \Delta x_j \rho_{jk} \Delta x_k.$$

Instead of standard errors one can also use relative standard errors $\Delta x_j/x_j$ and the corresponding relative variances and covariances. There are thus four equivalent ways to file the uncertainty information for given evaluated data:

1. either as variances and covariances (combined in covariance matrices),
2. or as relative variances and relative covariances,
3. or as standard errors and correlation coefficients,
4. or as relative standard errors and correlation coefficients.

By far the most convenient and mnemotechnically safest way is the last one. First, relative (or percent) errors are more easily grasped, compared, and remembered than absolute ones. Second, relative uncertainties and correlation coefficients have a clear intuitive meaning in contrast to variances and covariances. A 2% standard error tells immediately that the associated value is quite accurate, and a correlation coefficient of -0.9 tells that the associated two values are strongly anticorrelated. The corresponding variance and covariance, on the other hand, cannot be understood without the evaluated values themselves, and a square root must be calculated before the same insight is achieved.

It is hard to understand why the present ENDF format admits only absolute and relative variances and covariances. A format extension admitting also standard errors and correlation coefficients would enable evaluators and users to work with uncertainty files that are not bulkier than the existing ones but much more easily constructed, read, understood, debugged and updated, hence much less error-prone. The format extension that suggests itself would consist of one or two tables for the uncertainty information:

Table I, standard errors (one-dimensional array)

This table containing the Δx_j or the $\Delta x_j/x_j$ could be in essentially the same format as the values x_j themselves. A special error format would not be necessary.

Table II, correlation coefficients (two-dimensional triangular array)

This table would follow if and only if information about correlations is actually available. Any of the present formats for covariance matrices should be adequate. Because of $\rho_{jk} = \rho_{kj}$ and $\rho_{jj} = 1$ only the triangular matrix above (or below) the diagonal must be given.

2. First Priority: Standard Errors.

The construction of complete error ("covariance") files for all the data types of a given isotope is difficult, time-consuming, hence expensive. Especially correlations are difficult to establish, being caused by common ("systematic") experimental errors or by theoretical (model) constraints, whereas the assignment of uncorrelated standard errors is much more straightforward. In the present situation of dwindling manpower and funding, the strategy of data evaluators should therefore be to provide standard errors (or variances) first, for all nuclides and data types. Correlation coefficients would be second, given at first only for key nuclides and key data types. The error files would then mostly contain the equivalent of diagonal covariance matrices which is not optimal but sufficient for many purposes – and certainly better than no uncertainty information at all.

3. Manageable Error Files for Resolved Resonances.

Modern evaluations contain resonance parameters (energies, partial widths, spins, parities) for hundreds of resonances, from which Doppler-broadened cross sections and cross section functionals can be calulated, such as transmission, activation, or group cross sections for infinite dilution and self-shielding factors, for arbitrary isotopic mixtures and temperatures. The covariance matrices for the resonance parameters are enormous, and those for computed high-resolution point cross sections even more so. So much detail is not wanted in most technological applications.

The statistical model of nuclear resonance reactions (Hauser-Feshbach theory with width fluctuations) suggests reasonable simplifications. Instead of all the parameters of individual resonances it uses only average resonance parameters – average partial widths $\langle\Gamma_c\rangle$ for all open reaction channels c (for scattering, capture, fission etc.) and mean level spacings D_c. The resonance-averaged partial cross section for reactions leading from entrance channel a to exit channel $b \neq a$ is obtained in the so-called many-level Breit-Wigner approximation as

$$\langle\sigma_{ab}\rangle \simeq \pi\lambda\!\!\!^{-2}\,\frac{1}{D_a}\left\langle\frac{\Gamma_a\Gamma_b}{\Gamma}\right\rangle \equiv \pi\lambda\!\!\!^{-2}\,\frac{\langle\Gamma_a\rangle\langle\Gamma_b\rangle}{D_a\langle\Gamma\rangle}S_{ab}$$

with $\Gamma \equiv \sum_c \Gamma_c$. The Dresner factor S_{ab} accounts for fluctuations of the partial (neutron, radiation, fission etc.) widths and is of order one. The average total cross section is found to be

$$\langle\sigma_a\rangle = \sum_b\langle\sigma_{ab}\rangle \simeq 4\pi\lambda\!\!\!^{-2}\sin^2\phi'_a + 2\pi^2\lambda\!\!\!^{-2}\,\frac{\langle\Gamma_a\rangle}{D_a}\cos 2\phi'_a$$

$$\to 4\pi R'^2_a + 2\pi^2\lambda\!\!\!^{-2}\,\frac{\langle\Gamma_a\rangle}{D_a} \qquad \text{for} \qquad E \to 0,$$

where ϕ'_a is the hard-sphere scattering phase of resonance theory modified by distant levels, and R'_a the effective nuclear radius. Using these equations one can easily propagate errors of the average parameters to get errors of average cross sections. For averaging intervals ΔE containing very many resonances (labeled by λ) one has

$$\langle\Gamma_a\rangle \simeq \frac{1}{\Delta E}\sum_{\lambda\in\Delta E}\Gamma_{\lambda a}.$$

In this approximation one can estimate uncertainties in average widths from given uncertainties in individual resonance widths.

With these formulae one can go from uncertainties of individual resonance parameters to uncertainties of average resonance parameters to final uncertainties of average cross sections, adding systematic and statistical errors in quadrature where relevant. This works not only in the case of good statistics, with many resonances in the averaging interval, but also, at least approximately, and adequate for uncertainty estimation purposes, in case of not so many resonances. One can thus provide error files of manageable size for the resolved resonance range, containing standard errors and, via estimated common errors, correlation coefficients for cross sections averaged in broad intervals, corresponding to the ABBN or similar group structures used in reactor physics.

Although this recipe should work well for the bulk of the resolved resonances, it is clear that usually the first few resonances, especially those of key nuclides such as ^{238}U or ^{240}Pu, are so important practically that their parameter uncertainties must be given explicitly, without averaging.

For more details about uncertainty assignment, statistical and systematic errors, construction of covariance matrices and error propagation see the following reference.

F.H. Fröhner, Nucl. Sci. Eng. **126** (1997) 1-18

Session Summary (Paper C1 to C3)

A.Hasegawa(JAERI)

This session is dedicated for the application of Covariance Matrices. There are three presentations and one unregistered presentation. This session is next to the yesterday's long heated discussions about the fundamental problems of Covariance Matrices especially for the extension of the FORMAT and representation methods of data. The presentations made here are throwing light from the application side for the yesterday's discussions.

Dr. E. Fort (CEA) presented about lessons drawn from JEF-2 validation processes. He discussed on the point whether the nuclear data can be improved by adjustment on integral measurements. He showed many examples along with his experiences about the adjustments of the cross sections on the FBR core physics parameters such as Keff, spectral indices, and some reactivity coefficients important for the safety. He touched on the point of systematic errors of the integral data, which play important role for the adjustments. He insisted that systematic errors are mainly treated by the expert judgments and are not formally treated up to now. He showed his method how to reduce systematic errors by eliminating inconsistent integral data. In the example, he concluded that the current Na data like ENDF/B-VI or JENDL-3.2 are not validated by the adjustments. And also Pu-239(n,2n) data of JEF-2 were erroneously evaluated and have been corrected properly by the suggestion made by the adjustments. In the coarse of his presentation, he stressed importance of setting up of worldwide integral data database to preserve the valuable measured integral data piled up in these 30 years.

Dr. McKnight(LANL) presented a review of the application of data adjustment methodology to evaluation of reactor design quantities at ARGONNE. He presented an outline of the approach to provide a best estimate and uncertainty for the reactor applications, mainly reactor physics parameters, taken in ANL. As an example, application of critical experiment to LMR design by the formal data adjustments methods was presented. He showed uncertainties in the calculations are reduced significantly by the adjustments. He also stressed importance of worldwide integral data database for improving design qualities and as well as the importance of covariance data.

Dr. Broadhead(ORNL) presented about an application of covariance data to criticality safety data validation. He stressed the importance of covariance data especially for the estimation of criticality for the systems where no experimental data are available. He also told the development of formal range of applicability in the determination of criticality safety. This presentation was reflecting strong needs in this field.

One additional talk about application of covariance matrices on dosimetry was presented by Dr. Remec.

According to the session schedule, technical (free) discussions are combined to the discussions at the next session.

Lessons learned from the JEF2 validation
Possible perspectives

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ABSTRACT

The statistical consistent adjustment technique is used, among other applications,to realize the transfer of information from the integral data towards the nuclear data. This operation is called nuclear data validation against integral data.

This technique, based on the maximum Entropy Principle is well established but the conditions for an exact application are numerous.

These conditions are very difficult to be rigourously respected in the practical cases. They concern, in particular but not only, the generation of realistic covariance matrices. Another difficult problem, never solved so far, is the treatment of inconsistent (or incorrect) reference data.

Some solutions, used for the exhaustive JEF2 validation are described.

INTRODUCTION

Since long, the formal adjustment of nuclear data libraries on integral measurements is a controversial issue.

This was true mainly in the 70' and 80's when the activity on this item was in full development everywhere in the world. But the situation has evolved and significant improvements arose in neutronics calculational methods, in nuclear reaction modelling, in the methods to generate the covariance matrices and the knowledge of their performances, suggesting that a satisfactory solution could be in view.

For the sake of demonstration it will be referred to the conditions and the results of the extensive validation of JEF2.

The objective of a statistical adjustment is to organize the transfer of the specific information contained in the integral experiments towards the microscopic data in order to improve them.

As a matter of fact the integral data correspond to the observation of the same reaction mechanisms but in a different way that is rich in information :

- Several nuclei are present simultaneously.

- The energy of incident neutrons, instead of being monocinetic belong to a spectral distribution that can be large.

The peculiarities of the integral data, namely values averaged over a large energy spectrum and very low statistical uncertainties, are exactly complementary to the properties of the microscopic data.

GENERAL CONDITIONS

When looking at the consistency of the microscopic data and the integral measures the crucial point is the ability of the codes and algorithms to exactly calculate the neutron flux $\phi(E,\vec{r})$ in each point of bulk media characterized by complex geometries and heterogeneous compositions. This point was questioned in the past and this was probably one reason, among others, of the scepticism against the adjustment procedure as an efficient tool to transport the Physics information.

Numerous conditions have to be satisfied for a statistical adjustment to be meaningful. They can be expressed as follows :

1. The integral data are numerous, clean, of different types and representative of the different reaction mechanism over the whole energy range of interest.

2. The calculational methods in neutronics have limited biases.

3. The microscopic data treatment is such that there is no loss or distortion of information.

4. The uncertainty information is as realistic and complete as possible.

5. There is an efficient theoretical tool to perform the adjustment.

Some departure from these conditions can probably be tolerated but it is difficult to give an estimate of its amplitude.

Let's consider the example of the exhaustive validation of the JEF2.2 general purpose file, obtained by adjustment involving group cross sections.

1. CONDITION 1:COMPLETE INTEGRAL DATA BASE

This condition has to be understood as a constraint to obtain $\Phi(E,\vec{r})$ determined as accurately as possible for any integral configuration. The set of integral data has to be such that there are enough information on the competition of all the basic neutronic processes : production, absorption, slowing down and leakage over the whole energy range.

For the JEF2 validation it has been used 485 integral parameters from 78 different systems. The integral parameters were : critical masses, bucklings, spectral indices, response function data for neutron transmission, reactivity worth's.

2. CONDITION 2:CALCULATIONAL METHODS

The progresses in this field are impressive and, taking advantage of the development of the numerical technics and computer capabilities, they concern both the algorithms to calculate the integral parameter themselves and their sensitivity to the basic parameters.

In the validation there has been repeated tests, checkings, continuous validation and qualification. The well known biases of the deterministic methods due to the modelization of complex geometries are now under control thanks to comparison with the more « exact » MONTE CARLO methods which are progressively and systematically introduced.

There are a few exceptions, mainly due to algorithms problems, in this optimistic picture and they are related to particular items ; the neutron deep penetration is one example.

The sensitivity calculations were based on the Perturbation theory, S.P.T. for keff, G.P.T. for reaction rate or EGPT for reactivity variation ($\Delta\rho$).

The coefficients have been carefully and systematically checked, in particular by referring to direct calculations performed in ad hoc conditions (although sensitivities and relative variations are not formally identical).

The Perturbation theory imposes that the modifications on nuclear data are of small amplitude, which is a condition required elsewhere (see adjustment).

The shape of the sensitivity profiles are guides in deciding the most appropriate energy scheme for the adjustment procedure : the adjustment is the most efficient if the nuclear parameters have different behaviour with energy in a same macro-group. In addition, important nuclear features, like threshold or presence of important resonances, have to be taken into account. The number of macro-groups is also an important parameter which depends on the number of integral parameters to be considered in the adjustment.

Any energy scheme is a compromise and the one which has been chosen for the JEF2 validation (see table 1) presents at least 2 defects :

Table 1 : Macro-group scheme used for the JEF2 validation and justifications

Macro-group number	Upper limit	Lower limit	Comments
1	19.64 MeV	6.06 MeV	(n,xn) reactions 2nd and 3rd chance fissions
2	6.06 MeV	2.23 MeV	Fast range
3	2.23 MeV	1.35 MeV	
4	1.35 MeV	498 keV	
5	498 keV	183 keV	First resonance ^{16}O
6	183 keV	67.4 keV	Fast range
7	67.4 keV	24.8 keV	
8	24.8 keV	9.12 keV	U.R. for heavy nuclei
9	9.12 keV	2.03 keV	Resolved Range
10	2.03 keV	454 keV	Resolved Range
11	454 eV	22.6 eV	Resolved Range
12	22.6 eV	4 eV	First resonance of ^{238}U, other important resonances
13	4 eV	0.53 eV	First resonance of ^{240}Pu, ^{242}Pu
14	0.53 eV	0.1 eV	First resonance of ^{235}U, ^{239}Pu, ^{241}Pu
15	0.1 eV	0.0001 eV	Thermal range

- The group 1 should be splitted into 2 parts with a boundary at 10 MeV so as to share the information on the (n,2n) cross-section into two significant groups.

- In addition, another boundary should be introduced at 0.862 MeV in order to explicit the inelastic threshold of ^{56}Fe supposed to be the one of natural Fe.

3. CONDITION 3: MICROSCOPIC DATA TREATMENT

The necessary Q.A in data treatment should start first with the exact translation of the evaluation work into the formatted evaluated file.

The JEF2 library has been treated into a 1968 g scheme (1/120 in lethargy) using a validated version of NJOY (NJOY 89.69*) to obtain the infinite dilute group cross sections. The conditions imposed to the code give the guarantee that all group constants represent within an error of less than 0.1 %, the content of the evaluations. But even if great care has been taken one cannot exclude the probability of existence of unknown systematic errors.
As an example the option SHORTCUT 5.18 of NJOY 89 for the fission spectrum treatment adopts for the reference incident energy the value of 1 MeV while the version 91 adopts 10^{-5} eV. (In other words 2 different fission spectra have been used as a veighting function).

The change results in 125 pcm in k* of one simple UO_2 (3.5 % in U235) thermal cell[1].

4. CONDITION 4: UNCERTAINTY TREATMENT

The statistical adjustment requires uncertainty information for both integral data and microscopic parameters.

This information is crucial and has to be as realistic and complete as possible.

Although there is basically no problem on how to generate covariance matrices, their production is, by far, the most troublesome topic of today because it requires a significant amount of work and a complete source of information.

Complete covariance means that the off diagonal terms cannot be ignored since they play a significant role in the adjustment procedure as largely observed during the JEF2 validation.

4.1 COVARIANCE DATA FOR INTEGRAL « OBSERVABLES »

Most of the data used in this validation have been produced one or two decades (or more) ago when there was a poor concern about the uncertainties and their exact calculation.

Very often there is only short information about the sources of errors and in most cases an optimistic statistical error is given.

This is the reason why the published uncertainty values have been systematically reconsidered.

Systematic errors they are relevant either to experimental technique or to the calculational methods to analyse the raw data have been estimated on the basis of personal Judgment.

Full correlations ($\rho_{ij} = 1$) were admitted for all the error components relevant to calculations. For what concerns the errors related to the experimental techniques, correlations were admitted for data obtained with the same technique on the same critical. The magnitude of the correlation coefficient depends on the observable type.

For example, let's consider the category of fission spectral indices Is referring to the fission cross section of U-235. There are 2 sub-categories :

a) Spectral Indices involving fissiles nuclei : $\frac{Pu-239}{U-235}, \frac{Pu-241}{U-235}\ldots,$

b) Spectral Indices involving fertiles (or fissile with threshold) ; $\frac{U-238}{U-235}, \ldots$

Assuming average uncertainties of 1 % on counting rates and of 3 % on the isotopes masses, one can demonstrate :

- for indices belonging both to (a) the correlation is strong : ~ 0.6,
- for indices belonging one to (a), the other to (b) the correlation is weak : 0.01,
- for indices belonging both to (b) the correlation is not.

The final global covariance Matrix [I] for the integral data is

$$[I] = [E] + \sum_K [S_e]_K + \sum_\ell [S_c]_\ell \qquad (1)$$

where : $[E]$ stands for the statistical covariance matrix, constructed with the published « statistical » errors. This is a diagonal matrix.

$[S_e]_k$ is the « systematic » experimental covariance matrix for a parameter of a given type k (example : critical mass, Buckling, ...).

$[S_c]_\ell$ is the « systematic » covariance matrix associated to the calculated component for a parameter of a given type ℓ.

