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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

PROCEEDINGS OF THE IAEA CONSULTANTS' MEETING

ON

THE ASSESSMENT OF THE RESULTS OF THE REAL-84 EXERCISE

Prepared by E.M. Zsolnay and H.J. Nolthenius

Edited by V. Piksaikin

March 1987

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

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Table of Contents

Opening

The Consultants' Meeting on the Assessment of the Results of the REAL84 exercise was opened by Prof. Gy. Csom, Director of the Training Nuclear Reactor of the Budapest Technical University.

The meeting appointed W.L. Zijp as chairman. The scientific secretary of the IAEA was V. Piksaikin.

É.M. Zsolnay and H.J. Nolthenius were asked to prepare the report on the results of the meeting with contribution of the participants.

Program
for the IAEA Consultants' Meeting on the
Assessment of the Results of the
REAL84 Exercise

8...10 September 1986
Budapest, Hungary

Monday

9:00 - 17:00

1. Opening of Meeting
   Approval of Agenda
2. Summary of results of the REAL84 exercise
3. Improvement in uncertainty assessment of damage parameters due to REAL84
   3.1. Nuclear data aspects

Tuesday

8:30 - 16:30

   3.2. Mathematics procedures
   3.3. Physics procedures (i)

Wednesday

8:30 - 16:30

   Physics procedures (ii)
4. Evaluation procedures
5. Practical applications
6. Future actions and recommendations

1. Introduction

A Consultants' Meeting was organized by the Nuclear Data Section of the IAEA to discuss the assessment of the results of the REAL84 exercise on estimation of accuracies in radiation damage predictions. Host of the meeting was the Technical University of Budapest. The purpose of the meeting was to consider the progress, the presentation of the results, the interpretation of them and the discussion of scientific phenomena as well as to develop recommendations for future actions by IAEA and participants of the exercise.

The REAL84 exercise is a follow-up of the REAL80 exercise /1/ and is organized by the Nuclear Data Section of the International Atomic Energy Agency. The aim of the exercise is to improve the assessment of accuracies in radiation damage predictions by various laboratories using good quality input data and proper calculation methods. The emphasis lies on radiation damage to reactor pressure vessels and related nuclear technology. Therefore, the neutron energy range of interest is below 20 MeV. The long term aim of REAL84 is to strive towards establishment of standardized metrology procedures and recommended nuclear data for use in spectrum adjustments and damage parameter calculations. The short term aim is improvement of the information. In addition, the exercise will allow to assess and validate the accuracy of the methods and computer codes used. The joint effort of the participants of the exercise will contribute in solving some basic mathematical and physical problems that occur in neutron spectrum adjustment procedures for radiation damage purpose. The exercise has been described in detail in information sheets /2/ and /3/ which were distributed to candidate participants.

A first progress report /4/ on the REAL84 exercise was published in February 1986; it discussed the most important characteristics of 26 solutions, which were received before December 1985 from 8 participants. A second progress report /5/ was prepared for presentation at the 13th International Symposium on the Effects of Radiation on Materials, Seattle, June 23-25, 1986. This summarizing paper, entitled "Improvement of accuracy assessment in radiation damage predictions" gave some early results, based on the examination of 39 solutions from 10 participants, which were received before February 1986.

A third progress report /6/ (June 1986) gives a summary of the participants' results such as

- the presentation and ordering of the results submitted by the participants;
- the intercomparison of the numerical results;
- the consideration of specific problems mentioned by the participants in the neutron spectrum adjustment.

The evaluation of the data and writing of these progress reports was done by a joint team from ECN (Petten, the Netherlands) and BME (Budapest, Hungary).

The discussions of this meeting - related to the topical problems of the neutron spectrum adjustment and uncertainty assessment of integral (damage) parameters - were based on references /4-9/, furthermore on Appendices 1-3.

Future actions and recommmendations stated during the meeting are also involved in this report.

2. Summary of results

In frame of the REAL84 exercise 7 neutron spectra were investigated. Uptil the 25th February, 1986 39 different solutions from 10 laboratories were obtained. Numerical results and other information on the solutions are presented in /6/.

The main conclusions as mentioned in /6/ are as follows.

2.1. The situation with respect to consistency and quality of the input data is disappointing. Sometimes large inconsistencies in the input data set were found (PS1, PS2, CFR), detected e.g. by the χ^2-value (Table 1) or by deviating reaction rates. The participants had different actions for the solution of this problem. They changed the weight (variance) of some reaction rates in the calculations, deleted reactions from the adjustment, or modified the input spectrum.

2.2. For all seven spectra (ANO, PS1, PS2, TAN, RTN, U35, CFR) finer group structure in the low energy region, in other cases (ANO, U35, CFR) in the high energy region (above 3-6 MeV) would have been required for a better characterization of these parts of the spectra.

2.3. The uncertainty of the input spectrum was very large for ANO, and very small for U35 and CFR. As a result, no real spectrum adjustment could be expected in the latter cases.

2.4. Physics based, calculated correlation matrices were available for the spectra ANO, PS1, PS2, U35, CFR. In other cases "good estimates" or artificially created correlation matrices were used. As the input (and output) spectrum covariance matrix has an important role in the uncertainty assessment of the damage parameters, the lack of realistic data will lead to an incorrect estimate of the corresponding standard deviations.

2.5. Identical input spectrum correlation matrices were given for the spectra PS1 and PS2. As these spectra represent different irradiation positions, the two correlation matrices can not be the same. At this moment it is not yet clear which of the two positions the given correlation information is belonging to.

2.6. All input spectrum covariance matrices were found to be singular within computer accuracy. (Table 2)

2.7. In some cases (e.g. spectrum ANO and PS1) very large uncertainties for the measured reaction rates were found.

2.8. Only variances for the measured reaction rates were given for many of the spectra . In these cases diagonal covariance matrices had to be used in the calculations.

2.9. Sometimes not enough experimentally determined reaction rates were available (e.g.in case of ANO).

2.10. In a number of cases clearly inadequate values for cross-sections and cross-section uncertainties deriving from the most up-to-date version of ENDF/B-V and IRDF85 libraries were found by several participants.

2.11. In a late phase of the exercise it was communicated that in case of the spectrum PS1 all detectors were irradiated in a gadolinium cover. However, the total

Table 1

RANGE of χ^2 VALUES for input data sets

SPECTRUM	LOWEST VALUE		HIGHEST VALUE	
ANO	0.16*	SET5; m = 55	0.36	SET3; m = 100
PS1	1.00	SET6; m = 37	1.63	SET3; m = 98
PS2	0.52	SET6; m = 37	17.4	SET5; m = 37
TAN	0.98*	SET3; m =100	2.57	SET6; m = 39
RTN	0.47*	SET3A;m = 89	3.39	SET7; m = 60
U35	1.47	SET9; m = 24	0.58	SET7; m = 22
CFR	1.59	SET5; m = 26	7.07	SET6; m = 26

* : exclusive SET10 (SAND-MX; m = 215)
m : number of groups

Table 2

EFFECTIVE RANK of CORRELATION MATRICES

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

m : number of groups

λ_i : eigenvalues

cross-section of the Gd was made available, not all participants were in the position to perform the necessary corrections.

2.12. The solutions were in a number of cases given in a group structure (eg. 98, 100, 215) different from the given input. Sometimes more solutions by a participant for the same spectrum were supplied,using different adjustment codes and/or different energy group structures.

2.13. Most of the calculations were performed by codes based on the generalized least squares procedure, exept the two cases, were a SAND-type code - in one case combined with Monte-Carlo uncertainty analysis - was used. This case gave practically the same results as the least squares ones.

2.14. Different normalizations on the input reaction rates were in many cases used by the participants. This fact resulted in different input spectra, which of course led to deviating solutions.

2.15. Often large spread in the calculated input and output reaction rates can be observed (PS1, PS2, CFR). This fact indicates the presence of inconsistencies in the input data set and/or reflects the effect of different data treatment and calculation procedures applied by the participants.

2.16. The aim of the exercise was to get an impression of the interlaboratory differences in the estimates for the integral (damage) parameters and their uncertainties used in the lifetime assessment of reactor pressure vessels in order to arrive at better and reproducible methods. Ideally, one would like to obtain for the given data set only one unique answer (one unique final parameter value with one final value for its standard deviation).

Nevertheless, the comparison of the results shows that the participants' values have some spread (Table 4). Differences in the outcomes might be due to differences in mathematical-statistical procedures (rounding uncertainties, word length, matrix inversion procedures, optimalization procedures, etc.) or in physics based modifications (group structure, spectrum extrapolations, deletion of reaction rates,

Table 3

ROLE of CROSS-SECTION UNCERTAINTIES

	ANO	PS1	PS2	TAN	RTN	U35	CFR	φ_{th}	$\varphi_{1/E}$	φ_{fiss}
$^{6}Li(n,\alpha)$							0	0	0	0
$^{10}B\ (n,\alpha)$							0	0	0	-
$^{27}Al(n,p)$						-	-			-
$^{27}Al(n,\alpha)$				0	0	-	-			-
$^{45}Sc(n,\gamma)$		0	0	-	0		0	0	0	0
$^{46}Ti(n,p)$	--	--	--	--	--	--	--			--
$^{47}Ti(n,p)$				--	--	--	--		--	--
$^{48}Ti(n,p)$				--	--	--	--			--
$^{54}Fe(n,p)$	0	0	0	0	-	0	0		-	0
$^{55}Mn(n,2n)$						--				--
$^{56}Fe(n,p)$				0		0				0
$^{58}Fe(n,\gamma)$		--	--				--	-	--	--
$^{58}Ni(n,p)$		-	-	-	--	-	-		-	-
$^{58}Ni(n,2n)$	-			--	--	--				--
$^{59}Co(n,\gamma)$		0	0	-	0		0	0	0	0
$^{59}Co(n,\alpha)$				0		0				0
$^{59}Co(n,2n)$				-	-					--
$^{60}Ni(n,p)$				-	-					-
$^{63}Cu(n,\gamma)$						--	-	0	0	--
$^{63}Cu(n,\alpha)$	-	-				-				-
$^{115}In(n,\gamma)$						0	0	-	-	0
$^{115}In(n,n')$				--		--	--		--	--
$^{127}I\ (n,2n)$						--				--
$^{197}Au(n,\gamma)$				--	0	-	0	0	0	-
$^{232}Th(n,\gamma)$							--	-	--	--
$^{232}Th(n,f)$						-	-		-	-
$^{235}U\ (n,f)$		0		0		0	0	0	0	0
$^{237}Np(n,f)$		-				-	-	--	--	-
$^{238}U\ (n,\gamma)$				--			0	0	0	0
$^{238}U\ (n,f)$	0	0		0		0	0	--	-	0
$^{239}Pu(n,f)$	-					0	0	0	-	0

0 : uncertainty 0- 5%

- : uncertainty 5-10%

-- : uncertainty > 10%

modification of covariance matrices, introduction of other cross-section sets, etc.).

In evaluation of the participants' responses one should keep in mind that these results are not independent data, but they are all based on the same input set of observations.

The deviation in the results - apart from some clearly outlying data - is within the average of the predicted standard deviation of the given parameter for all the spectra. That means that the different procedures applied by the participants did not lead in the present cases to significant differences in the results. Nevertheless, the observed deviations are considered as "unwelcome" events, as they lead to undesirable differences in the lifetime prediction of reactor pressure vessels.