To note that $[S_e]_k$ and $[S_c]_\ell$ are not of same rank as $[E]$. Completion is obtained by lines and columns of 0 in adequate positions.

4.2 COVARIANCE DATA FOR MICROSCOPIC DATA

It is admitted since the talk of R.E. HODGSON and co-workers[2] on preequilibrium process in nuclear reactions at the SANTA-FE Conference (1985) that the modelling of nuclear interactions is now well mature with correct Physical basis and no practical limitation below 20 MeV. A similar improvement followed for the generation of covariance matrices which are now produced during the evaluation itself by a two steps procedure. This one is well described in the literature[3,4,5,..].

It is as follows :

A set of experimental data (critically analysed and possibly modified) is represented by a vector M. An experimental data vector δ, called in the literature « refinement » vector, is derived by a least squares fit.

$$\delta = \left(A^T C_m^{-1} A\right)\left(A^T C_m^{-1} M\right) \qquad (2)$$

with a covariance matrix :

$$C_\delta = \left(A^T C_m^{-1} A\right)^{-1} \qquad (3)$$

(A : Design matrix, C_m : Covariance matrix of experimental data).

The nuclear models are used in a second step to fit into the vector δ, again by a least squares procedure.

Let be $\hat{p}$ the a priori parameter vector of the nuclear model f and $C_{\hat{p}}$ its covariance matrix. The fit leads to a new parameter vector p.

$$p = \left(D^T C_{\hat{p}}^{-1} D\right)\left(D^T C_{\hat{p}}^{-1}\, \hat{p}\right) \qquad (4)$$

and a new covariance matrix $C_p = \left(D^T C_{\hat{p}}^{-1} D\right)^{-1}$ (5),

where D stands for the derivative matrix of f.

The covariance matrix C_f of the evaluated quantities $f_{(p)}$ is obtained by error propagation.

$$C_f = [D^T C_p D] \qquad (6).$$

For the JEF2 evaluations the covariance have been established for U-238 (covariance C_p type) and for Pu-239 (covariances C_f type). (For this last nucleus the covariances are not in the file but have been used in the adjustment).

For the other nuclei and for the purpose of the adjustment the covariance matrices have been generated from information in the literature for what concerns the thermal data[6] from evaluators specialists of the resonance range[7] and for the rest of the energy range on the basis of my personal judgment resulting from my experience as experimentalist and evaluator.

The correlations have been systematically assumed to be of medium importance (max $\rho_{ij} = 0.66$) and of medium range with a linear variation, ie, over 3 groups of the 15 group scheme described above.

Finally the covariance matrix C_f for JEF2 was obtained by :

$$C_f = [\Sigma]\,[COR]\,[\Sigma] \qquad (7)$$

In this relationship $[\Sigma]$ is the relative standard deviation matrix (diagonal) and [COR] is the correlation matrix.

It is suggested to store in the evaluated file the uncertainty information in this comprehensible form from which one gets immediately a good picture on the incident situation. This is consistent with a proposal made by F. FRÖHNER (« Format proposal for ENDF File 32 » - Sept. 94) and also with the input formats for various codes dealing with covariance matrices (DANGELO2, ...) and which are in current use.

Although I am convinced that the order of magnitude of standard deviations are perfectly realistic for each nucleus it is obvious that the covariance data for the evaluated nuclear constants may be regarded as one weak point of the JEF2 validation.

Fortunately it appears that the need for quality for the covariance matrices is less stringent concerning the parameters than concerning the observables when these ones are significantly numerous.

5. CONDITION 5: EFFICIENT THEORETICAL TOOL TO REALIZE THE INFORMATION TRANSFER

5.1 GENERAL CONDITIONS

The statistical consistent adjustment procedure is well known and in current use everywhere in the world. This satisfactory situation is the result of numerous and continuous studies starting from 1939 with the pioneering work of DUNNINGTON. But very few synthetic works are available except those by F. FRÖHNER[8] or D. SMITH[9].

As shown by F. FRÖHNER, the basis is the Maximum Entropy Principle which defines a probability density p when part of information is lacking.

The entropy principle is defined by SHANNON in the formula.

$$W = -\sum_{\nu} p_\nu \,\mathrm{Ln}\, p_\nu \qquad (1)$$

given probabilities p_ν for alternatives ν, extended by JAYNES to continuous distributions :

$$W = -\int p(x)\,\mathrm{Ln}\big(p(x)\big)\,dx \qquad (2)$$

When a part of information relative to (x) is lacking p(x) has to be chosen in such a way that W is maximised, subject to the contraints due to the available information.

For example[8], if a probability distribution is a priori described only by an average value <x> and a standard deviation Δx the Maximum Entropy Principle (M.E.P.) gives :

$$p\left(x|<x>,\Delta x\right)dx=\frac{1}{\sqrt{2(\Delta x)^2}}\exp\left[-\frac{1}{2}\left(\frac{x-<x>}{\Delta x}\right)^2\right]dx \qquad -\infty<x<+\infty$$

The extension to several quantities x_i with average values $<x_i>$ and a covariance matrix relating Δx_i to Δx_j leads to the multivariate Gaussian :

$$p\left(x|<x>,C\right)d(x)=\frac{1}{\sqrt{\det(2\pi C)^2}}\exp\left[-\frac{1}{2}(x-<x>)^T\,C^{-1}\,(x-<x>)\,d(x)\right]$$

The nuclear parameter x_μ, $\mu = 1, 2, ..., M$ are represented by a vector x.

The vector x (TRUTH) is unknown. The evaluated data define a vector ξ and a covariance C_ξ which are an a priori information on x (or a first approach to the TRUTH).

Applying M.E.P a probability distribution p(x) can be defined :

$$p\left(x|\xi,C_\xi\right)d^M(x)\simeq\exp\left[-\frac{1}{2}(x-\xi)^T\,C_\xi^{-1}\,(x-\xi)\right]d^M(x) \qquad (4)$$

(The upperscript T stands for Transpose)

The set of integral parameters (observables) y_i, $i = 1, 2, ... M$ is represented by a vector y for which there is also an a priori information represented by measured values η and associated covariance $C\eta$(althoug this possibility is not excluded).

The relationship between x and y is denoted y(x).

The likelihood to obtain the η values from the x values is given by :

$$p\left(\eta|y(x),C_\eta\right)d^I\eta\equiv\exp\left[-\frac{1}{2}(\eta-y(x))^T\,C_\eta^{-1}\,(\eta-y(x))\right]d^I\eta \qquad (5)$$

(to note this is nothing else but again M.E.P)

It is wanted to complete the a priori information on x by an information from integral experiments. The application of the BAYES rules (product of the a priori distribution times the likelihood function) leads to the following probability density distribution.

$$p\left(x \middle| C_\xi, \xi, C_\eta, y(x)\right) dM \equiv \exp -\frac{1}{2}\left[(x-\xi)^T C_\xi^{-1} (x-\xi) + (\eta - y(x))^T C_\eta^{-1} (\eta - y(x))\right] dM \quad (6)$$

This important relationship expresses the transfer of information from the integral data to the microscopic's.

The transfer is optimum when the r.h.s term is maximized, i.e when the quantity :

$$(x-\xi)^T C_\xi^{-1} (x-\xi) + (\eta - y(x))^T C_\eta^{-1} (\eta - y(x)) \text{ is minimum} \quad (7)$$

The optimum transfer defines the best estimate of the vector x (or most probable vector $\tilde{x}$), i.e the nuclear data vector improved by a transfer of information from integral data.

The quadratic form (7) which involves the parameters and the « observables » is the so called generalized KHI2 (χ^2).

Then, we have to consider the system :

$$\begin{cases} \chi^2 = (x-\xi)^T C_\xi^{-1} (x-\xi) + \left((\eta - y(x))^T C_\eta^{-1} (\eta - y(x)\right) \min & (a) \\ y(x) - y(\xi) = S\,(x-\xi) & (b) \end{cases} \quad (8)$$

S is the sensitivity matrix whose terms are the derivatives values of y(x) at values ξ of x.

The equation (8b) contains the implicit so called linearity condition which limits the amplitude of $(x-\xi)$ perturbation in order to preserve the consistency with GPT.

One has to note that the most probable vector $\tilde{x}$ solution of the system (8) is a vector of minimum variance. This is a general characteristic of the minimum KHI2 estimator, also demonstrated by WALD by introducing a « loss function » varnishing at the true value, positive elsewhere : the expected loss of information is minimized for minimum variance.

The solution of the system (8) is classically obtained by using the LAGRANGE's multipliers method.

Normally it should produce estimator values acceptable in the statistics sense.

The degree of freedom for the KH12 distribution equals the number N of observables. For large values of N (a few hundred) the KH12 distribution can reasonnably by approximated by a Gaussian.

In these conditions, if it is defined $2\alpha = 2 \times 1.35\ 10^{-3}$, the χ^2 values such :

$$N - 3\sqrt{2N} \leq \chi^2 \leq N + 3\sqrt{2N} \qquad (9)$$

have a probability $(1-2\alpha) = 0.9973$ to be correct minimum KHI2 estimators (MKE).

Actually KHI2 reduced values $\left(\frac{\chi^2}{N} = \chi_r^2\right)$ are used, so that the condition (9) writes :

$$1 - 3\sqrt{\frac{2}{N}} \leq \chi_r^2 \leq 1 + 3\sqrt{\frac{2}{N}} \qquad (9')$$

The interval $\left[-3\sqrt{\frac{2}{N}}, +3\sqrt{\frac{2}{N}}\right]$ defines the confidence interval for the estimated mean value of the reduced KH12 distribution with a probability of 99.73% .

With 483 Integral data (N=483) one obtains before adjustment ($x = \xi$) :

$$^{prior}\chi_r^2 = (\eta - y(\xi))^T\, C_\eta^{-1}\, (\eta - y(\xi)) = 20.$$

After adjustment the posterior value of KHI2 is :

$$^{post}\chi_r^2 = 7.$$

This high value is not a correct M.K.E. according to condition (9') and suggests the presence of systematic errors, in the [n - y(x)] vector rather than in $C\eta$.

5.2 - TREATMENT OF SYSTEMATIC ERRORS IN INTEGRAL DATA -

Handling systematic errors is difficult, requires sophisticated statistical techniques. Since the presence of systematic errors is revealed by high χ_r^2 values a recipe is sometimes suggested consisting of rescaling all the errors by the proper factor. This recipe is non adequate (or even dangerous) since the errors on integral and on nuclear data have different origins and have to be treated differently.

In what follows it is suggested a recipe used for the JEF2 validation as a substitute to more exact methods.

This recipe has been defined under the pressure of time, but with the willingness to respect at least the « spirit » of the statistical consistent method.

At this stage it is worthwhile to recall the objectives of an adjustment by the statistical consistent method, which is to obtain a minimized value of KHI2 obtained for a minimum variation δx of the parameter vector.

The actual question is :

Are the posterior values obtained for χ_r^2 and δx^2 optimal minima which permit the determination of the best estimate of the vector x ?

If the idea is accepted that some inconsistent data exist in the integral data base, the only possible decision (on a statistical point of view) is to « discard » them since their systematic errors are translated into irrealistic adjustments.

Consequently, the set of integral data has to be splitted into 2 subsets one with « correct » or consistent data, the other one gathering the discarded or inconsistent data.

The decision to switch on one subset or to the other one is based on a test and a criterion with a risk (to be also minimized) inherent to any statistical decision. The set of χ_r^2 and δx^2 has been used as criteria.

It is proposed the following definitions (N as underscript stands for an implicit dependence, N as a variable expresses an explicit dependence).

$\chi^2_{\mathrm{mic}_N} = (x-\xi)^T\, C_\xi^{-1}\, (x-\xi)$ for N data in the integral data base

$\chi^2_{\mathrm{mac}}(N) = (n-y(x))^T\, C_\eta^{-1}\, (n-y(x))$ for N data in the integral data base

$dx^2{}_N = (x-\xi)^T\, (x-\xi)$ the variance of x for N data in the integral data base.

One has :

$$\chi_r^2(N) = \chi^2_{\mathrm{mic}_N} + \chi^2_{\mathrm{mac}}(N).$$

By adjustment a vector x' is defined :

$$\chi^2_{mac} = \frac{1}{N}\left[(\eta - y(x'))^T \, C_\eta^{-1} \, (\eta - y(x'))\right]$$
$$= \frac{1}{N}\sum_{i=1}^{N} X_i^2 + e$$

X_i is the residual after adjustment for a given integral parameter i. The residuals are ordered by increasing values :

$$N\,\chi^2_{mac}(N) = X_1^2 + X_2^2 + \ldots + X_i^2 \ldots + X_N^2 + E$$

If χ_r^2 is outside the fixed limits (ie the probability for the present distribution of χ_r^2 is less than 1-2.7 10^{-3} to be a correct KHI2 distribution), the largest term of the previous series identifies the integral parameter to be first discarded. The adjustment procedure is repeated with N' = N-1 integral data and so on...

The Figure 1 shows the evolution of the various statistical parameters as a result of the progressive elimination of integral data.

The variance dx^2 decreases with N down to a plateau value (invariance of the variance) obtained from a No value of the number of integral data. The constancy of the variance means that only consistent data are implied in the adjustment procedure. Consequently, No corresponds to the total number of consistent data in the integral data base.

If the elimination process is pursued, useful information is progressively suppressed, less and less nuclear parameters are adjusted leading to smaller and smaller dx^2. Several plateau particular appear during the elimination process each corresponding to a particular subset of adjusted nuclear data. The size of these « concentric » subsets decreases in the same time as N.
In the present approach the best estimate $\tilde{x}$ of the vector x is obtained by making use of the maximum likelihood : it is defined a particular χ^2_{mac} related to the No integral data , $\chi^2_{mac(N_0,N_1)}$,calculated with the data resulting from the adjustment involving N_1 integral data in the N_0 set . The N_1 set is a subset of the N_0 set ($N_1 < N_0$) obtained by the « elimination » process defined just above which is stopped when $\chi^2_{mac(N_0,N_1)}$ is minimum.

$\chi^2_{mac(N_0,N_1)}$ minimum -> $\tilde{x}$.

It should be remembered that the Maximum Likelihood Estimator (M.L.E) has the following properties :

- There is no reason for it to be unique.
  (Such a feature can be observed on the figure 1).
- It is not unbiased.

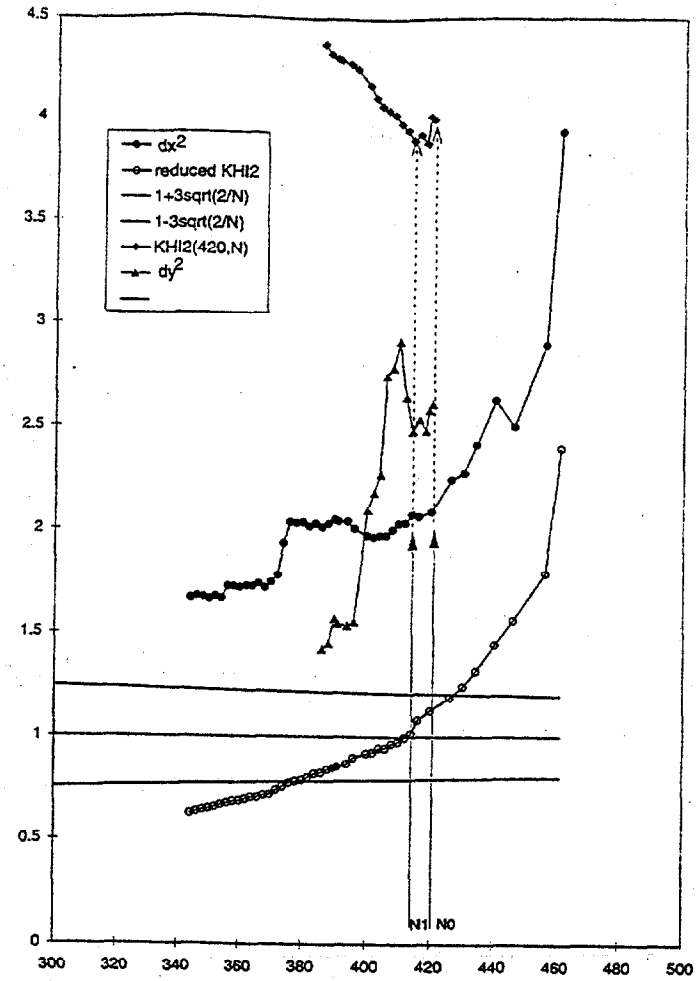

Fig. 1. Evolution of the various statistical parameters as a function of the number of the integral data ordered according to the suggested methodology.

Because of the numerous question marks related to the covariance matrices and the handling of systematic errors the final results of the adjustment have to be carefully checked. This has been done :

- Most of the « discarded » integral data have been reanalyzed by Reactor Physicists and explanations have been found. Some have been corrected and re-introduced in the adjustment procedure with successful results.

- Most of the cross section adjustments have been confirmed either by recent measurements or by recent evaluations. Some (example of the correction on $\sigma_{n,n'}$ of Fe) are still awaiting for a confirmation.

5.3 ADJUSTMENT INVOLVING NUCLEAR BASIC PARAMETERS.

Some words have to be said about the relevance of groups cross sections in an adjustment procedure.

- The adjustment, which is performed using a limited number of macro-groups, has to be unfolded in the fine scheme of the application libraries. This operation is generally done by means of procedures based on the use of cubic splines.

This way of doing, that is quick and sometimes useful, doesn't respect either the basic nature of the adjustment that is statistical or the basic physics information as it can be understood from the Figure 2. Even, it can lead to dangerous results especially when the original cross section shape is not monotonous.