2.17. For a number of cases the uncertainty values of integral parameters determined by the different laboratories show a large spread (Table 5). Differences by a factor greater than 3 do sometimes occur between standard deviations reported by the different participants. For the thermal and intermediate neutron energy region these data have a limited importance due to the rough energy group structure in this part of the spectrum. The observed very large spread in the standard deviation of

Table 4

INTERLABORATORY VARIATION

Spread in results for important output parameters

The symbol n denotes the number of solutions for each case

SPECTRUM	ANO	PS1	PS2	TAN
φ (> 0.1 MeV)	3.1%* (n=10)	5.0% (n=4)	15.4% (n=5)	8.5% (n=4)
R_{dpa} (Fe)	3.8% (n=10)	3.5% (n=3)	13.1% (n=5)	**
R_{He} (steel)	3.3% (n=8)	6.5% (n=3)	8.3% (n=4)	**
R_H (steel)	2.6% (n=8)	3.6% (n=3)	8.6% (n=4)	**

SPECTRUM	RTN	U35	CFR
φ (> 0.1MeV)	4.5% (n=6)	1.9% (n=6)	4.0% (n=3)
R_{dpa} (Fe)	1.5% (n=2)	2.4% (n=6)	2.3% (n=3)
R_{He} (steel)	4.1% (n=2)	4.9% (n=6)	17.3% (n=3)
R_H (steel)	4.1% (n=2)	3.0% (n=6)	5.6% (n=3)

* : exclusive one outlier
** : only one solution

Table 5

RANGE of REPORTED VARIATION COEFFIECIENTS

n = number of solutions

SPECTRUM	ANO	PS1	PS2	TAN
σ in φ (> 0.1MeV)	9.3-12.1% n=10	5.9- 6.3% n=3	5.5-16.7% n=5	2.3-2.4% n=3
σ in R_{dpa} (Fe)	7.7-13.3% n=10	8.9-11.5% n=3	5.5-13.7% n=5	0.5% n=1
σ in R_{He} (steel)	5.7-20.8% n=7	9.4-13.1% n=2	5.5-12.6% n=3	-
σ in R_H (steel)	5.7-19.8% n=7	8.5-11.6% n=2	5.3-11.7% n=3	-

SPECTRUM	RTN	U35	CFR
σ in φ (> 0.1MeV)	3.2- 4.5% n=5	0.1- 1.4% n=3	0.5- 0.6% n=3
σ in R_{dpa} (Fe)	10.5-10.6% n=2	8.4-10.8% n=6	7.2-10.8% n=3
σ in R_{He} (steel)	7.9% n=1	8.3-10.6% n=5	8.6-10.5% n=2
σ in R_H (steel)	7.8% n=1	7.6-10.3% n=5	7.9-10.2% n=2

integral (damage) parameters indicates that they are very sensitive to the different data treatment and calculation procedures. Basically, they are determined by the covariance information of the cross-section and spectrum data applied. Any deviation from the input covariance information specified for the exercise will be reflected by the uncertainty values discussed here. This circumstance underlines the importance of this exercise in the improvement of uncertainty predictions for damage parameters, furthermore, it indicates the necessity of some kind of standardization for the adjustment data treatment and uncertainty assessment of radiation damage data.

2.18. After adjustment, the spectrum contribution to the standard deviation of the integral data has significantly decreased. Therefore, the uncertainty of the output reaction rates and damage parameters is in most cases determined by the uncertainty contribution of the corresponding displacement and gas production cross-sections.

At the same time, the cross-section uncertainties (derived from the ENDF/B-V file) are for a number of reactions rather high and no uncertainties for the damage cross-sections are at this moment available. Artificial data (10 % for Fe, 12 % for Ni and 18 % for Cr) were chosen for this exercise.

3. Improvement in uncertainty assessment of damage parameters due to REAL84

In the course of the exercise a number of points were observed which have the effect of increasing the uncertainty values of the damage parameters. A few of these points were elaborated.

3.1. Nuclear data aspects

Inadequate and lacking cross-section values

In the REAL84 exercise the distributed input data contained among others cross-section files for the reactions of interest. The most complete cross-section file in the exercise is the IRDF-85. But even in this library a number of reactions which can be important for neutron metrology is lacking. For instance cross-section data are not available for he reactions: $^{45}Sc(n,2n)$, $^{52}Cr(n,p)$, $^{54}Fe(n,p)$, $^{65}Zn(n,\gamma)$, $^{59}Co(n,p)$, $^{88}Y(n,2n)$, $^{93}Nb(n,\gamma)$, $^{93}Nb(n,2n)$, $^{109}Ag(n,\gamma)$, $^{169}Tm(n,2n)$, $^{197}Au(n,2n)$, $^{197}Au(n,3n)$ and $^{238}U(n,2n)$.

These reactions are especially important in the case of fusion neutron metrology. In this exercise several reaction rates had to be deleted from the input due to lack of cross-section data.

For a number of these reactions evaluations are available which are not yet incorporated in metrology cross-section files.

Another source of cross-section files is the Lepricon library /10/, which contains adjusted cross-section data. The consequence of the application of these adjusted data can not be overseen so easily owing to the possible correlations introduced by the procedure of deriving this set.

The cross-section data in the IRDF-85 are not always correct. Clearly inadequate cross-section data were found by several participants for a number of reactions, e.g. $^{47}Ti(n,p)^{47}Sc$, $^{58}Fe(n,\gamma)^{59}Fe$. Furthermore, the cross-section values for the reaction $^{115}In(n,\gamma)^{116}In^{m}$ had to be calculated from the total capture cross-section of ^{115}In given in the IRDF-85 file.

The application of the cross-section data for $^{58}Fe(n,\gamma)$, may lead to inconsistent results when in the metrology procedure not the same isotopic abundance is applied as in the evaluation of the cross-section data. Of course this holds also for other nuclides but in the case of $^{58}Fe(n,\gamma)$ reaction an important change in the abundances has occurred.

In case of the $^{47}Ti(n,p)$ reaction deviations up to 30% can be found in the measured and calculated reaction rates of an adjustment run depending on the spectrum.

A confusion is present due to the release of two versions of the ENDF/B-V dosimetry file (TAPE 531). These versions show a number of changes for various reactions. Among others this can be observed for the threshold reactions $^{58}Co(n,p)$ and $^{54}Fe(n,p)$. The first version showed a small sub-threshold cross-section for these two reactions while the corrected second version missed this contribution.

The IRDF-85 as applied in REAL84 contains the second version of the ENDF/B-V dosimetry file.

Inadequate and lacking cross-section uncertainties

In the adjustment procedure cross-section uncertainties in the form of covariance values are needed. A number of reactions in the IRDF-85 has this information (Table 3). But for several cross-sections including gas production and displacement cross-sections uncertainty data are completely missing which excludes these reactions from the input of a neutron spectrum adjustment, or does not allow proper estimate of the uncertainty of the damage parameters. The uncertainty of damage cross-section values is especially important if damage parameters for different neutron spectra have to be compared.

The quality of the uncertainty data in IRDF-85 is difficult to judge. But the opinion of the meeting was that the definition of the untertainties was probably not the same for all the reactions, and this might be a source of inconsistencies observed during the spectrum adjustment. Also the too coarse group structure with large jumps in the uncertainty data seems to be not realistic (e.g. $^{197}Au(n,\gamma)$ reaction). For all reactions the numerical rank (i.e the effective rank) of the uncertainty matrix is relatively small so that for most of the group structures singular covariance matrices will be obtained. Table 3 shows also that the reaction rate uncertainties calculated for reference spectra are rather large; this fact indicates of course large uncertainties for the cross-sections. These reactions with large uncertainties will in general not contribute much information in the adjustment when also reactions with small uncertainty data are applied.

This can be illustrated with the incorrect cross-section data for $^{47}Ti(n,p)$. When the deviation of the calculated and measured reaction rates for this reaction in

an adjusment run is divided by the uncertainty of its cross-section, a relatively small number is obtained This number does not show the presence of incorrect cross-section values in this case.

A clear numerical error is present in the uncertainty data of $^{93}Nb(n,n')$ of the IRDF-85. This was detected by several participants.

In a few cases cross-correlations are present between various reaction cross-sections of the IRDF-85 library. These data were not used by the participants. The influence of the neglection of these cross-correlations on the results cannot be estimated yet, but presumably its effect is rather small.

3.2. Mathematics aspects

Singularaty and rank of covariance matrices

For characterizing the covariance information, the standardized form of the $\underline{C}$ covariance and $\underline{R}$ correlation matrices can be used:

$$\underline{C} = \underline{U}_c \underline{\Lambda}_c \underline{U}_c^T \quad \text{and} \quad \underline{R} = \underline{U}_R \underline{\Lambda}_R \underline{U}_R^T$$

where $\underline{U}$ is a matrix consisting of the eigenvectors and where $\underline{\Lambda}$ is a diagonal matrix with the eigenvalues λ_i as elements. In sense of mathematical statistics the covariance and correlation matrices are positive definite matrices, i.e. for the ordered eigenvalues one has the relations

$$\lambda_1 \geqslant \lambda_2 \geqslant \lambda_3 \geqslant \ldots \geqslant \lambda_n > 0$$

However in most of the input spectrum covariance matrices of the REAL84 exercise, zero and negative eigenvalues have been found in the matrix (see Appendix 2). In the following part of this chapter we use the expressions "covariance" and "correlation" matrix also in those cases, when the referred information does not fulfil the requirements of covariance (and correlation) matrices in sense of mathematical statistics.

The numerical treatment of these matrices leads to difficulties. Some of the eigenvalues can be smaller by several order of magnitudes than the largest one. These values will be substituted by the computers with zeros, due to the underflow during their processing. One can determine the number of eigenvalues treated by the computer as non-zero values. This number represents the numerical (i.e. effective) rank. This number will depend to some extent on the computer precision.

The use of the correlation matrix instead of the covariance matrix in the chi-square calculation can solve certain numerical problems. One can generally write:

$$\chi^2 = \underline{d}^T \underline{C}^{-1} \underline{d}$$

where $\underline{d}$ is a vector of the differences between the observed and the expected values, and $\underline{C}$ is the corresponding related covariance matrix. At the same time,

$$\underline{C} = \underline{S}\,\underline{R}\,\underline{S}$$

where $\underline{S}$ is a diagonal matrix containing the standard deviations. Then

$$\chi^2 = (\underline{d}^T \underline{S}^{-1})\ \underline{R}^{-1}\ (\underline{S}^{-1} \underline{d})$$

This means, that the correlation matrix should be inverted instead of the covariance matrix, transforming the eigenvalues of the matrix to be inverted into a narrower range. The differences in $\underline{d}$ are then given in "confidence units".

Another way to determine the numerical rank of a correlation matrix consists in counting the number of ordered eigenvalues constituting nearly 100 per cent of the trace of the matrix /8,12/. (See Table 2)

In general, the rank of a covariance or correlation matrix is a measure for the "amount of physical information". The rank gives information about the essential number of independent variables involved. Therefore it is related the number of degrees of freedom for spectrum modifications in the adjustment procedure.