- The classical group cross section adjustment is meaningless when dealing with integral data largely affected by self shielding effects. As a matter of fact the classical formalism doesn't allow taking into account properly the self shielding effect that depends on the resonance parameters which have to be adjusted.

One solution and seemingly the only one to the problem related to self shielding and group constants adjustment deconvolution is given by the adjustment of the basic parameters involved in the nuclear models.

In this case the sensitivity coefficient matrix $[^{P}S_{p}]$ of the integral parameters P to the nuclear parameters p is obtained in a way simple but time consuming.

Let be : $[^{P}S_{\sigma g}]$, the sensitivity matrix of integral parameters P to the effective group cross sections.
$[^{\sigma g}S_{p}]$, the sensitivity matrix of the effective group cross sections σg to the nuclear model parameters.

We have :

$$[^{P}S_{p}] = [^{P}S_{\sigma g}] \times [^{\sigma g}S_{p}]$$

The linearity of the dependance of the integral parameter P to the microscopic parameter p has to be seriously demonstrated and is not automatically guaranteed by the linearity occuring in the 2 independent steps.

The production of « adjusted » pointwise nuclear data libraries are not anymore hypothetic, with cross section data and covariance data produced in the format already available.

So far, this promising methodology (adjustment of nuclear parameters), to which no serious arguments can be opposed but the cost, has been applied in very few cases to the restricted area of resonance parameters[10,11,12].

But it can be generalized to any energy range and to any basic parameter type.

This implies a common reference to the same physical nuclear models which are now well mature even if some phenomenological aspects are still persistent in the description of the fission process.

The number of parameters to be considered in this type of formal adjustment will not be excessive if the resolved range is limited to the first few resonances of practical interest. The other resonances will be included in the unresolved range described by average parameters. This number could be still reduced to a very manageable size if one excludes from the list of adjustable parameters, the parameters of the optical model as a result of the high quality work performed at Bruyeres le chatel.

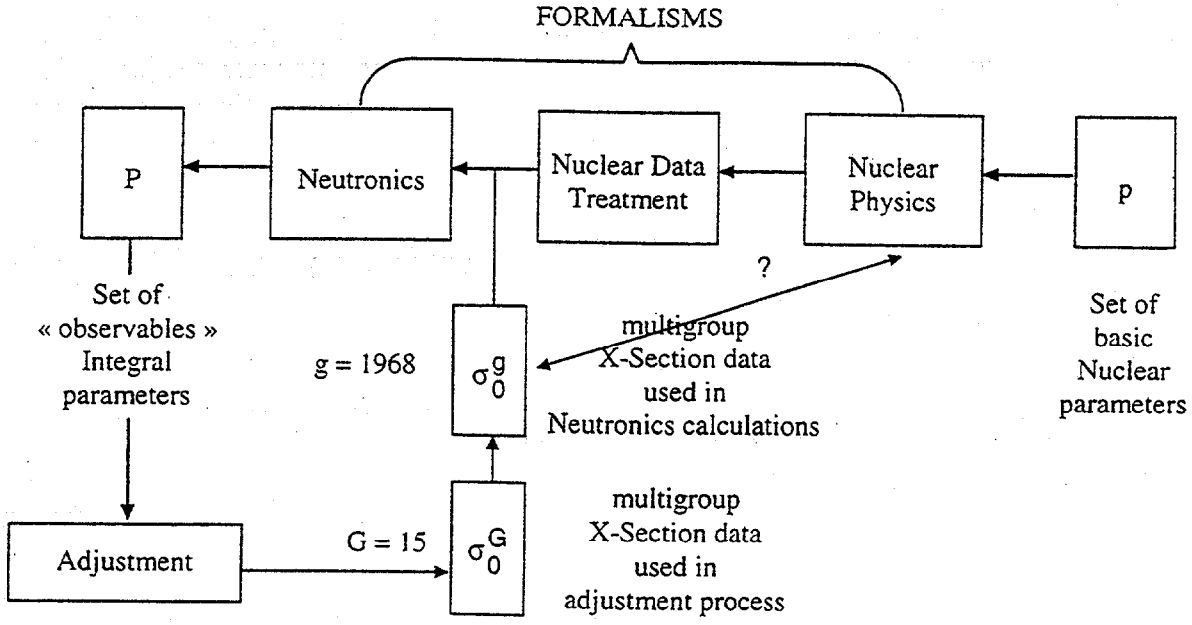

FIGURE 2

The problem of covariance data for the nuclear parameters has to be investigated with presumably no more complexity than in the present situation.

In the unresolved range there is nothing new and the present suggestion should help in the covariance size limitation (reduction of the number of resonances). One possible difficulty lies in the evaluation of the uncertainty correlations between resolved and average parameters.

One has to note that the step of group cross section generation to calculate the sensitivity coefficients is unavoidable. It is possible to use it for a composition of adjustments (adjustment of group cross sections followed by the model parameter adjustment).

But it is demonstrated[13] that, the direct adjustment of model parameters on integral data. should be the preferred route.

CONCLUSION

The exhaustive validation of the JEF 2.2 file is probably the first example of an adjustement performed with almost sufficient statistics, such that the resultant changes to the data are significant.

The corrections on the nuclear data have been confirmed by recent evaluations and/or measurements.

The feedback on the integral observables also received a clear confirmation : several integral data identified as inconsistent data by the suggested methodology have been carefully reanalyzed and all recognized as erroneous.

All these positive results support the improvements proposed for the application of the well established consistent statistical adjustment method.

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A Review of the Application of Data Adjustment Methodology to Evaluation of Reactor Design Quantities at Argonne

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Abstract

Throughout the 1980's, many organizations throughout the world developed programs to use data adjustment methodologies with integral data from critical assemblies in the reactor design process. Many of the speakers at this workshop were active participants in that effort. The present speaker, more of an observer in this area, has been asked to review some of the work performed at Argonne National Laboratory (ANL) during that period.

The fast reactor program at ANL sought the best means to employ the integral data obtained from the Zero Power Reactor (ZPR) critical assemblies in assessing and reducing the uncertainties in calculated parameters in fast reactor design. The work at ANL was the effort of many people, but lead roles were taken by P. Collins, W. Poenitz, R. Hwang, D. Wade, G. Grasseschi, among others. Their work has been published in many references, but perhaps the best source is the *Proceedings of the NEACRP Specialists' Meeting on Application of Critical Experiments and Operating Data to Core Design via Formal Methods of Cross Section Data Adjustment* (NEACRP-L-307). This meeting was held at Snow King Resort, Jackson Hole, Wyoming, on September 23-24, 1988. These proceedings contain not only several papers by the ANL participants which describe in detail their activities, they also contain many excellent papers from experts throughout the world describing their own work.

The talk presented at this workshop by R. D. McKnight was simply a summary and review of the work presented by the ANL authors at this 1988 NEACRP Specialists' Meeting. The following pages contain the visual material used in that talk. Interested readers are encouraged to review the original reference quoted above to see the full details of this work.

A REVIEW OF THE APPLICATION OF DATA ADJUSTMENT METHODOLOGY TO EVALUATION OF REACTOR DESIGN QUANTITIES AT ARGONNE

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Outline

- Introductory Comments.
- Data Adjustment Methodology at ANL.
- ANL Integral Database.
- Application of Critical Experiments to LMR Design via Formal Methods of Cross Section Data Adjustment.
- Conclusions and Caveats.

Note: All of this discussion represents a review of work done by others at ANL (Collins, Poenitz, Hwang, Wade, Grasseschi, Schaefer, Lell, ...).

"Data Adjustment"

- Evaluated cross section library gives a unique result for any parameter.
- An integral measurement provides additional information - System is over-determined.
- Determine "best" unbiased estimate of minimum variances to certain observed quantities with known errors.
- Fit is largely controlled by C/E biases of integral measurements with smallest uncertainties.

"Data Adjustment" -- Continued

- Provides a best estimate and uncertainty for any integral parameter.
- Sound theoretical basis for these estimates.
- Identifies suspect data (integral, differential, measured, and calculated).
- Provides estimates of parameters not directly measured.
- Quantitative indication of relevance of measurement in one system relative to a measurement in another.

Data Adjustment Methodology at ANL

- In Generalized Least Square Form:

$$\delta = C_p S^T W^{-1} M$$

$$C_p' = C_p - C_p S^T W^{-1} S C_p$$

$$W = S C_p S^T + C_I$$

where δ = adjustment vector to an apriori parameter vector.

- This procedure is used to utilize integral experimental data (as done by Gandini, Salvatores, Rowlands, Mitani, Kuroi, Dragt, Marable, Weisbin, Usachev, …).

ANL Integral Database

- Large Integral Database Established.
  - ~300 integral values
  - Hard (Godiva, Jezebel) to soft (Zebra-8A) spectra
  - 6 kg (Flattop-Pu) to 3700 kg (ZPPR-18) fissile loading
  - 5% to 95% fissile enrichment
- Data from Various Sources.
  - Measurements using different techniques and from different experimental facilities
  - Randomizing systematic uncertainties/biases
  - Clean Physics Benchmarks to EMC Assemblies
  - Typical LMR compositions to Diagnostic Cores

ANL Integral Database -- Continued

- Various Data Types.
  - K_{eff} (enrichment)
  - Reaction Rate Ratios (breeding ratio, burnup swing)
  - Spatial Reaction Rates (power distribution)
  - Control Rod Worths (safety)
  - Na Void Reactivity (safety)
  - Flux Ratios (Doppler)

    (versus the conventional k_{eff} and RRR's)
- C/E values ≠ 1 as well as C/E values = 1.

Application of Critical Experiments to LMR Design via Formal Methods of Data Adjustment

K-eff -- Calculated and Fitted Data					
Assembly	C/E-1,%	σ[C],%	A/E-1,%	σ[A],%	σ[E],%
Godiva	-0.3	1.6	0.1	0.13	0.1
Flattop-25	0.4	1.2	-0.1	0.11	0.1
Big-10	1.6	2.0	0.1	0.15	0.2
ZPR-U9	1.4	2.2	0.2	0.12	0.2
Scherzo	0.9	3.4	-0.1	0.21	0.4
Zebra-8H	0.3	3.1	-0.5	0.19	0.4
ZPPR-15D	-0.1	1.1	0.0	0.16	0.2
ZPR-6/6A	-1.2	1.2	-0.1	0.16	0.2
Jezebel	-0.2	1.8	-0.1	0.18	0.2
Jezebel-Pu	-0.8	1.6	-0.5	0.18	0.2
Flattop-Pu	0.7	1.6	0.4	0.14	0.2
ZPPR-12V	0.1	1.4	0.0	0.14	0.3
ZPPR-12	-0.1	1.4	-0.1	0.12	0.3
ZPPR-15B	-0.5	1.7	0.1	0.14	0.3
ZPPR-15A	-0.5	1.6	0.2	0.14	0.3
ZPR-3/56B	-1.0	1.5	-0.5	0.16	0.3
Zebra-8B	1.0	3.2	0.7	0.15	0.4
Zebra-8E	-1.6	2.7	-0.7	0.21	0.4
Zebra-8D	0.1	2.6	0.7	0.19	0.5
Zebra-8C	-2.2	1.9	-0.4	0.27	0.5
ZPR-6/7	-0/8	1.6	-0.1	0.13	0.2
ZPPR-13C	-0.7	1.6	-0.1	0.12	0.3
Zebra-8A	-1.4	2.0	-0.9	0.33	0.7
Zebra-8F	-0.3	1.9	0.4	0.33	0.5

Application of Critical Experiments to LMR Design via Formal Methods of Data Adjustment

ZPPR-15D Data-- Fitted and Predicted							
Quantity	C/E-1,%	σ[C],%	A/E-1,%	σ[A],%	σ[E],%	P/E-1,%	σ[P],%
K_{eff}	-0.7	1.1	-0.1	0.16	0.3	-0.2	0.19
F28/F49	0.2	5.1	-2.0	1.06	2.3	-2.3	1.18
F25/F49	0.9	2.3	0.6	0.44	1.6	0.5	0.45
C28/F49	5.9	3.0	1.8	0.58	1.8	2.0	0.62
Radial F28	-2.7	1.5	-1.2	0.49	2.0	-1.2	0.56
Radial F25	-0.6	1.0	1.1	0.31	1.7	1.2	0.38
Radial F49	0.2	1.0	1.8	0.31	2.3	1.9	0.35
Radial C28	1.3	0.9	2.3	0.34	1.5	2.4	0.38
SSW B10	-9.8	3.2	0.2	1.17	5.8	0.2	1.34
SSW U5	1.2	1.7	2.4	0.63	5.8	2.6	0.66
SSW U8	-1.5	4.5	0.1	0.91	6.2	0.4	1.00
SSW Pu9	2.1	2.9	2.6	0.98	5.8	3.1	1.03
Na Void	48.1	14.6	0.5	2.27	6.0	2.5	6.74
CR Worth	-11.3	2.0	-3.6	0.84	5.9	-3.8	0.89

Typical Improvements in Calculated Parameters Achieved via GLS Fitting

• Critical Mass	factor of 10
• Reaction Rate Ratios	factor of 3
• Reaction Rate Distributions	within $\sigma(E)$
• Small Sample Worths	factor of 2-4

Note: Uncertainties in calculations are reduced. This is achieved by the correlations of the cross sections as permitted by their covariances.

Conclusions and Caveats

- The worldwide database of integral data represents a valuable resource for improving calculated design quantities.
- Prior work at ANL (and elsewhere) has demonstrated the advantages of applying GLS methods with integral data (and its covariances) and differential data (and its covariances).
- A large and diverse set of integral data is necessary.

Conclusions and Caveats -- Continued

- Systematic errors (that is, errors which affect all measurements/calculations of a certain type in the same way) are very important.
- Improvements in predictions depend on the extent to which uncertainties in the integral data and the calculational methods are understood and accounted for.
- Improvement is needed in all of the covariance data (viz., for the nuclear data, the integral experiments, and the calculational methods).

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Application of Covariance Data to Criticality Safety Data Validation

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Application of Covariance Data to Criticality Safety Data Validation

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Abstract

The use of cross-section covariance data has long been a key part of traditional sensitivity and uncertainty analyses (S/U). This paper presents the application of S/U methodologies to the data validation tasks of a criticality safety computational study. The S/U methods presented are designed to provide a formal means of establishing the area (or range) of applicability for criticality safety data validation studies. The goal of this work is to develop parameters that can be used to formally determine the "similarity" of a benchmark experiment (or a set of benchmark experiments individually) and the application area that is to be validated. These parameters are termed D parameters, which represent the differences by energy group of S/U-generated sensitivity profiles, and c_k parameters, which are the correlation coefficients, each of which gives information relative to the similarity between pairs of selected systems. The application of a Generalized Linear Least-Squares Methodology (GLLSM) tool to criticality safety validation tasks is also described in this paper. These methods and guidelines are also applied to a sample validation for uranium systems with enrichments greater than 5 wt %.

1. INTRODUCTION

Traditional approaches to the validation of criticality safety calculations use a statistical approach where the calculated values of the system multiplication factor, k_{eff}, for a series of "benchmark" critical experiments are trended against a physical system parameter, such as the moderator-to-fissile material ratio, the fissile material concentration, etc. Observed trends in these systems are then used to estimate a bias for a given application system. The underlying assumptions in these types of analyses are that the critical experiments are "similar" to the given application area, and, therefore, the resulting bias predictions are valid for the application area.

The validation requirements concerning criticality safety in the United States are described in ANSI/ANS-8.1-1998, which defines these area(s) of applicability. However, the establishment of these areas are vague in that no guidance is given with respect to determining what constitutes a valid range, or under what conditions the range is breached. The current work seeks first to provide a formal means of quantifying similarity between systems, and to further develop methods that can be used to validate systems that are outside the traditional areas of applicability (i.e., validate systems in which there are no known measurements of similar systems available).

A useful tool in establishing similarities between systems is the use of sensitivity coefficients. In this application, the full-sensitivity profiles are generated in the selected problem neutron-energy-group structure for each material and reaction type (i.e., ^{235}U fission, scatter, $\bar{\nu}$, χ, capture, etc.). In a criticality safety validation study, typically some 30–50 critical benchmarks are used. Sensitivity profiles give a great deal of information about the particular system; however, the amount of information is too large to be of general use (20 profiles for each system, with about 40

values each, i.e., one for each energy group). Therefore, a method of obtaining the differences between the sensitivity profiles for pairs of systems was devised to reduce the amount of needed information to only a few parameters, while maintaining the uniqueness of the information present in the full-sensitivity profiles. The most promising set of parameters are a family of "D" values as defined below:

$$D_n = \sum_{i=1}^{g} |S_{nai} - S_{nei}| \qquad D_c = \sum_{i=1}^{g} |S_{cai} - S_{cei}| \qquad D_s = \sum_{i=1}^{g} |S_{sai} - S_{sei}| ,$$

where S is the sensitivity of k_{eff} for the safety application, a, or experimental configuration, e, to $\bar{\nu}$, or to the capture, or scattering cross sections (n, c, or s, respectively) for group i. These coefficients are useful in making a quick determination of the similarity between pairs of systems.

An alternative approach to exploring the similarity of systems is to use uncertainty analyses. This procedure involves the propagation of estimated cross-section uncertainty information to the calculated k_{eff} value of a given system via the sensitivity coefficients. Mathematically, this is accomplished by a quadratic product of the sensitivity profile vectors for each system, material, and reaction type with the cross-section uncertainty matrices by material and reaction type. The result of this procedure is not only an estimate of the uncertainty in the system, k_{eff}, for a *given* system, but also an estimate of the correlated uncertainty *between* systems. This parameter, denoted as c_k, has not only the desirability of a single quantity relating the two systems, but the similarity of the systems is measured in terms of uncertainty, not just sensitivity.

A final approach to the traditional trending analysis for determination of biases is the use of the Generalized Linear Least-Squares Methodology (GLLSM). Physically, the GLLSM is designed to "force agreement" between the measured and calculated values of k_{eff} for the entire set of criticals used in the data validation process. The inputs needed for such an analysis are almost identical to the concepts presented thus far; the sensitivity coefficients, the cross-section uncertainties, the actual calculated and measured k_{eff} values, with the addition of an estimate of the uncertainty in the measured k_{eff} values. Mathematically, the GLLSM represents a combination of measurements. These measurements include the experimental values of k_{eff} for each critical benchmark and the calculated value of k_{eff} obtained via functional analysis of the cross-section measurements. The "data changes" that result from the application of the GLLSM can then be used to predict the biases for *any* similar application where the area of application corresponds to an interpolation or extrapolation scenario.

This paper describes an illustrative application of both the S/U and GLLSM procedures to the validation of criticality safety studies for facilities processing commercial reactor fuels with uranium enrichments greater than 5 wt %. In the past, these processing facilities have been limited to enrichments at or below 5 wt %. Hence, much of the critical experiment data correspond to these lower enrichments. The use of S/U and GLLSM methods in validation studies was demonstrated by performing a validation of a hypothetical set of application scenarios, which consist of 14 systems, each having $U(11)O_2$ fuel with H/X values varying from 0 to 1000. The 11-wt % enrichment was chosen so that critical systems that exist over the entire range of moderations, including dry, could be studied. The data validation included both the traditional trending analyses, trending analysis with the D and c_k parameters, and finally the full GLLSM approach. Advantages and disadvantages of each approach were explored, and guidance for the general use of these techniques was developed.

2. SENSITIVITY COEFFICIENT METHODS

The techniques used in this work to generate sensitivity information for the various critical benchmarks is based on the widely used perturbation theory approach.[1-4] The full derivation of the general procedure will not be given here; however, for the specific theory and code development for the generation of k_{eff} sensitivities, the reader is referred to the accompanying paper.[5]

The k_{eff} sensitivity, as described above, has been implemented by modifying a version of the FORSS[6] (Fantastic Oak Ridge Sensitivity System) package. The FORSS system was developed in the late 1970s, primarily for use in the development of fast reactor systems. This project has reactivated the individual FORSS modules, with the goal of putting portions of the original system into the SCALE[7] system. A one-dimensional (1-D) sensitivity sequence, SEN1,[8] was produced for use in this project and for subsequent general use. The capacity to generate 2-D sensitivities is also available via the SEN2 module. More complete information on SEN1 and SEN2, the progress to date on 3-D Monte Carlo methods, and some results of using the SEN1 and SEN2 capabilities are the subject of a companion paper.[5]

3. UNCERTAINTY ANALYSIS THEORY

The determination of uncertainties in the calculated values of the system multiplication factor is accomplished by two steps: the estimation/processing of uncertainties in the underlying cross-section data and the propagation of those uncertainties to the system k_{eff} value. The techniques for processing cross-section uncertainty data are well-known,[9,10] and will not be discussed here.

Once cross-section uncertainty information for all materials and reaction processes that are important to the systems of concern are available, it is then possible to estimate the uncertainty in the system multiplication factor due to these data uncertainties. If we denote the matrices of uncertainty information for all of the cross sections as $C_{\alpha\alpha}$ and the sensitivity matrices relating changes in each constituent material and process to the system k_{eff} as S_k, the uncertainty matrix for the system k_{eff} values, C_{kk} is given as:

$$C_{kk} = S_k \, C_{\alpha\alpha} \, S_k^T .$$

The S_k matrix is I × N, where I is the number of critical systems being considered, and N is the number of nuclear data parameters in the problem. Typically, N is the number of material/reaction processes times the number of energy groups. The $C_{\alpha\alpha}$ matrix is an N × N matrix, with the resulting C_{kk} matrix I × I. The C_{kk} matrix consists of variance values for each of the critical systems under consideration (the diagonal elements), as well as the "covariance" between systems (the off-diagonal elements). These off-diagonal elements represent the shared or common variance, hence the term covariance, between the various systems. For presentation, these off-diagonal elements are typically divided by the square root of the corresponding diagonal elements (i.e., the respective standard deviations) to generate a correlation coefficient matrix.

These c_k values are felt to be most appropriate for correlation with error trends in a criticality safety validation analysis because they are essentially the sensitivities to the individual cross sections weighted by their uncertainties. Thus, the c_k values represent the systems similarity with respect to materials with the highest sensitivity/uncertainty combination.

4. GENERALIZED LINEAR-LEAST-SQUARES METHODOLOGY

The final procedure utilized in this work is based on the generalized linear-least-squares method (GLLSM) introduced by Gandini,[11] Dragt et al.,[12] and Barhen, Wagschal, and Yeivin.[13,14] The GLLSM has been referred to as a data adjustment procedure, a data consistency analysis, and even a data evaluation technique. The most appropriate description of this particular application would be a generalized trending analysis tool. Physically, the GLLSM is designed to force agreement between the measured and calculated values of k_{eff} for the entire set of criticals used in the data validation process. The resulting "data changes" that result from the application of the GLLSM can then be used to predict the biases for *any* similar application where the area of application corresponds to an interpolation or extrapolation scenario.

The derivation of the GLLSM equations in this work follows the general notation from Ref. 15. The vector $m \equiv (m_i)$, $i = 1, 2, \ldots I$ represents a series of k_{eff} measurements on critical benchmark experiments that are to be used in the validation of a dataset for criticality safety computations. This vector m has a corresponding symmetric $I \times I$ uncertainty matrix associated with it which we denote as $C_{mm} \equiv \mathrm{cov}(m_i,m_j) \equiv \langle \delta m_i \delta m_j \rangle$. Further, we denote the vector $k \equiv (k_i)$ as the corresponding series of calculated values of k_{eff} for each of these experiments. The vector $\alpha \equiv (\alpha_n)$, $n = 1, 2, \ldots N$, with its corresponding symmetric $N \times N$ uncertainty matrix $C_{\alpha\alpha} \equiv \mathrm{cov}(\alpha_n\alpha_m) \equiv \langle \delta\alpha_n \delta\alpha_m \rangle$, represents the differential data used in the calculations (i.e., nuclear data, such as fission, capture, and scattering cross sections, the fission spectrum and neutrons per fission quantities) and, additionally, the material densities used in the problem description. This procedure also allows for the possibility of correlations between the integral and differential quantities, which may be present at times in the analysis. These correlations are denoted by the $N \times I$ covariance matrix $C_{\alpha m} \equiv \langle \delta\alpha_n \delta m_i \rangle$.

The sensitivities of the calculated k_{eff} to the α parameters are given as $S_k \equiv \partial k_i / \partial \alpha_n$, with S_k being an $I \times N$ matrix. Representing perturbation of the α parameters as linear changes in the calculated k_{eff} value, yields the following:

$$k(\alpha') = k(\alpha + \delta\alpha) = k(\alpha) + \delta k \simeq k(\alpha) + S_k \delta\alpha, \tag{1}$$

with the corresponding uncertainty matrix of the calculated values of

$$C_{kk} \equiv \langle \delta k_i \delta k_j \rangle = S_k \langle \delta\alpha_n \delta\alpha_m \rangle S_k^T = S_k \, C_{\alpha\alpha} \, S_k^T. \tag{2}$$

If we denote the deviations of the measured responses from their corresponding calculated values by the vector $d \equiv (d_i) = k(\alpha) - m$, then the uncertainty matrix for the deviation vector d, denoted by C_{dd}, is the following:

$$\begin{aligned} C_{dd} &= C_{kk} + C_{mm} - S_k \, C_{\alpha m} - C_{m\alpha} \, S_k^T, \\ &= S_k \, C_{\alpha\alpha} \, S_k^T + C_{mm} - S_k \, C_{\alpha m} - C_{m\alpha} \, S_k^T. \end{aligned} \tag{3}$$

Denoting $x = \alpha' - \alpha$, and $y = m' - m = k(\alpha') - m$, we can rewrite Eq. (1) as

$$y = d + S_k x. \tag{4}$$

The measured k_{eff} values m_i and the measured (or evaluated from measurements) parameter values α_n both have their corresponding uncertainties. The best evaluated parameters α_n' and the best evaluated k_{eff} values m_i' will be those values that are consistent with each other, namely $m_i' = k_i(\alpha'_n)$, and are consistent with their estimated values and uncertainties (i.e., they do not deviate too much from their current best estimates m_i and α_n, respectively).

The GLLSM procedure involves minimizing the quadratic loss function

$$Q(x,y) = (y,x)^T \begin{pmatrix} C_{mm} & C_{m\alpha} \\ C_{\alpha m} & C_{\alpha\alpha} \end{pmatrix}^{-1} (y,x), \tag{5}$$

where $(y,x)^T \equiv (y_1, y_2, ..., y_I, x_1, x_2, ..., x_N)$, subject to the constraint expressed by Eq. (4). Adopting the procedure of Refs. 14–16, the above conditional minimum formulation is equivalent to unconditionally minimizing the function R(x,y), where

$$R(x,y) = Q(x,y) + 2\lambda^T(S_k x - y), \tag{6}$$

and 2λ is an I-dimensional vector of Lagrange multipliers. Thus x and y satisfy the equations

$$\partial R(x,y)/\partial x = \partial R(x,y)/\partial y = 0. \tag{7}$$

Solving the resulting equations for x and y, we obtain

$$\alpha' = \alpha + (C_{\alpha m} - C_{\alpha\alpha} S_k^T) C_{dd}^{-1} d, \text{ and}$$

$$m' = m + (C_{mm} - C_{m\alpha} S_k^T) C_{dd}^{-1} d, \tag{8}$$

where C_{dd}^{-1} is obtained by taking the inverse of Eq. (3) and is a matrix of dimension I × I.

This could of course suggest that any criticality application that is similar to the benchmarks used should be calculated using the modified cross sections and thus have a reduced uncertainty. However, even if we want to stick to "conventional" criticality estimates using "established" cross sections and trend curves, the GLLSM approach can be beneficial, as will be demonstrated in the next section.

In summary, the GLLSM procedure, as applied to the validation of cross-section libraries for criticality safety applications, is designed to predict the data changes, x, such that the differences between measured and calculated k_{eff} values (i.e., the quantity, y) is minimized. These original k_{eff} differences give rise to the trends observed in the trending analyses. Removal of these trends and identification of the data responsible for them is the key to the application of GLLSM techniques to criticality safety data validation.

4.1 APPLICATION OF GLLSM TO DATA VALIDATION

The solution of Eq. (8) allows us to evaluate the x and y quantities in Eq. (4). Of particular interest is the quantity d which has been defined as (k - m). This quantity is the calculated-versus-measured discrepancy in k_{eff} as determined from the as-specified experimental benchmark description and given cross sections. Rarely do the actual criticality safety scenarios match exactly with one of the experimental benchmarks. Thus, the actual quantity of interest is an estimate of the quantity d for the criticality safety scenario of interest, denoted the "application."

The systematic application of GLLSM to criticality scenarios described above amounts to a formal procedure for evaluation of the quantity d for the applications of interest. Since the application is assumed to be similar but *not* exactly like one of the experimental benchmarks, the key to the procedure is that we can rewrite Eq. (4) for the application as:

$$k_a(\alpha') - m_a' = [k_a(\alpha) - m_a'] + S_a(\alpha' - \alpha) , \tag{9}$$

where S_a are the calculated sensitivities for the application. The GLLSM theory predicts that if a sufficient number of experiments are similar to the application of interest, the calculated value of k_{eff} using the "best" cross sections, α', will indeed approach the value m_a', and thus, Eq. (9) yields the predicted value of the application bias $d_a = k_a(\alpha) - m_a'$, which is obtained when using the given cross sections α as

$$d_a \simeq -S_a(\alpha' - \alpha) , \tag{10}$$

where $\alpha' - \alpha$ was obtained in Eq. (8) using similar benchmark criticality measurements.

5. APPLICATION OF METHODOLOGY TO ENRICHMENTS ABOVE 5 WT %

This current report presents an illustrative application of both the S/U and GLLSM procedures to an area of current interest. The application being studied in this report is the validation of criticality safety studies for facilities processing uranium fuels with enrichments greater than 5 wt %. In the past, these processing facilities have been limited to enrichments at or below 5 wt %. Hence, much of the critical experiment data correspond to these lower enrichments. As a part of this study, a number of critical experiments in the 5–20-wt % range performed in Russia were identified. A number of these experiments were obtained and documented as a result of this work.[16]

As with any criticality data validation, the goal is to estimate the bias trends for ranges over which criticality safety calculational studies are to be performed. The use of S/U and GLLSM methods in validation studies was demonstrated by performing a validation of a hypothetical set of application scenarios, which consists of 14 systems, each having $U(11)O_2$ fuel with H/X values varying from 0 to 1000. The validation effort included both the traditional trending analyses, trending analysis with the D and c_k parameters, and finally the full GLLSM approach. Advantages and disadvantages of each approach were explored, and guidance for general use of these techniques was developed.

5.1 TRADITIONAL TRENDING ANALYSIS

In order to clearly show the relationship between the GLLSM techniques and the more traditional techniques for criticality safety validation, a traditional trending analysis using a validation set of 68 benchmark experiments[17] is presented. In Fig. 1, k_{eff} is trended versus the energy of average lethargy causing fission (EALF). The prediction from this analysis would be a nearly constant positive bias of about 0.3%. The standard deviations on these bias trends would vary from about 1% for low energies to about 2% at high energies. Trend plots were also generated for H/X and enrichment parameters. The H/X trend plot shows a slight trend, with the predicted Δk bias near zero for high H/X values and about + 0.005 for low H/X values. The trend with enrichment is similar, but not enough data are present for the intermediate enrichments to confirm the trend.

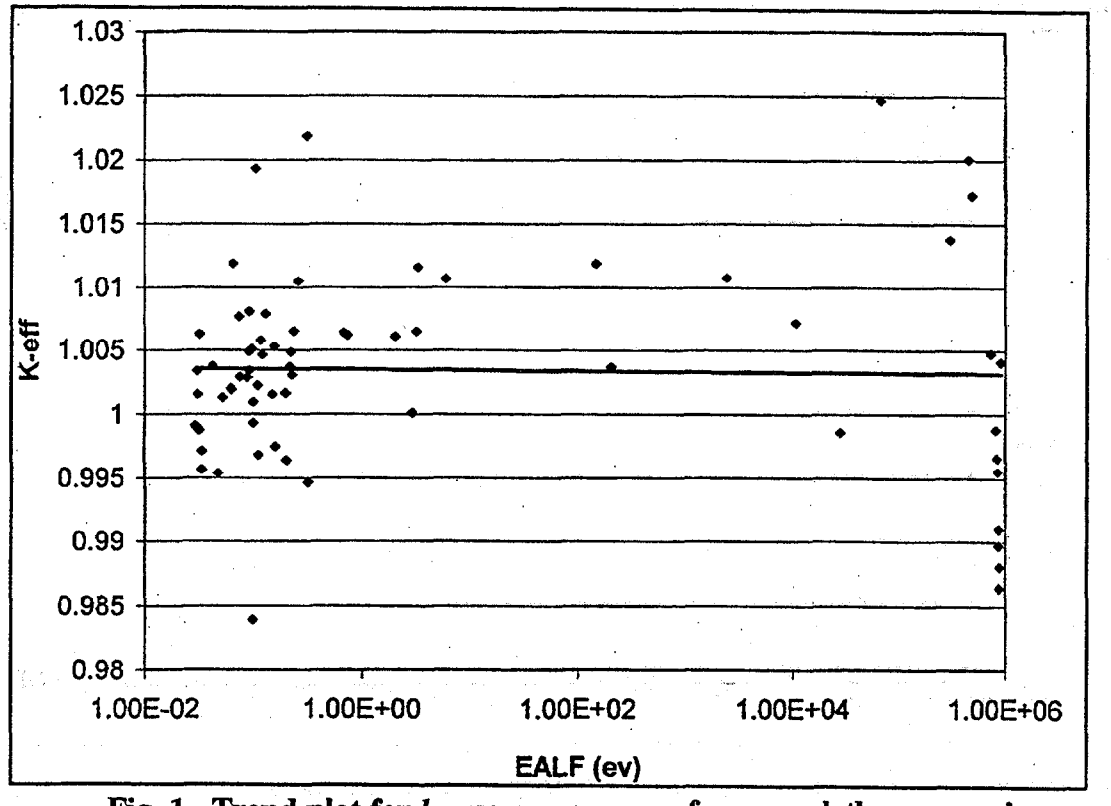

Fig. 1. Trend plot for k_{eff}-versus-energy of average lethargy causing fission (EALF).

It was noted that the largest variations (± 2%) about the trend lines were seen for fast systems (i.e., the right-hand portion of the EALF trend plot and the lower portion of the H/X trend plot). Upon examination, it was observed for H/X = 0 systems that the predicted k_{eff} values less than unity were from the HEUMET set of criticals, while the systems with predicted eigenvalues greater than unity were from the Big-10 and ZPR sets. The effects of the high-versus-low enrichments are believed to be responsible for this variation; however, no definite cause has been identified.