Table 6

EVALUATION PROCEDURES USED
by the PARTICIPANTS of the REAL84 EXERCISE

CODES USED

many STAY'SL types
NEUPAC
LEPRICON-methodology
SAND II type + Monte Carlo (SET9 ; SET10)

NORMALIZATION

SET5 $\quad f_1 = [\Sigma \alpha_i^c \alpha_i^m]/[\Sigma \alpha_i^c \alpha_i^c]$

SET1, SET9; SET10 $\quad f_2 = \Sigma [\alpha_i^m/\alpha_i^c]/n$

SET2; SET6, SET7 $\quad f_\Delta = [(\underline{A}_c)^T \underline{W} (A_c)]^{-1} [(A^c)^T W(A^m)]$

FITTING PARAMETER

SET1; SET2

SET3; SET7, SET5; SET6; SET8 $\quad \chi^2 = (\underline{A}^m - \underline{A}^c)^T \underline{W} (\underline{A}^m - \underline{A}^c)$

where A^c is based on input data

SET9 $\quad \sqrt{\frac{1}{n} \Sigma [(A_i^m - A_i^c)^2/\mathrm{var}(A_i^m)]}$

SET10 $\quad \sqrt{\frac{1}{n} \Sigma [(A_i^c - A_i^m)/A_i^m]^2}$

Conversion of covariance (correlation) matrices from one to another group structure

Both the neutron fluence rate per energy and the energy dependent cross-sections are continuous functions. These are approximated in most of the neutron spectrum adjustment codes by histogram-like functions defining certain "group-averaged" quantities.

The cross-section values are available in the libraries of the ENDF/B structure (e.g.IRDF-85) in continuous form, by means of point values and interpolation rules. Similar situations can be present with respect of the calculated neutron spectra derived with certain neutron transport codes.

It should be stated, that the cross-section covariance matrices (at least of the type of File 33) are given as two dimensional histograms. If one needs a finer energy grid

than is given in the library, the correlation coefficients in all fine groups within a coarse group will be equal, making in this way the new correlation (covariance) matrix singular. The situation in connection with the neutron spectrum covariance matrices is similar. In both cases,extra physical information is required to obtain regular matrices.

Further investigations of these covariance matrices should provide a list of conditions which must be fulfilled in transforming a covariance matrix from one group structure to another one. Computer programs for such transformation - handling the data in a consistent way - seem not to be available yet.

The participants of the Consultants' Meeting agreed that the interpolation procedure should preserve the physical information given in the covariance matrix, e.g. keep the same numerical (e.g. 98%) rank. The extra information originating from the interpolation procedure should not exceed a low limit (e.g. 2%). The modified matrix should be positive definite. If these conditions are fulfilled, then a correct uncertainty propagation analysis can be performed to determine the uncertainty of the output. Nevertheless, if negative eigenvalues of rather high absolute value are present, this process should not be used; the original matrix has then to be checked from physics point of view and may be modified so that adjusted and acceptable eigenvalues are obtained.

Least squares algorithms

In the exercise least squares codes of STAY'SL type were often used. These codes apply a linearized model, and invert only reaction rate covariance matrices. In cases when no inconsistencies in the input data set are present this method gives a good result. For other cases development of a code using a non-linear model for the χ^2 calculation had formerly been suggested /11/. The advantages and present status of this code (called EAGLE) are detailed in Appendix 3. At the same time one should keep in mind that inversion of (both input spectrum and cross-section) covariance matrices is necessary for the calculations in this case, which requires the availability of positive definite matrices. For the majority of covariance matrices available in frame of the REAL84 exercise this assumption does not hold.

In case of using STAY'SL type codes from a mathematical point of view the rank of the output fluence rate covariance matrix should be lower or equal to the rank of the input matrix. Any increase of the rank by the adjustment procedure (see REAL80 results (possibly REAL84 results)) corresponds to the addition of non-relevant information to the spectrum by the computing procedure. The increase in rank between input and output covariance matrices therefore quantifies the modelling and rounding errors involved in the calculations.

3.3. Physics procedures

Uncertainties for displacement damage

The calculation of displacement damage cross-sections involves an integral over the recoil atom energy distribution and a secondary displacement model. The recoil distributions are calculated directly from nuclear interaction cross-sections and angular distributions. Uncertainties and correlations can be rigorously assigned to both the cros-ssections and angular distributions. Consequently, uncertainties and correlations can be determined for the recoil atom energy distribution. The secondary displacement function on the other hand is only a model, usually due to Lindhard, and no uncertainty information assignment is possible. Hence, it is recommended that uncertainties and correlations have to be developed for the nuclear data part of the damage calculation. These values can then be combined with the neutron fluence rate uncertainties and correlations to result in a more reliable estimate of the uncertainties in damage calculations. This is especially needed for the comparison of damage between different facilities. This effort may also be facilitated by the release of new recoil atom distribution with uncertainty files in ENDF/B-VI (date of release uncertain).

Displacement damage for compound materials

There has been some concern about the calculation of displacement damage for compound materials. In lieu of better calculation a linear combination of the elements is often used. A new computer code, SPECOMP has been developed / 13 /, wich calculates compound damage directly. This code makes use of the SPECTER recoil atom energy distribution and integrates over all possible combinations of recoil ion and matrix atoms. Preliminary results show that there are large differences (30-40%) compared to the linear sum for compounds having a large difference in the mass of the elements (e.g. LiO_2, $LiAlO_2$) but smaller differences (< 10%) for compounds with similar element masses (e.g. SiO_2, Al_2O_3); see Figures 1 and 2 and Table 7. Calculations for other compounds are in progress and results will be reported in Jackson Hole at the next ASTM-EURATOM Symposium on Reactor Dosimetry, May 1987. However, it is expected that differences between SPECOMP and a linear sum from SPECTER will not be very large for alloys such as stainless steel.

The consequences for the damage cross-section of different material structures of the same chemical composition of a certain type stainless steel have not been investigated yet.