As a result of the trending analysis, a prediction of the Δk bias and its uncertainty can be obtained for each of the $U(11)O_2$ systems. Predictions using the USLSTATS[18] procedure for $U(11)O_2$ systems with H/X values of 0, 3, 40, and 500 are given in Table 1.

Table 1. Comparison of predicted Δk bias and its standard deviation[a] for various procedures

	H/X = 0 System		H/X = 3 System		H/X = 40 System		H/X = 500 System	
Procedure	Bias (%)	Std. dev. in biased k_{eff} (%)	Bias (%)	Std. dev. in biased k_{eff} (%)	Bias (%)	Std. dev. in biased k_{eff} (%)	Bias (%)	Std. dev. in biased k_{eff} (%)
EALF	0.32	0.74	0.45	0.74	0.46	0.74	0.46	0.74
H/X	0.49	0.77	0.49	0.77	0.47	0.77	0.31	0.77
D_{sum}	-	-	1.26	0.76	0.66	0.78	0.28	0.78
c_k	1.28	0.73	1.40	0.69	0.69	0.76	0.39	0.78
GLLSM	2.56	0.38	1.30	0.33	0.77	0.40	0.63	0.37

[a]For all but GLLSM, the standard deviations correspond to the "pooled standard deviation" as specified in Ref. 18 because this definition was judged to best match that provided by GLLSM.

5.2 TRENDING ANALYSIS USING D VALUES

This section will discuss trending analyses using the same set of 68 benchmarks as the traditional analyses shown above; however, the trending parameters are now the D coefficients, described earlier. Even though it is possible to perform the trending on each of the D coefficients independently, it was decided to trend k_{eff} versus the sum of these coefficients (i.e., $D_{sum} = D_c + D_n + D_s$). This method reduces the number of trends plots to be examined.

The trend plot of k_{eff} versus D_{sum} is given in Fig. 2 for the $U(11)O_2$ H/X = 3 system. These plots are analyzed in quite a different method from the traditional approach. A D_{sum} value of zero corresponds to the $U(11)O_2$ H/X = 3 system. The trend line must therefore be extrapolated to zero in order to estimate the Δk bias. A D_{sum} value of 1.2 or less has been shown to indicate similar systems.[17] Therefore, the slope of the trend line is important, as well as how many systems are in the region of D_{sum} less than 1.2. From this plot it is clear that perhaps only one other system could be considered similar to the $U(11)O_2$ H/X = 3 system (i.e., D_{sum} less than 1.2). Hence, the predicted bias will have a large degree of uncertainty associated with it. The trend plot for the $U(11)O_2$ H/X = 40 system was also generated. Here the coverage near a D_{sum} value of zero is much better than that shown in Fig. 2. In this case, there are at least 8 systems with D_{sum} values of 1.2 or less. The trend plot for the last system (i.e., $U(11)O_2$ H/X = 500) gives conclusions that are very similar to those for the H/X = 40 example. There are a large number of systems within a D_{sum} value of 1.2, with a resulting good prediction of the Δk bias for this system.

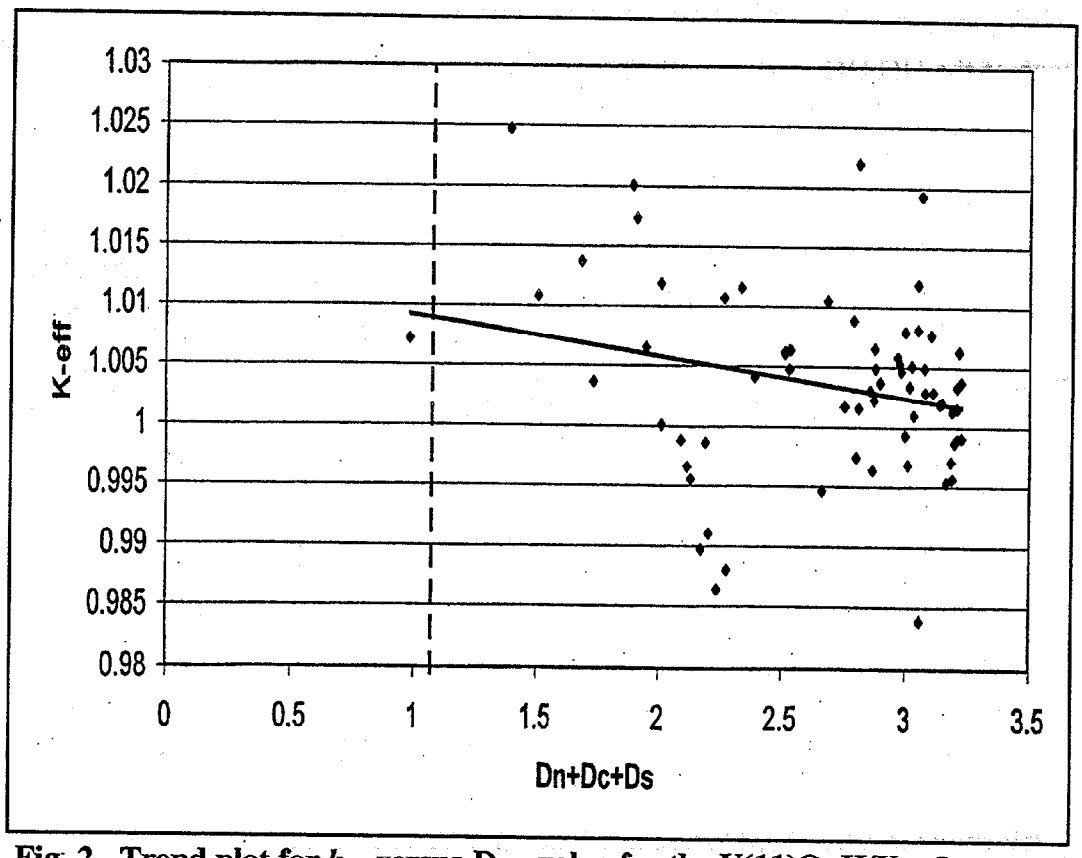

Fig. 2. Trend plot for k_{eff}-versus-D_{sum} value for the $U(11)O_2$ H/X = 3 system.

These trending analysis results are generated using the same software that was used in the traditional trending approach previously [see Ref. 18]. Therefore, the estimates of the Δk bias and its uncertainty are available for these analyses. These bias predictions and their uncertainties are given in Table 1.

5.3 TRENDING ANALYSIS USING C_K VALUES

The trending analyses using the c_k values follows very closely to the analyses using the D coefficients discussed in the previous section. Here the trend curves are interpreted as an extrapolation to a c_k value of unity, which corresponds to the particular application system of interest. A determination of system similarity is a c_k value of 0.8 or higher.[17] The slope of the trend curve is again important; however, the items of primary importance are the number of systems with a c_k value greater than 0.8 and the value of the predicted Δk bias at a c_k value of unity.

The k_{eff} trend plot for c_k of a $U(11)O_2$ H/X = 0 system is shown in Fig. 3. This trend plot is interesting when compared with the traditional trend plot shown in Fig. 1. The four data points in the upper-right-hand portion of both plots correspond to the same four systems (three ZPR and Big-10 systems). In Fig. 1, the predicted Δk bias is about 0.4% because the overprediction of k_{eff} for these four systems is counteracted by the underprediction of the HEUMET systems which all have very similar values of EALF. However, the trend seen for k_{eff} in Fig. 3 is caused by the lack of similarity between the $U(11)O_2$ H/X = 0 and HEUMET systems. These HEUMET systems can be seen in Fig. 3 with a c_k value of about 0.5–0.6, indicating only minor correlations with the $U(11)O_2$

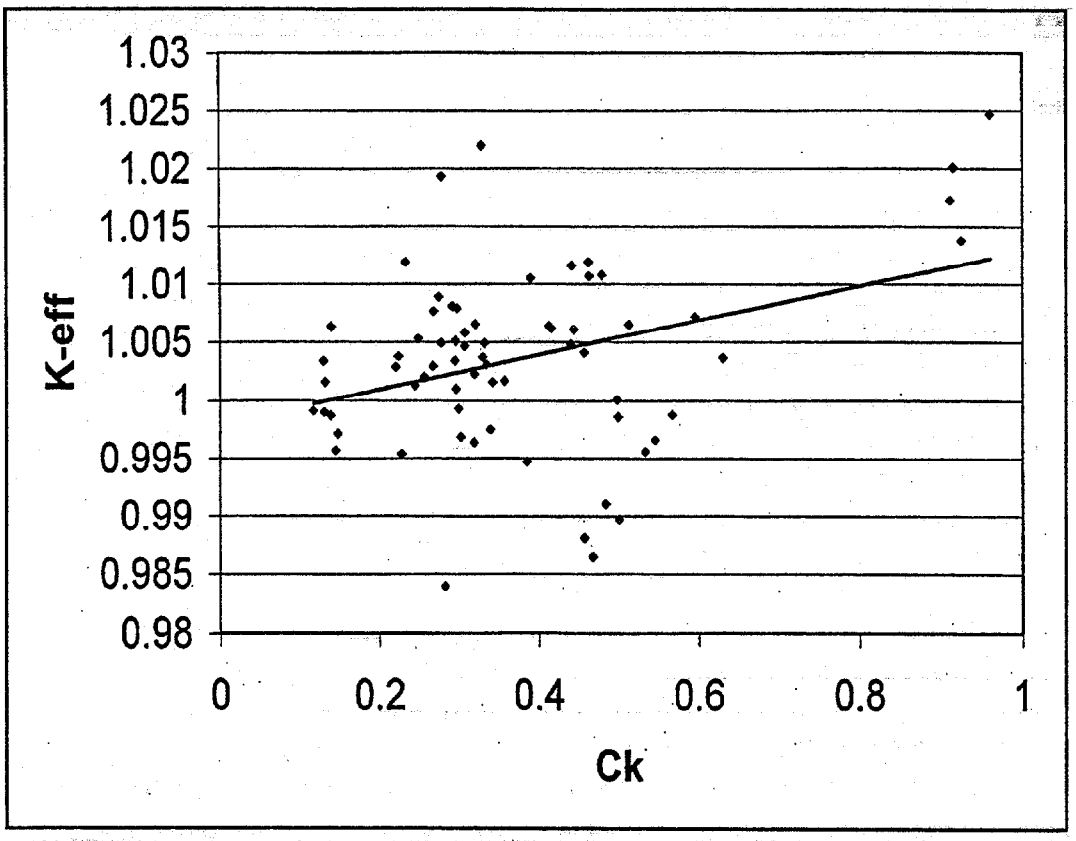

Fig. 3. Trend plot for k_{eff}-versus-c_k value for the U(11)O_2 H/X = 0 system.

H/X = 0 system. This example shows the potential improvement from the use of a trending analysis with these new parameters, since trends can be observed as a function of systems that are expressly determined to be similar. It is clear from the preceding analyses that sometimes the traditional parameters indicate that systems should be similar, but are not. In this particular case, the predicted bias is much larger than that predicted by the standard techniques.

The trend plots for the remaining U(11)O_2 systems with H/X values of 3, 40, and 500 were also studied using c_k values. For the systems with H/X values of 3 and 40, the predicted biases are higher than those predicted by the standard techniques. The specific reasons for these differences were not explored in depth as with the H/X of 0 cases, but are believed to be caused by the separation of effects that tended to cancel each other in the traditional approach. The Δk bias predicted for the H/X = 500 system are in line with those of the standard techniques since a large number of experiments are considered to be similar, and no cancellation of effects is seen.

These trending analysis results are generated using the same software that was used previously. Estimates of the Δk bias and its uncertainty from this trending approach are given in Table 1.

6. SUMMARY

In the preceding sections, results from a number of approaches to criticality safety data validation were presented. The GLLSM results shown in Table 1 were taken directly from Ref. 17. Quite interestingly, they give very different answers for the low-H/X problems chosen for study. The primary reason for these differences seems to be the inclusion of systems that may "look" very similar from the standpoint of certain parameters, but are in fact very different with respect to other parameters. In particular, according to both the H/X and EALF parameters, both the HEUMET and ZPR/Big-10 problems are similar. However, with respect to the sensitivities and uncertainties, they appear to be quite different. Cancellation of effects due to systems that "appear" to be similar causes the *traditional trending approaches to underpredict the actual bias for low-moderation systems with intermediate enrichments.* This underprediction is evident in Table 1, where the results are presented in summary form. The predicted bias from these applications are all positive (overpredict k_{eff}). Therefore, the variation in results is not a concern for these applications. However, a similar situation can be easily postulated where a predicted positive bias is actually a negative bias. With the inclusion of strict confidence levels along with an additional margin of subcriticality, the cumulative effect of these factors should still be conservative. However, *prudent application of trending procedures is very important in criticality safety validation exercises.*

The new criticality safety data validation procedures discussed in this paper should be useful for a wide variety of application areas. The advantage of these procedures is that the determination of similar systems is automatic because the systems are trended with the D and c_k values. Also, the inclusion of a wide variety of benchmarks in the validation set is possible, since the trending parameters will selectively fit only systems that are similar to the particular application area. Further guidance on the use of these new techniques is given in Ref. 17.

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Session D
Applications for Covariance Matrices II
Friday, 23 April 1999

Session Chair: Phillip J. Finck

Three formal presentations were allocated to this session of the Workshop (Applications for Covariance Matrices II) and informal discussions on matters related to applications for covariance information continued from the preceding session on the same topic (Applications for Covariance Matrices I).

Prof. H. Vonach, Institute fuer Radiumforschung und Kernphysik, discussed his recent work on double-differential measurements for the 9Be(n,2n) reaction, i.e., determination of both energy and angular distributions for the emitted neutrons. He noted that the angular distributions were strongly dominated by reaction kinematics. His method of analysis was based on the use of constrained least squares and made liberal use of covariance matrices. Some possible modifications to the ENDF formats were suggested to accommodate information of this nature.

Dr. K. Shibata , JAERI Nuclear Data Center - Tokai, described an effort in Japan to provide covariance information for JENDL in response to strong requests from users. No covariance data are available in JENDL-3.2. Rather than retrofitting the existing evaluations with covariances, it was decided that the proper (technically correct) approach was to redo all the selected evaluations using least-squares methodologies which produce covariance results in a natural way. Two computer tools are used. For experimental data, the code GMA is applied. For evaluations based mainly on theory (nuclear modeling) the code KALMAN is used to adjust model parameters to fit available data. It is found that very strong correlations arise in the covariance files generated in evaluations based on nuclear models.

Dr. T. Kawano, Kiyushu University, presented an overview of the KALMAN system used in Japan for evaluations based largely on nuclear models, as mentioned by the preceding speaker. A suite of nuclear modeling codes, including such well-known ones as CASTHY, ECIS, ELIESE, and GNASH, are used in this work. Dr. Kawano noted that the strong correlations (mentioned earlier by Dr. Shibata) arise because of functional relationships inherent in the nuclear models. Application of this technique involves deriving estimates of the uncertainties of nuclear model parameters. An important example are the Optical Model parameters for which it has been estimated that the uncertainty is about 10%.

Discussions on the role of covariance information in applications continued from the earlier session. Two important themes were evident in these discussions. One is that requests from users for basic nuclear data (experimental or theoretical) or evaluated nuclear data for applications are of limited value unless the accuracy requests are stated in a realistic and convincing manner. In order to do this, detailed sensitivity analyses pertinent to the intended application are needed. This is seldom done. Since reliable nuclear data information are often technically difficult - and thus expensive - to generate, it will be essential in the future to emphasize the issue of sensitivity analysis if real progress is to be made

in improving nuclear data for applications. Another issue discussed stems from the observation that many users continue to employ older versions of evaluated files even after new (presumably superior) ones have been made available. The well known argument that the processing of new files is costly and time consuming was mentioned. However, one cannot help but suspect that one of the real reasons for this behavior is that there is not much confidence that the new files will yield better results. If users were confident that the new files would lead to significantly improved performance, it is very likely that they would be motivated to expend the effort and cost needed to process them without question or complaint.

JENDL-3.2 Covariance File

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Abstract

Covariances of neutron nuclear data have been estimated for 14 nuclides contained in JENDL-3.2. The physical quantities for which covariances are deduced are cross sections, resolved and unresolved resonance parameters, the first order Legendre-polynomial coefficient for the angular distribution of elastically scattered neutrons, and fission neutron spectra. As for ^{235}U and ^{241}Pu, covariances were obtained also for the average number of neutrons emitted in fission. Generalized least-squares methods were applied to obtain the covariances of those cross sections which were based on expermental data. A simultaneous evaluation method yielded uncertainties in the fission cross sections of ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu and ^{241}Pu. Covariances of nuclear model calculations were determined from uncertainties in model parameters. The covariance file thus obtained is processed by a system which has been developed, and will be used for the adjustment of group cross sections.

1. INTRODUCTION

Uncertainties in evaluated data are needed not only to estimate margins in design

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and safety of nuclear facilities, but also to adjust group constants by considering integral measurements. There was a strong request of covariance data from those who were involved in fast reactor development. However, the second revision of JENDL-3 (JENDL-3.2)[1] does not contain covariance data, while ENDF/B-VI[2] and JEF-2.2[3] have covariances files for a limited number of nuclides. To overcome such a situation, a working group on covariance estimation was organized in Japanese Nuclear Data Committee. This group has a task of developing methods and tools for covariance estimation. They have also made a covariance file of JENDL-3.2 for the adjustment of group cross sections needed for fast reactor applications.

The physical quantities for which covariances are required are cross sections, average number of emitted neutrons in fission, resolved and unresolved resonance parameters, the first order Legendre-polynomial coefficient for the elastically scattered neutrons, and fission neutron spectra. Covariances were prepared for 14 nuclides: ^{10}B, ^{11}B, ^{16}O, ^{23}Na, Cr, ^{55}Mn, Fe, Ni, ^{233}U, ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu and ^{241}Pu.

Covariances were estimated on the basis of the same methods that had been adopted in the JENDL-3.2 evaluation. In cases where the evaluated data were obtained by a curve fitting to experimental data, the covariances were also obtained from the experimental data. On the other hand, a computer code system KALMAN[4], which was developed at Kyushu University, enabled one to estimate covariances of nuclear model calculations from uncertainties in model parameters. Covariances of fission cross sections of fissile and fertile nuclides were obtained by the simultaneous evaluation[5] together with mean values.

This paper deals with how the covariances of the JENDL-3.2 data were estimated. Moreover, a processing system of covariances is briefly described.

2. COVARIANCE ESTIMATION

2.1 RESONANCE PARAMETERS

Covariances of resolved resonance parameters were given for ^{23}Na, ^{55}Mn, Fe, ^{233}U, ^{238}U, ^{239}Pu, ^{240}Pu and ^{241}Pu. Standard deviations of the parameters were estimated from the analyses of experimental data. No correlation of the parameters is given except for Fe, ^{233}U and ^{241}Pu. In general, correlation between different resonances is weak. As a result, uncertainties in group cross sections calculated from resonance parameters and their covariances were found[6] to be very small, i.e., less than 1% when a lot of resonances were included in a group. This is a problem when the adjustment is performed in the

resonance region; no good solution has been found yet.

As for unresolved resonance, the covariances of the parameters were calculated by the ASREP code[7] on the KALMAN system[4]. Table 1 gives the estimated covariances of the level spacing, neutron widths, capture widths and fission widths for ^{240}Pu.

Table 1. Covariances of unresolved resonance parameters for ^{240}Pu

Parameter*	Error(%)	Correlation coefficient							
D_0	6.4	1.00							
$\Gamma_n(s)$	7.9	0.56	1.00						
$\Gamma_n(p)$	15.2	0.70	0.16	1.00					
$\Gamma_\gamma(s)$	9.6	0.45	0.24	-0.10	1.00				
$\Gamma_\gamma(p)$	8.4	0.37	0.35	-0.01	0.06	1.00			
$\Gamma_f(1/2+)$	23.9	0.36	0.21	-0.03	0.41	0.38	1.00		
$\Gamma_f(1/2-)$	16.6	0.06	0.04	-0.01	0.08	0.08	-0.08	1.00	
$\Gamma_f(3/2-)$	15.8	0.14	0.11	-0.03	0.18	0.22	-0.19	-0.06	1.00

* The symbols are defined as follows: D_0: s-wave level spacing, $\Gamma_n(s)$ and $\Gamma_n(p)$: s- and p-wave neutron widths, $\Gamma_\gamma(s)$ and $\Gamma_\gamma(p)$: s- and p-wave capture widths, $\Gamma_f(1/2^+)$: s-wave fission width with $J^\pi=1/2^+$, $\Gamma_f(1/2^-)$: p-wave fission width with $J^\pi=1/2^-$, $\Gamma_f(3/2^-)$: p-wave fission width with $J^\pi=3/2^-$.

Figure 1 shows the standard deviations of the capture cross section for ^{240}Pu in the unresolved resonance region.

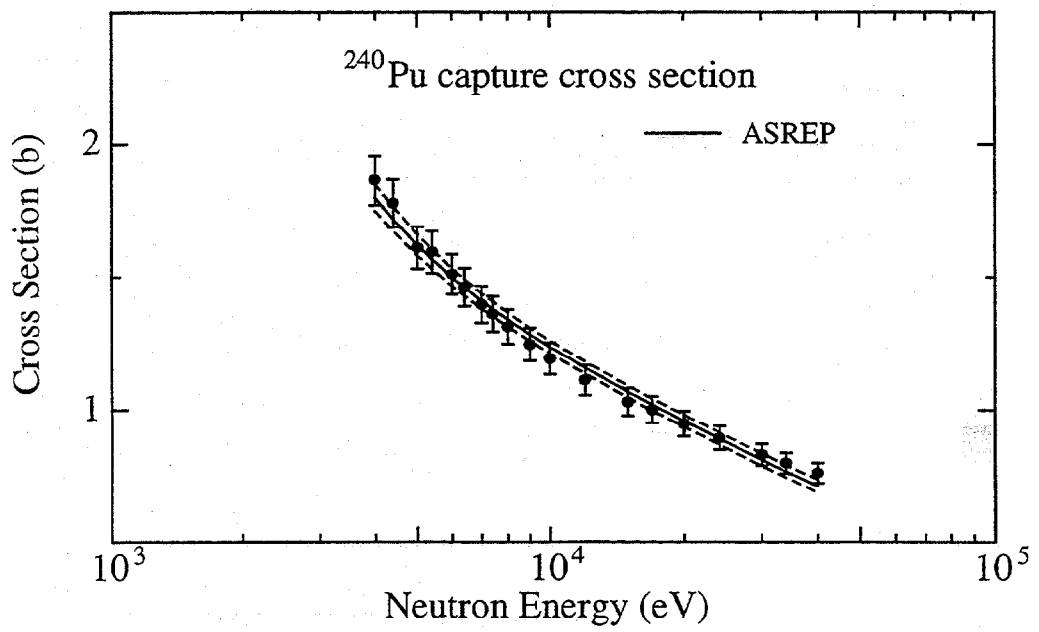

Fig. 1. Capture cross section of ^{240}Pu in the unresolved resonance region.

2.2 SMOOTH CROSS SECTIONS

2.2.1 COVARIANCE ESTIMATED FROM MEASUREMENTS

Important cross sections of fissile and fertile nuclides had been obtained in the simultaneous evaluation[5] for JENDL-3. The cross sections obtained are fission cross sections of ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, and ^{241}Pu in the energy range from 50 keV to 20 MeV. The simultaneous evaluation is based on the generalized least-squares methods, and it can estimate not only cross sections but also covariances associated with them. The experimental data used in the simultaneous evaluation were absolute and ratio measurements. The generalized least-squares fitting based on the Bayes' theorem with the second order B-spline functions was applied to these experimental data. The covariances for the measurements were prepared from the experimental information of individual data on the basis of common criteria in which each partial error was categorized to a few groups having specific correlation factors. The correlation of the data only between the different neutron energies was considered and other correlation was neglected. Figures 2 and 3 show the standard deviations and correlation matrices for the fission cross sections of ^{235}U and ^{238}U obtained in the simultaneous evaluation, respectively.

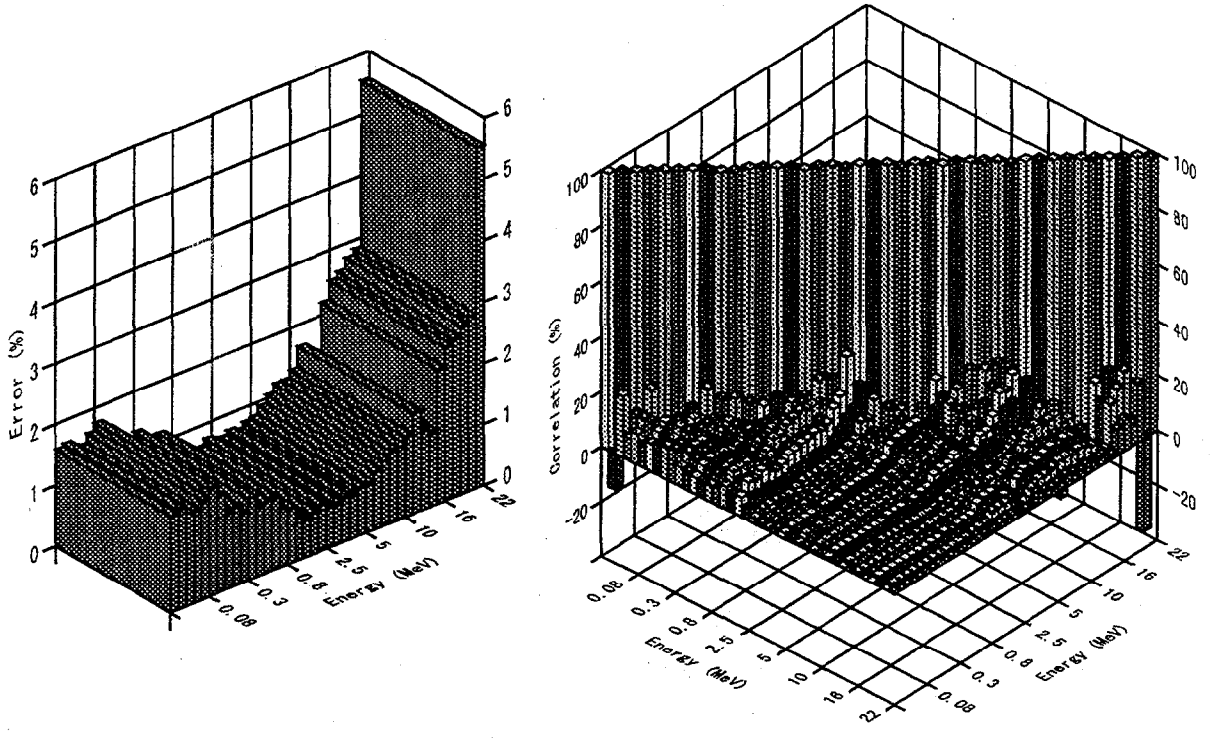

Fig. 2. Covariances of $^{235}U(n,f)$ cross sections.

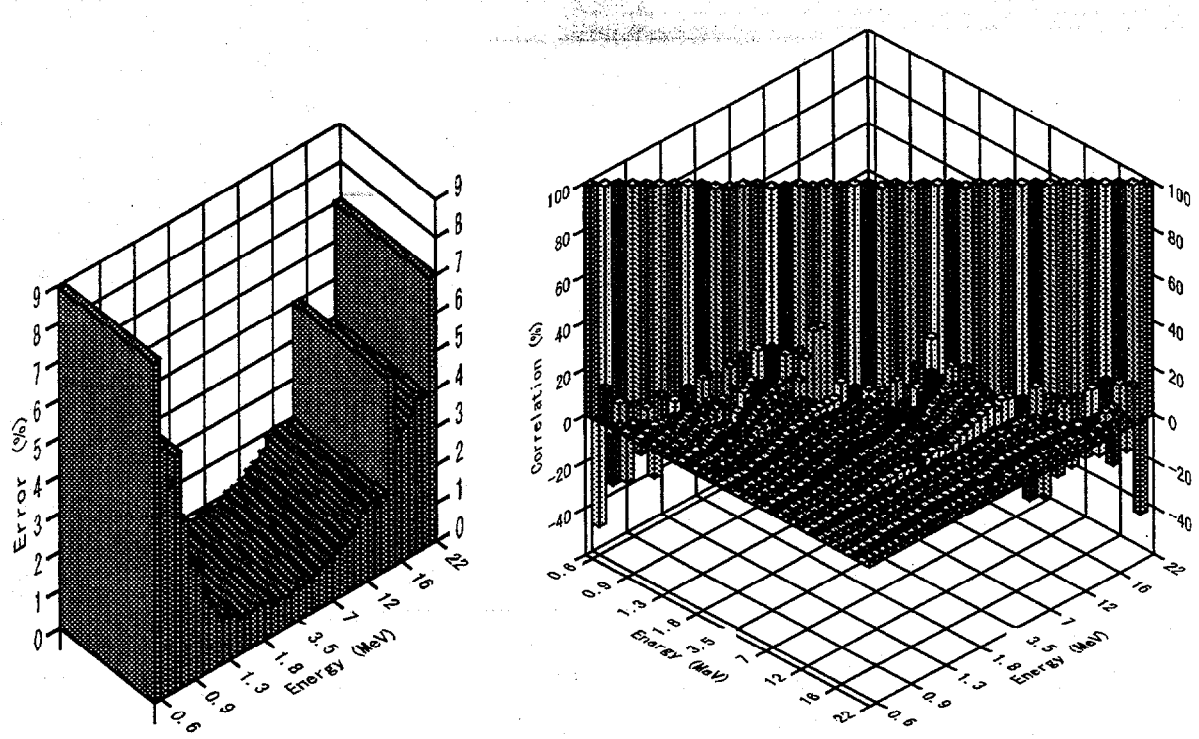

Fig. 3. Covariances of ^{238}U(n,f) cross sections.

Least-squares fitting is often used in data evaluation in cases where a lot of measurements are available. We have applied the GMA code[7] to estimate uncertainties in various cross sections and average number of emitted neutron in fission. With this code, the percentage of the systematic error to the total error is required as input. The correlation matrix for data points in each measurement is calculated from this percentage. In the GMA analysis, energy grids are defined by prior data. Experimental values from one data set are extrapolated to neighboring energy grids by using the shape of prior cross sections, and then the weighted average value is calculated at the energy grid. The cross-section error at this grid consists of a systematic error given by input and a reduced statistical error calculated from contributing data. The procedure is simple and appropriate for producing covariance files. Figure 4 shows the uncertainties in the total cross section of elemental Ni obtained by GMA. The GMA code was also applied to estimate the standard deviations of the average number of neutrons emitted in the neutron-induced fission of ^{235}U, as seen in Fig. 5.

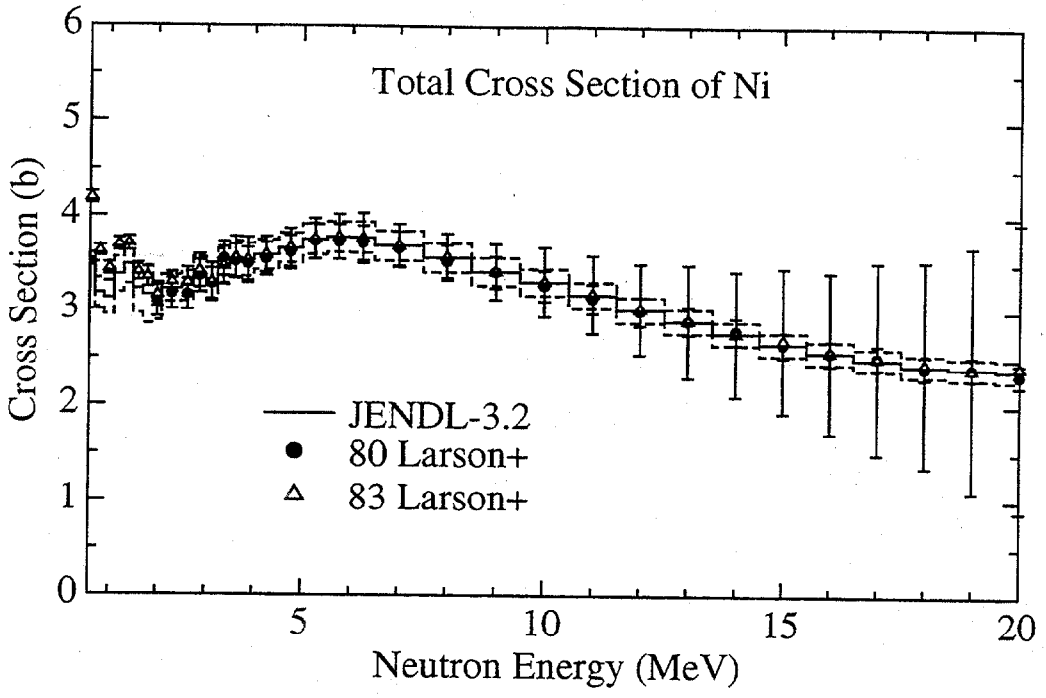

Fig. 4. Total cross section of elemental Ni. Standard deviations are shown by dashed lines.

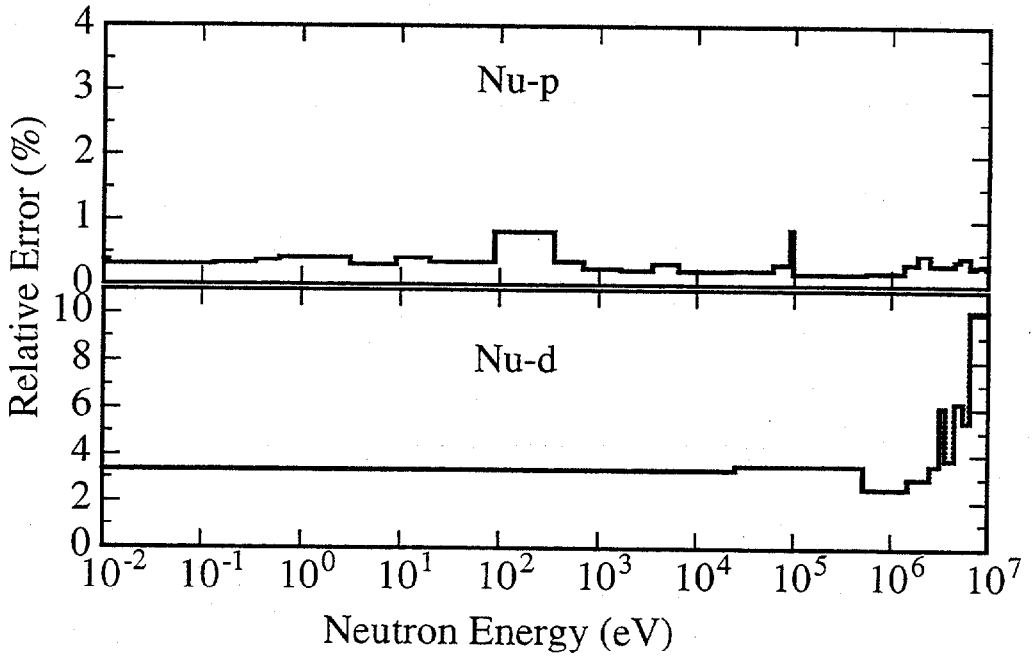

Fig. 5. Uncertainties in the average number of neutrons emitted in the $^{235}U(n,f)$ reaction.