The weighting spectrum

The relatively large interlaboratory spread which is found in the results will be partly due to the definition by participants of the weighting spectrum. The weighting spectrum has an important role in the conversion of the continuous cross-section information and its covariances to group values required in the adjustment. Differences in definiton of the input spectrum may lead to deviations in the group values which can seriously effect the results. Of course this phenomenon is the strongest in energy regions with sharp changes in the spectrum or cross-section values. The solution of this problem is not so simple because in general the input spectrum is calculated in a rather coarse group structure in a limited energy region. This input spectrum has then to be extrapolated in the low and high energy regions using an appropriate procedure supplying a smooth character for the calculated spectrum. The conversion and smoothing procedure should conserve the input spectrum information and the extra

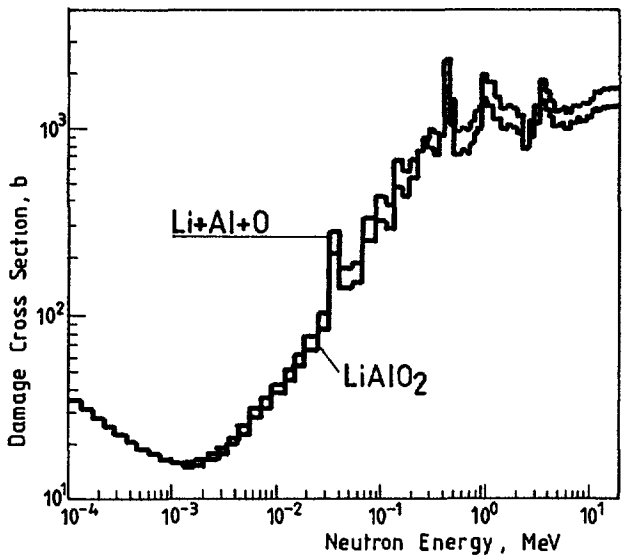

Fig 1
Displacement damage cross-sections

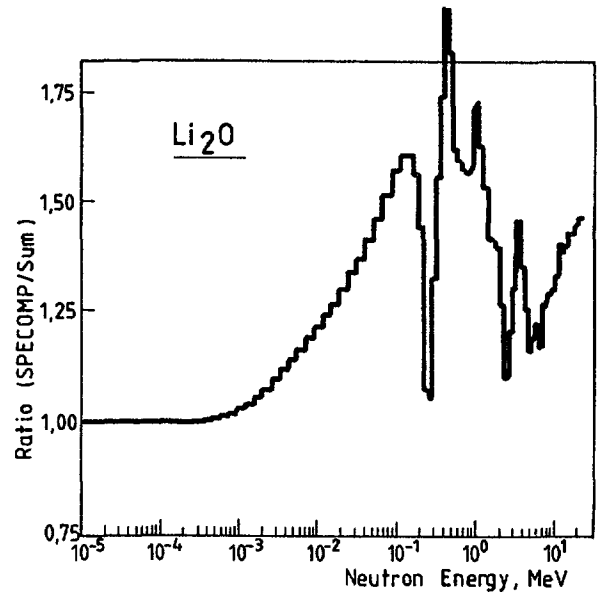

Fig. 2.
Displacement damage cross-section

Table 7

SPECOMP Results

Spectral-averaged dpa cross sections, b

Compound		14 MeV	Fusion	HFIR	EBR II
Li_2O	SPECOMP	1040.	754.	2410.	939.
	Sum	728.	517.	2321.	636.
$LiAlO_2$	SPECOMP	1648.	978.	1120.	1031.
	Sum	1336.	777.	1050.	808.
Al_2O_3	SPECOMP	1685.	935.	303.	924.
	Sum	1718.	945.	304.	925.
Si_2O	SPECOMP	1700.	938.	305.	944.
	Sum	1764.	955.	306.	943.

information added by the exptrapolation should be reliable. Of course, this procedure will give inaccurate results if the group structure of the input spectrum masks already spectrum details due to its coarseness. In principle an iteration procedure might be tested in which the output spectrum information is used again as weighting spectrum etc.

It is felt that an improved input spectrum definition will reduce the spread in the results of the various laboratories. The required extra input spectrum information (i.e. extrapolation and smoothing procedures) should be made available to the participants in a tested form to reduce the interlaboratory spread. It would be a step forward if software for this smoothing and extrapolation could also be further developed and made available to the neutron metrology community.

Covariance matrices for reaction rates

In the development of covariance matrices a careful uncertainty analysis has to be performed. For semiconductor spectrometers uncertainty contribution due to e.g. the interpolation of efficiency curves and to the gamma ray emission probabilities of the radionuclides involved in calibration and measurement should be taken into account. There might be a cross-correlation between the measured activity and cross-section values resulting from the gamma ray emission probability.

The presence and importance of cross-correlations between reaction rates and cross-sections should also be investigated. Due to all these effects the relative importance of the different reaction rates in the adjustment procedure can be altered.

The existing computer codes in this field (e.g. /9,14/) have to be tested and some improvements have to be made if necessary.

Inconsistencies of input data

In the input data of the REAL84 several inconsistencies were detected by the participants. In most cases the inconsistencies were detected from a too high (or too low) value of the chi-square value or from an outlying reaction rate ratio in the adjustment run. The reason of the inconsistency was stated in a number of cases (e.g. incorrect cross-section for $^{47}Ti(n,p)$, a too coarse input spectrum structure for de CFRMF in the resonance region of $^{59}Co(n,\gamma)$ and for the fusion spectra in the high energy region). In other cases the reason of the inconsistency could not be traced.

To eliminate the inconsistency a variety of methods were applied which contributed also to the relatively large inter-laboratory spread. The methods comprised:

- deletion of reaction rate(s),
- increase of standard deviation of measured activity in the adjustment run,
- modification of input spectrum (in one or more groups),
- modification of the uncertainty of the input spectrum (in one or more groups).

It was felt in the meeting that a more systematic way to treat inconsistencies of the input data in the adjustment is needed. Of course this method should comprise the investigation of the physics background of the data.