2.2.2 COVARIANCE ESTIMATED FROM NUCLEAR MODEL CALCULATIONS

Nuclear model calculations were rigorously adopted in the JENDL-3 evaluation. In such cases, one should estimate uncertainties in nuclear model calculations. There must be an uncertainty in the model itself, i.e., model deficiency. However, nobody can tell the deficiency exactly. The only thing we can do is to incorporate the deficiency into uncertainties in the model parameters, although a chi-square value after fitting is a measure of the model deficiency.

The parameters required for model calculations are adjustable within a certain acceptable limit which is given by *a priori* knowledge and theoretical consideration. This is expressed by prior covariances of the parameters. When the nuclear model calculation is fitted to experimental data, uncertainties in the model parameters are determined according to the prior covariances of the parameters and covariances of experimental data used. Uncertainties in the parameters lead to uncertainties in calculated cross sections by the law of error propagation. Therefore, one can obtain a covariance matrix of evaluated data based on nuclear model calculations.

Covariances of model calculations have been studied by a group of Kyushu University, and they developed a computer system KALMAN[4], which enabled one to estimate covariances of various model calculations. The total cross section of ^{239}Pu was analyzed by the spherical optical model on the KALMAN system, as an example. The optical model parameters were adjusted so as to reproduce measurements. Table 2 gives the prior and posterior parameter values together with their covariances. From the table, a strong correlation is seen between a real depth V and a real radius r_v, which is predicted by the fact that small changes in V and r_v will not change the scattering provided that the product Vr_v^2 is kept constant. This is known as discrete ambiguities of the optical model.

Table 2. Optical model parameters for ^{239}Pu

Parameter*	Prior	Posterior	Error(%)	Correlation (×1000)					
V (MeV)	40.7	41.3	0.95	1000					
r_v (fm)	1.32	1.31	0.99	-966	1000				
a_v (fm)	0.47	0.46	4.87	651	-611	1000			
W_s (MeV)	6.78	6.22	4.23	-558	492	-20	1000		
r_s (fm)	1.38	1.39	1.24	497	-627	4	-252	1000	
a_s (fm)	0.47	0.42	4.92	-153	292	-47	-294	-818	1000

* Energy-dependent depths and a spin-orbit term are not given in this table.

The calculated total cross section of ^{239}Pu is shown in Fig. 6.

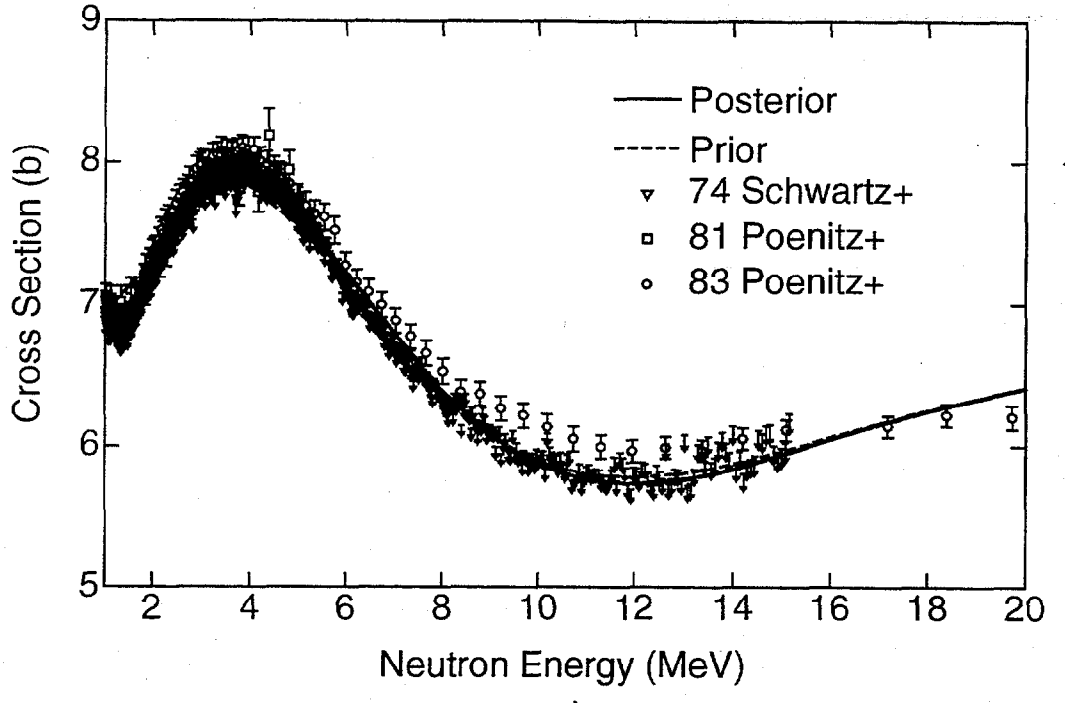

Fig. 6. Total cross section of ^{239}Pu.

The covariances for the ^{238}U(n,n$_1$) cross sections obtained by KALMAN are compared with those contained in ENDF/B-VI.2 and JEF-2.2, as shown in Fig. 7. Near the threshold, the presently estimated error is much larger than those of other libraries, whereas it is smaller than that of ENDF/B-VI in the energy region from 100 keV to 10 MeV. In JEF-2.2, uncertainties are given up to 309 keV.

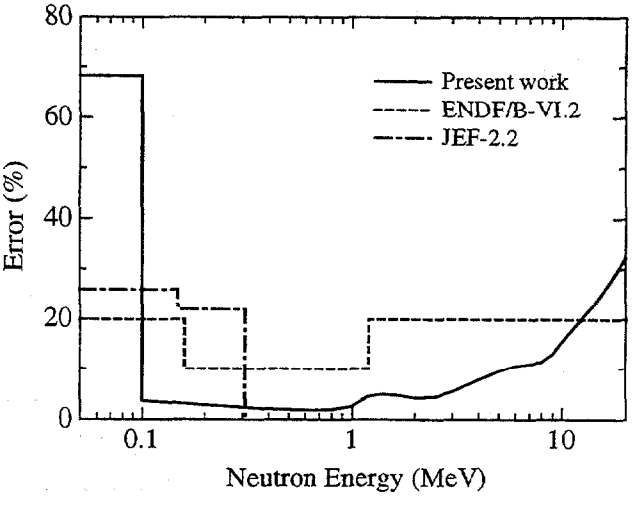

Fig. 7. Uncertainties in the ^{238}U(n,n$_1$) cross section.

3. PROCESSING OF COVARIANCES

Once the JENDL-3.2 covariance file is prepared, it should be processed for the adjustment of multi-group cross sections. Unfortunately, the NJOY code[8] was not complete as far as covariances were concerned. Therefore, we have developed a processing system for covariance which is relevant to the adjustment performed by the Japan Nuclear Cycle Development Institute.

As shown in Fig. 8, the covariance file is processed by the ERRORJ code which is essentially based on the ERRORR module of NJOY94.105. The ERRORJ code is capable of dealing with covariances of resolved (Breit-Wigner and Reich-Moore formulae) and unresolved resonance parameters. It can also produce an uncertainty in average cosine of elastic scattering angles from the data in MF/MT=34/2. Covariances of fission neutron spectra given in MF/MT=35/18 can be also processed by ERRORJ.

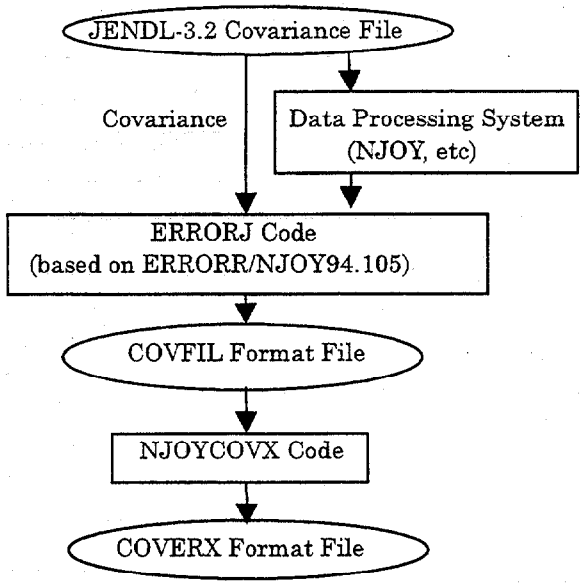

Fig. 8. Flow of processing.

4. CONCLUSIONS

Covariances were estimated for 14 nuclides contained in JENDL-3.2. We have developed methods of covariance estimation and some related computing tools. The covariance file is processed by the ERRORJ code which is a modified version of ERRORR in NJOY94. The multi-group covariance data will be used for the adjustment of group cross sections for fast reactor development.

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Covariance Evaluation with the KALMAN System

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Abstract

The KALMAN system has been developed to evaluate covariances of the evaluated nuclear data libraries. Calculation codes of an optical model, a Hauser-Feshbach model, an improved Madland-Nix model, and Reich-Moore R-matrix theory were incorporated into the system to generate the covariances of various quantities. The system is applied to some simple examples to show how the system works and how to estimate covariances in case few experimental data are available.

1. INTRODUCTION

Generation of covariance data with a model calculation is an extension of the generalized least-squares method. Uncertainties of the evaluated nuclear data obtained by the least-squares technique represent uncertainties of the fitting function used for the data evaluation. An interval-average or a linear-interpolation, those correspond to the 0-th order and the first order linear functions, are often used as the fitting function. The covariance obtained by the data fitting reflects an analytical property of those fitting function.

The basic idea is the same for use of the model calculations. When a nuclear model calculation is adopted as the fitting function, the uncertainties of the model parameters are determined by the uncertainties of the experimental data. The error-propagation from the parameters to the calculated quantities gives the covariance, and it reflects properties of the parameters in the model.

The program KALMAN[1] was designed to calculate covariances of the model parameters from experimental data. The program can be generally used for various models, and we have developed a system in which an optical model, Hauser-Feshbach model, and R-matrix calculation codes are incorporated to generate covariances of the nuclear data library.

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2. COVARIANCE EVALUATION

The starting point of the covariance evaluation with the KALMAN system is the same as the well-know generalized least-squares method, which is expressed as

$$\boldsymbol{x}_1 = \boldsymbol{x}_0 + \mathbf{P}\mathbf{C}^t\mathbf{V}^{-1}\left(\boldsymbol{y} - \boldsymbol{f}(\boldsymbol{x}_0)\right) = \boldsymbol{x}_0 + \mathbf{X}\mathbf{C}^t\left(\mathbf{C}\mathbf{X}\mathbf{C}^t + \mathbf{V}\right)^{-1}\left(\boldsymbol{y} - \boldsymbol{f}(\boldsymbol{x}_0)\right), \quad (1)$$

$$\mathbf{P} = \left(\mathbf{X}^{-1} + \mathbf{C}^t\mathbf{V}^{-1}\mathbf{C}\right)^{-1} = \mathbf{X} - \mathbf{X}\mathbf{C}^t\left(\mathbf{C}\mathbf{X}\mathbf{C}^t + \mathbf{V}\right)^{-1}\mathbf{C}\mathbf{X}, \quad (2)$$

where $\boldsymbol{x}$ is the vector of the model parameters, $\boldsymbol{x}_0$ the prior parameter, $\boldsymbol{x}_1$ the posterior parameter, $\boldsymbol{y}$ the vector of experimental data, $\mathbf{V}$ the covariance matrix of the experimental data, $\mathbf{X}$ the covariance matrix of $\boldsymbol{x}_0$, $\mathbf{P}$ the covariance matrix of $\boldsymbol{x}_1$, and $\mathbf{C}$ the sensitivity matrix. Nuclear reaction model calculation $\boldsymbol{f}(\boldsymbol{x})$ is linearized by the first-order Taylor expansion,

$$\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x}) \simeq \boldsymbol{f}(\boldsymbol{x}_0) + \mathbf{C}(\boldsymbol{x} - \boldsymbol{x}_0). \quad (3)$$

If uncertainties of the prior parameters are very small in comparison with those of the experimental data, the obtained $\mathbf{P}$ strongly depends on $\mathbf{X}$. On the other hand, $\mathbf{P}$ is mainly determined from the experimental errors if they are smaller than the uncertainties of the prior parameters, and this is the case for the covariance evaluation. The posterior covariance $\mathbf{P}$ contains information of uncertainties of the experimental data, and one can inter/extrapolate this information by means of the error-propagation $\mathbf{C}\mathbf{P}\mathbf{C}^t$ to a region where experimental data are inaccessible.

3. KALMAN SYSTEM

The KALMAN code solves Eqs. (1) and (2), but it does not have any nuclear model calculation part. Then, to evaluate a covariance of nuclear data, one has to prepare a model calculation code, and make a sensitivity matrix $\mathbf{C}$. We have developed the KALMAN system which consists of several nuclear model calculation codes and data processing tools. The nuclear model codes incorporated into the KALMAN system are show in Table 1. Some modifications were made for these codes in order to calculate the sensitivity coefficients.

4. EXAMPLES

4.1. COVARIANCE EVALUATION WITH A SIMPLE LORENTZIAN

In order to explain how does the KALMAN system work, we show some examples of the covariance evaluation. The first example is a covariance generation with a simple Lorentzian curve. Suppose the experimental data obey the function, $y = c/\{a+(x-b)^2\}$

Table 1: Nuclear model codes in the KALMAN system.

Code name	Type of covariances to be calculated	Reference
GNASH	Reaction Cross Section	[2]
ELIESE-3	Total Cross Section, P_1	[3]
ECIS88	Total and Inelastic Scattering Cross Section (DI)	[4]
CASTHY	Capture and Inelastic Scattering Cross Section (CN)	[5]
FISPEKL2	Fission Spectrum	[6]
gfr	Resonance Parameter (Reich-Moore)	[7]
ASREP	Unresolved Resonance Parameter	[8]

Table 2: Covariance of the parameters of the Lorentzian curve.

Parameter	Value	Error (%)	Correlation (%)		
a	1.00	17	100		
b	2.00	12	68	100	
c	3.00	15	81	90	100

where a, b and c are the parameters, and they have values of $a = 1$, $b = 2$ and $c = 3$ with the prior uncertainties of 100%. The sensitivity coefficients are easily obtained by $\partial y/\partial p_i$ where $p_i = a, b$ or c. When the experimental data are provided, one can calculate the covariance of the posterior parameters in Eq. (2).

When the provided experimental data are, (x, y)= (2, 3), (4, 0.6), (6, 0.1765) and (8, 0.08198), and the y values have uncertainties of 10%, the posterior covariance **P** is shown in Table 2. The obtained uncertainty of the Lorentz function is shown in Fig. 1, and its correlation matrix is in Fig. 2. The arrows in Fig. 1 stand for the positions of the data. At $x = 2$ and 4, the obtained uncertainties reproduce the errors of 10% those were given for the data.

4.2. COVARIANCE WITH THE OPTICAL MODEL

The next example shows an application of the KALMAN system to the covariance evaluation of an angular distribution of elastic scattering cross sections with the optical model. The optical model calculation is fitted to the experimental data of 10 MeV neutron induced ^{209}Bi(n, n) reaction[9]. The global optical potential of Rapaport, Kulkarni, and Finlay[10] is used for the prior parameters, and six optical potential parameters — V, r_v, a_v, W_s, r_w, and a_w — are adjusted to the experimental data. The uncertainties of the prior parameters are assumed to be 10%, and the correlations among them are zero. The obtained posterior covariance is shown in Table 3.

Figure 3 shows the comparison of the calculated uncertainties with those of the experimental data. The correlation matrix is shown in Fig. 4. In Fig. 3, peaks of

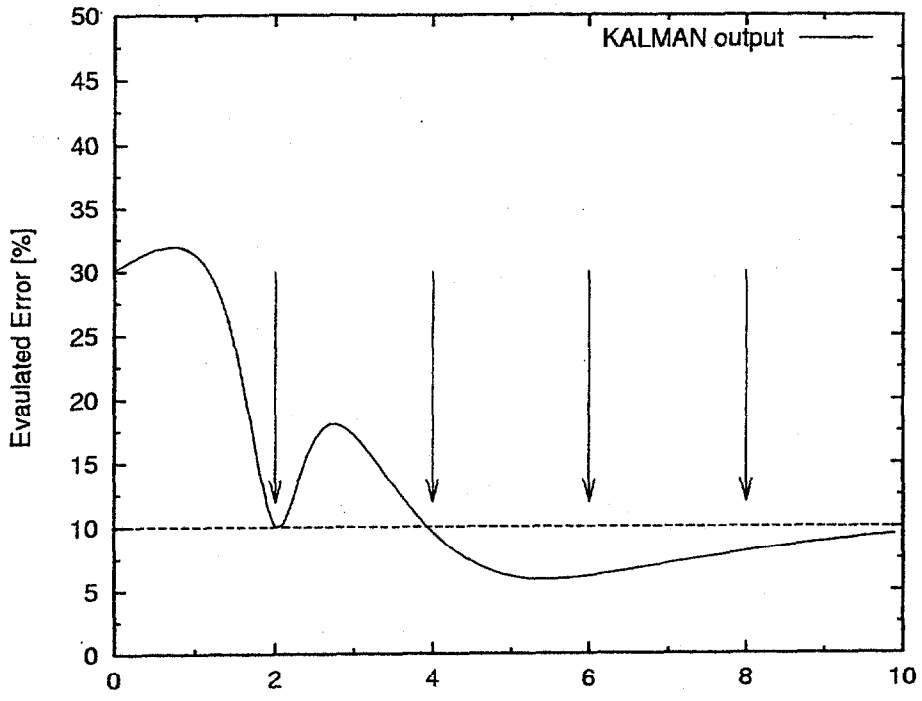

Fig.1: Uncertainties of the simple Lorentzian curve evaluated with the KALMAN system.

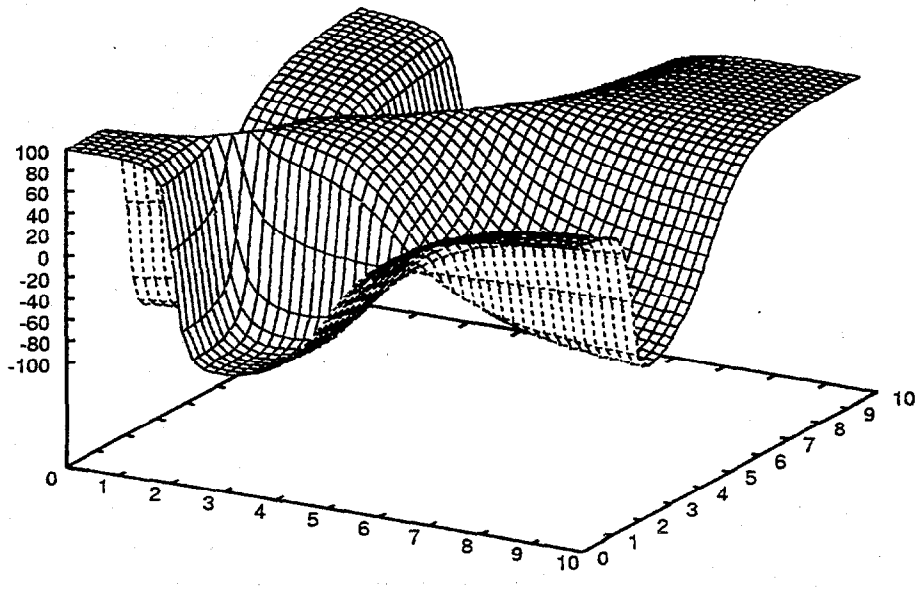

Fig.2: Correlation matrix of the simple Lorentzian curve.

Table 3: Covariance of the optical potential parameters.

Parameter	Error (%)	Correlation (%)					
V	2.60	100					
r_v	1.93	−98	100				
a_v	5.83	59	−67	100			
W_s	15.5	−70	67	0	100		
r_w	1.98	66	−75	71	−27	100	
a_w	9.25	42	−35	−29	−90	−14	100

the experimental error correspond to minima of the differential cross sections, and the KALMAN results follow this tendency. At the forward and backward angles ($\theta \leq 20°$ or $\theta \geq 160°$) where no measurements are available, one can extrapolate the KALMAN calculation into these region and predict uncertainties there. This is an advantage of use of model calculations. We can estimate uncertainties of parameters in some model, even if there exists only one measurement. Then it is possible to estimate a covariance matrix of the evaluated data with the obtained covariance of the parameters by means of the error propagation. This means an extrapolation of the uncertainty of the measurement.

4.3. COVARIANCE WITHOUT EXPERIMENTAL DATA

The next example shows how to generate a covariance matrix without experimental data. As explained above, one needs at least one measurement to estimate a covariance of the model parameters. There are, however, many kinds of nuclear data those cannot be measured but calculated values are only available, and we have to give a covariance of such a kind of quantities for practical applications.

A model calculation tells us a relative magnitude of uncertainties of the calculated quantities if a covariance of the parameters is provided. Generally, it is very difficult to assume the covariance of the parameters, however, if an error of the calculated value at a certain point is assumed, the covariance of the parameters can be obtained. This assumption acts as a normalization factor of the covariance of the calculated quantities.

Figure 5 shows an example of the renormalized errors of differential elastic scattering. The parameters used were the same as in Fig. 3, but the covariance was obtained by the normalization method. The assumed data error is 5% at 10°.

The other example is a covariance of fission spectrum[11]. Experimental data for the fission spectra are available for a few actinoid nuclei at the limited neutron-incident energies. However this is insufficient to make a covariance file for the fission spectra in a nuclear data library.

The fission spectra of U and Pu isotopes were evaluated with the FISPEKL2 code[6] in JENDL-3.2, and the covariance data for those spectra were calculated with the same code. Then the calculated uncertainties of the fission spectra were renormalized —

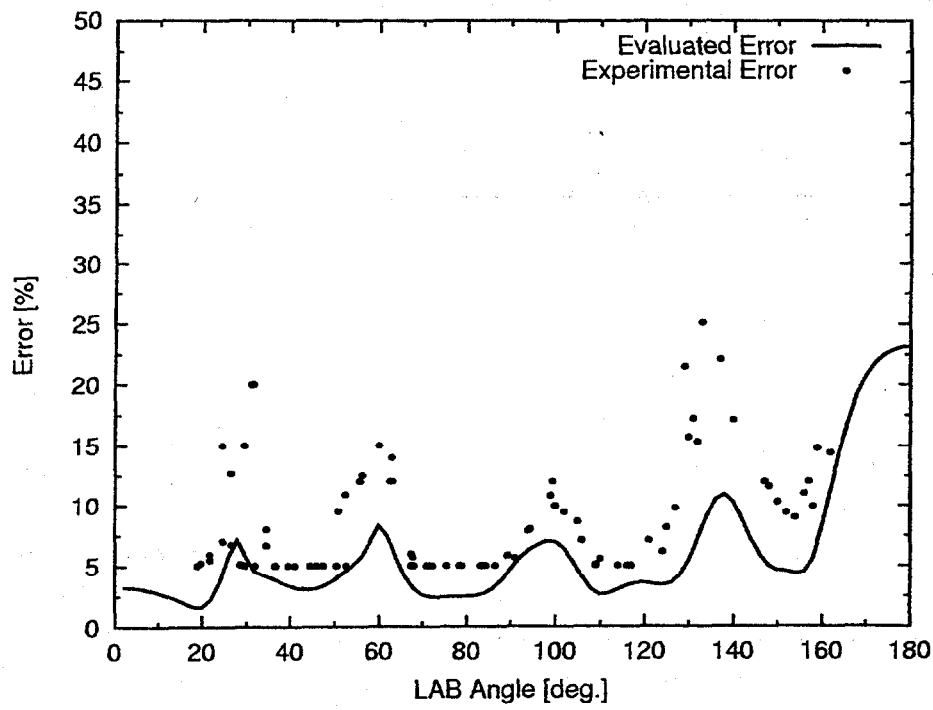

Fig.3: Comparison of the uncertainties of the experimental data of ^{209}Bi elastic scattering cross sections with the results of the KALMAN system.

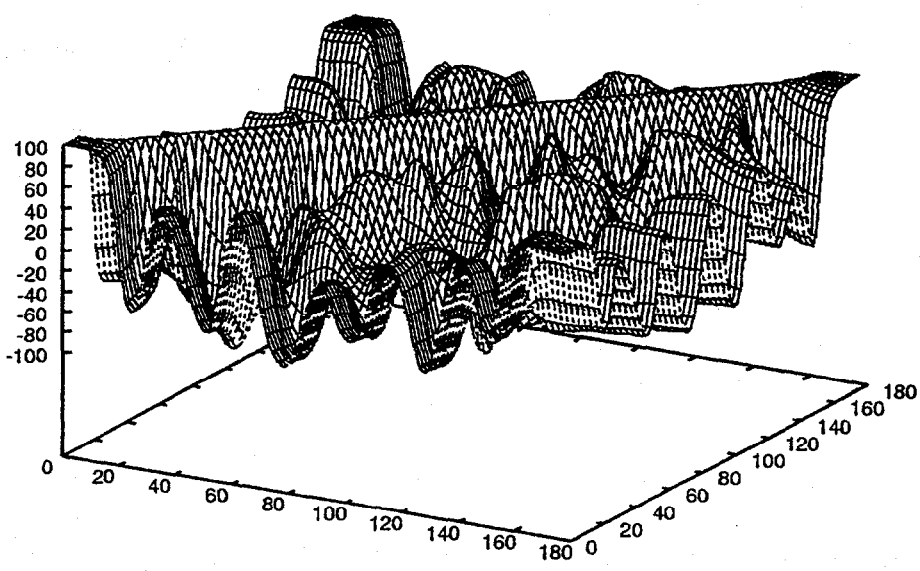

Fig.4: Correlation matrix of the angular distribution of the elastic scattering generated with the KALMAN system.

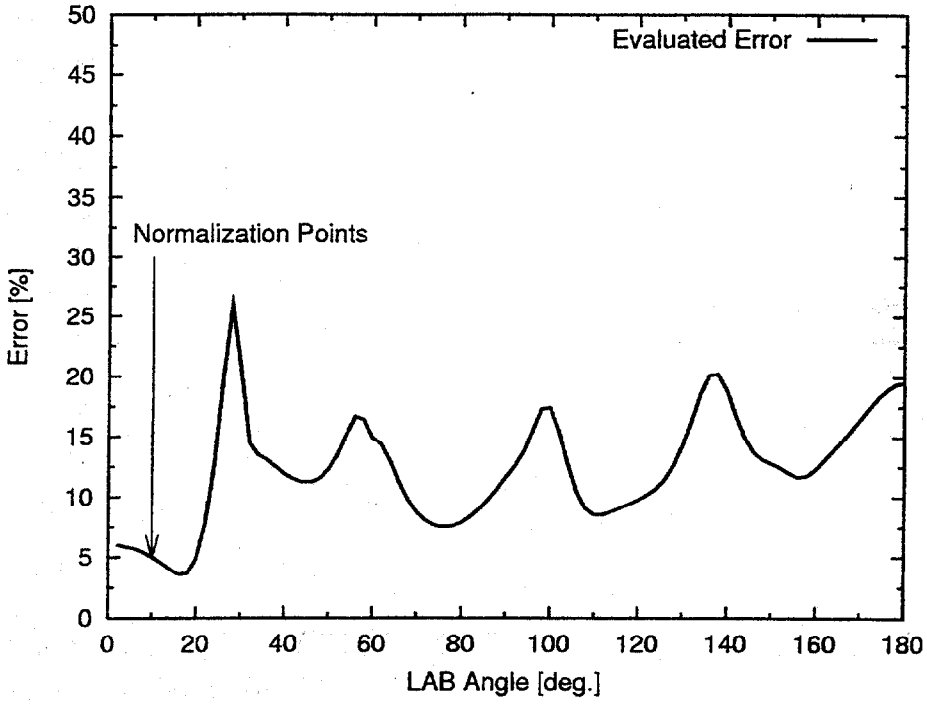

Fig.5: Calculated uncertainties of the ^{209}Bi elastic scattering cross sections. The obtained uncertainties were renormalized at 10°.

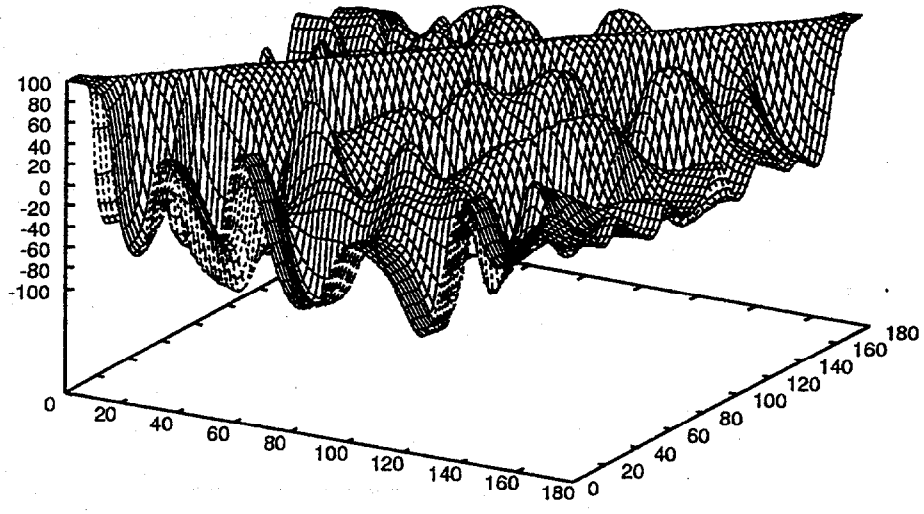

Fig.6: Correlation matrix of the angular distribution of the elastic scattering generated with the KALMAN system.

Table 4: Covariance matrix of the fission neutron spectrum of ^{235}U at thermal energy.

Energy [MeV]	Error [%]	Correlation [%]																
1.00e-08	7.73	100																
1.00e-07	7.73	100	100															
1.00e-06	7.73	100	100	100														
1.00e-05	7.73	100	100	100	100													
1.00e-04	7.73	100	100	100	100	100												
1.00e-03	7.74	100	100	100	100	100	100											
1.00e-02	7.85	100	100	100	100	100	100	100										
1.00e-01	7.47	100	100	100	100	100	100	100	100									
1.00e+00	2.09	83	83	83	83	83	83	83	84	100								
2.50e+00	2.52	-100	-100	-100	-100	-100	-100	-100	-100	-80	100							
5.00e+00	6.38	-81	-81	-81	-81	-81	-81	-81	-82	-100	78	100						
7.50e+00	11.00	-68	-68	-68	-68	-68	-68	-68	-70	-97	64	98	100					
1.00e+01	15.50	-55	-55	-55	-55	-55	-55	-55	-57	-92	50	94	98	100				
1.20e+01	19.20	-43	-43	-43	-43	-43	-43	-43	-45	-86	38	88	95	99	100			
1.40e+01	23.10	-28	-28	-28	-28	-28	-28	-27	-29	-76	22	78	89	95	99	100		
1.60e+01	27.80	-7	-7	-7	-7	-7	-7	-6	-9	-61	1	64	77	87	93	98	100	
1.80e+01	34.70	18	18	18	18	18	18	18	16	-40	-23	43	60	72	81	90	97	100
2.00e+01	45.80	41	41	41	41	41	41	41	39	-17	-46	20	39	53	65	76	88	97	100

3% at E'_n =0.7 MeV. This normalization factor was determined from the experimental data of Bojcov *et al.*[12], Johansson *et al.*[13], and Kornilov[14]. An investigation of Adams[15] was also taken into account. The obtained covariance of the fission spectrum of ^{235}U at thermal energy is shown in Table 4. Since the fission spectrum is expressed by a probability in the ENDF format, the integrated probabilities must be unity. This requirement yields strong anti-correlations between the higher and the lower energy regions.

5. CONCLUSION

An overview of the principle and the method of the covariance evaluation with the KALMAN system was described. A covariance evaluation with a simple Lorentz function and an optical model calculation demonstrated that the uncertainties generated with the KALMAN system reproduce those of the experimental data, and it is possible to extrapolate information of the experimental uncertainties into the region where no experimental data are available. Even no data are available, it is possible to estimate covariances with the KALMAN system if one assumes a normalization factor of the calculated uncertainties.

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APPENDIX A

Agenda for Covariance Workshop to be held at Brookhaven National Laboratory April 22-23, 1999		
Thursday April 22	**Medical Conference Room, Bldg. 490**	
0845	Convene Workshop	
0845-0900	Opening Remarks	Chairpersons: L.C. Leal and D.L. Smith
Session A:	**Generation of Covariance Matrices**	R. Roussin, Chair
0900-0930	Paper A. I	S. Tagesen (IRK - Austria)
0930-1000	Paper A.2	G. Manturov (IPPE - Russia) Presented by A. Ignatyuk
1000-1030	Paper A.3	S. Badikov (IPPE - Russia) Presented by A. Ignatyuk
1030-1100	Coffee Break	
1100-1230	Technical Discussions	All (1 hour 30 minutes)
1230-1330	Lunch BNL Cafeteria - Berkner Hall	
Session B:	**Representation and Processing of Covariance Matrices**	W. Mannhart, Chair
1330-1400	Paper B. I	D-Muir (IAEA - Austria)
1400-1430	Paper B.2	N. Larson (ORNL - U01-LI
1430-1500	Paper B.3	I. Kodeli (US - Slovenia)
1500-1530	Coffee Break	
1530-1800	Technical Discussions	All (2 hours 30 minutes)

Friday April 23	**Medical Conference Room, Bldg. 490**	
Session C:	**Applications for Covariance Matrices I**	A. Hasegawa, Chair
0900-0930	Paper C. I	E. Fort (CEA Cadarache - France)
0930-1000	Paper C.2	R. McKnight (ANL - USA)
1000-1030	Paper C.3	B. Broadhead (ORNL - USA)
1030-1100	Coffee Break	
1100-1230	Technical Discussions	All (2 hours)
1230-1330	Lunch BNL Cafeteria - Berkner Hall	
Session D:	**Applications for Covariance Matrices II**	P. Finck, Chair
1330-1400	Paper D. I	H. Vonach (IRK - Austria)
1400-1430	Paper D.2	K. Shibata (JAER1 - Japan)
1430-1500	Paper D.3	T. Kawano (Kyushu U. - Japan)
1500-1530	Coffee Break	
1530-1745	Technical Discussions	All (2 hours 15 minutes)
1745-1800	Closing Remarks	Chairpersons: L.C. Leal and D.L. Smith
1800	Adjourn Workshop	

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