Input spectrum

Most input specta used in the exercise suffered from the poorness of information in the low energy region. This sometimes originated from a too coarse group structure in the neutron energy range of interest (e.g. PS2, TAN, RTN and U35), while in other cases spectrum data below 0.5-1 eV were not present (e.g. ANO, PS1 and CFR).

Similar problems, e.g. rough group structure, were also encountered in the high energy region of some spectra.

Due to the inadequate spectrum information the participants had to perform extrapolations in the neutron energy region of interest. The type of the extrapolation was not defined. Thereafter different normalizations and scaling factors were applied leading to non-negligible deviations in the input spectra.

Therefore the participants of this meeting have the opinion that better (and more detailed i.e. finer group structure) information is needed both in the low and high energy range of the input spectra. Furthermore, normalization procedure based on the least squares procedure /15/ is recommended. The input neutron spectrum has to be accompanied by proper uncertainty information in the form of covariance matrices. It was stated, that in cases when no covariance information for the input spectrum is available it is better to use physics based approximation (from another similar type reactor) than an artifical band matrix. It may be useful to state the rank information of the input covariance matrix in order to estimate the number of independent "statistical" parameters involved.

Covers and neutron selfshielding

The exercise comprised sometimes reaction rates inside covers or reaction rates determined for thick foils. In this case cross-section values corrected for these effects should be applied. This correction was sometimes obtained with a rather simple mathematical relation. This approach does not always yield reliable results. The correction especially for thick ^{10}B covers and for the reaction $^{59}Co(n,\gamma)$ remains uncertain.

This situation can somewhat be improved by application of the total cross-section instead of the activation cross section in the selfshielding calculations. But even in this case the reliability remains low. If the correction is important the best way is probably to perform calculations with a reactor physics transport code. Nevertheless, one can decrease the selfshielding effects by applying diluted foils of the target material in the detector set. This has also the advantage that the original cross-section uncertainty information can be applied as a good estimate of the corrected cross-sections. At the same time, for an important cross-section correction a more complicated uncertainty calculation will be required, e.g. if corrections are introduced for more reactions, cross covariances have also to be taken into account.

The situation in this field is unsatisfactory at this moment, and needs more attention in the future. Also software should be made available to perform simple and complicated selfshielding corrections and to estimate the uncertainties of the resulting corrected cross-sections.

4. Evaluation procedures

Evaluation procedures for the exercise

The magnetic tape distributed to the participants of the exercise comprised the input data for the neutron spectra to be investigated, furthermore, utility programs for data processing were also available. The participants used their own adjustment code, normalization procedure and fitting parameter in evaluation of the neutron spectra. The most important procedures applied are listed in Table 6.

Interlaboratory spread

The intercomparison of the results for the damage parameters of the REAL84 exercise show that the participants' values have a few percent spread /6/. Differences in the outcomes might be due to:

a., The application of incorrect physical information
b., Algorithm (modelling) shortcomings
c., Computer accuracies
d., real mistakes

Especially large spread (sometimes a factor greater than 3) in the uncertainty values of integral parameters was observed in a number of cases. This indicates that they are very sensitive to the data treatment and calculation procedures. This circumstance underlines the importance of this exercise in the improvement of uncertainty predictions for damage parameters, furthermore it indicates the necessity of

some kind of standardization for the adjustment data treatment and uncertainty assessment of radiation damage data.

5. Practical aspects

Utility programs and libraries

In the meeting it was stated, that it was useful and an improvement in respect to REAL80, that now a few utility programs were made available also to the participants. Especially the two versions of the program UNC33 to convert the IRDF-85 uncertainty data to the required group structure proved to be a help. It was a pity that a few programming errors were present in the software. In general, the effect of these errors was small. Only in the case of $^{239}Pu(n,f)$ differences for the uncertainties in the low energy groups were encountered.

The programs being available were:

- UNC 33 (FORTRAN 77)
- UNC 33 (FORTRAN IV)
- FITOCO
- GROUPIE
- LINEAR

The libraries and utility programs to read the cross section and uncertainty libraries were:

- IRDF-85
- CS640
- Uncertainties of the resonance parameters for $^{237}Np(n,f)$, $^{58}Fe(n,\gamma)$ and $^{63}Cu(n,\gamma)$.

6. Recommendations

6.1. Recommendations for neutron spectrum adjustments

1. In computer calculations it is for numerical reasons better to work with correlation matrices than with covariance matrices.
2. For the characterization of input and output data for neutron spectrum adjustment one should quote:
   a) the measured (or calculated) values;
   b) their variances;
   c) the related correlation matrices;
   d) if possible, the numerical (i.e. effective) rank of the correlation matrix, and the way of defining it;
   e) the word length used in computer calculation (for estimation of rounding errors).

   With a view to further calculations, it is recommended to report correlation data in a precise form, and not rounded to 2 or 3 digits.
3. More attention should be given to elimination of inconsistencies in the input data set. In this respect one should try to involve more physics information.
4. In cases where no covariance matrix for the input neutron spectrum is available, one should preferably use a physics based approximation (from another similar type of reactor) rather than an artificial band matrix.
5. In neutron sepctrum adjustments one should distinguish between scaling and normalization. Scaling refers to the determination of a rough spectrum conversion factor (e.g. a power of 10) needed to arrive at comparable values of calculated and measured reaction rates. Normalization refers to the determination of a fine spectrum modifying factor (a factor near unity), needed to arrive at the best fit between calculated and measured reaction rates. The uncertainty of the spectrum normalization factor should be incorporated in the input spectrum covariance matrix (and its associated correlation matrix) before starting the final adjustment procedure.

6.2. Recommendations to the IAEA

1. The Consultants' Meeting recommends that the IAEA Nuclear Data Section prepares an updated version of the International Reactor Dosimetry File (IRDF-86 or IRDF-87), and distributes this version within two years with a good documentation.
2. In order to be able to perform improved uncertainty assessment of integral parameters, one needs for a number of reactions more accurate information than is present in file 33 of IRDF-85.
3. The Concultants' Meeting requests the IAEA Nuclear Data Section, the existing working groups involved in the work on ENDF, and all evaluators involved, to improve the scattering cross-section data and the cross-section variance and covariance data.
4. The Consultants' Meeting requests the IAEA to promote the preparation of a reference data set for neutron sepctrum adjustment procedures, based on the experience obtained in the REAL84 exercise, and comprising a modified and improved data set, preferably with the same spectrum cases as in REAL84 (ACTION: REAL88). The aim of such a reference data set is to provide a tool for testing neutron spectrum adjustment codes by means of an unambiguous test case. The reference data file should preferably comprise also important utility programs.

   The consultants were prepared to provide assistance to this action by running this well chosen and well defined scheduled reference data set on their laboratory computers (ANL, Argonne: VAX, IBM, GRAY; BME, Budapest: IBM; ECN, Petten: CDC; PTB, Braunschweig: Telefunken).

   New tables should be prepared showing the observed spread in results (comprising interlaboratory variation and range of reported variation coefficients) when this well defined reference data set was treated without changes by different laboratories with different adjustment codes with different computers.

   The IAEA should then distribute the resulting reference data set upon request to all experienced or new-coming laboratories interested in neutron spectrum adjustment procedures.

   The consultants recommended that this approach be discussed at the 6th ASTM-Euratom Symposium on Reactor Dosimetry, to be held in Jackson Hole,

Wyoming, USA, May 31 - June 5, 1987 (maybe in a special organized Consultants' Meeting).

5. The Consultants' Meeting recommends that the IAEA Nuclear Data Section convenes in Spring 1988 a next Consultants' Meeting on the REAL88 action, mentioned above.
6. The Consultants' Meeting requests the IAEA Nuclear Data Section to distribute the corrections for the numerical data of the covariance information of the reaction $^{93}Nb(n,n')$ to the users of the IRDF-85 file (see letter to Cullen from Zijp dated 850916).
7. The Consultants' Meeting recommends that the IAEA promotes the establishment and the distribution of a simple reactor physics code which neutron metrologists can use to calculate neutron self-shielding factors and cover attenuation factors, required when in irradiation experiments covers and relatively thick activation detectors (foils and wires) are used. For this purpose the IAEA could e.g. grant a research contract or a fellowship.
8. The Consultants' Meeting requests the IAEA Nuclear Data Section to distribute the report of this meeting.

6.3. Actions

1. ECN-Petten should contact R.E. Maerker at ORNL for making available the cross-section information used in application of the Lepricon methodology.
2. BME-Budapest should make available the modified version of the adjustment code EAGLE, in order to have it tested by a few other laboratories.
3. BME-Budapest should also perform an analysis of covariance matrices for the output neutron spectra.
4. The evaluation team should prepare the final report and the presentation at the Jackson Hole symposium according to the information present in the three progress reports. Attention should be given to the spread in results obtained by participants using exactly the same input data set, to possibilities for using a reduced set of activation detectors for nuclear power plant applications.
5. V. Piksaikin (IAEA-NDS) should communicate to the participants of the meeting the date and location of the next IAEA Advisory Group Meeting on Radiation Damage and Related Safety Aspects.
6. All participants of the meeting should send all available recent and relevant cross-section information to W.L. Zijp (ECN-Petten) before the end of October 1986.
7. L.R. Greenwood (ANL) should document and make available his SPECOM program and his self-shielding program.
8. A. Bosznay (BME) should investigate the proper methods for defining a proper weighting spectrum and, if possible, make available the software serving the purpose.
9. E. Szondi (BME) should make available his program ACORNS (for the calculation of the rank of correlation matrices).
10. H.J. Nolthenius (ECN) should make available an improved version of the programs UNC32 and UNC33 (for the preparation of covariance matrices from ENDF data). E.J. Szondi should then prepare and check an IBM version of these programs.
11. All participants should assist in the preparation of a reference data set (see REAL88 action mentioned in recommendation 4 to the IAEA).

7. Acknowledgement

At the end of the meeting the participants expressed their satisfaction with the results which were obtained by the evaluation team. Also the results of this meeting were considered very fruitful.

Furthermore, the participants thanked for the organisation and the hospitality from the side of the Technical University of Budapest.

V.Piksaikin on behalf of IAEA expressed his thanks to the evaluation team of the exercise, and to the participants of this meeting for their contributions.

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Appendix 1

Results of REAL84 Exercise

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Comments on REAL84 Data

- ANO

  Low-energy flux ill-defined (1 group below .1 MeV)
  - Np(n,f) sensitive to 5 keV
  - Capture damage (dpa) ?

  Large uncertainites in reaction rates

- PS1/PS2

  Normalization uncertain - effects adjustment

  $^{58}Fe(n,\gamma)$ too low?

  Low and high-energy fluxes poorly defined

- CFRMF

  $^{47}Ti(n,p)$ reaction dropped

  Coarse group problem with $^{59}Co(n,\gamma)$ resonance

  Need extrapolation above 10 MeV for some reactions

- U235

  High-energy spectrum inadequate for (n,2n) reactions

- RTN

  Self-shielding for Au (1.98), Co (1.08), and Sc (1.07)

  Low-energy flux not well-defined, but unimportant

- TAN

  Low-energy spectrum unknown, but unimportant

General Comments on REAL84

- Spectrum Definition

  Generally too coarse for some reactions

  Coarse groups require spectral-weighted cross sections

  Low-energy flux Maxwellian? Temperature?

  High-energy region effects (n,α),(n,2n) reaction rates

  Assumptions by participants effect results

- Spectral Covariances

  Not well-defined for finer group structure

  Definition of variances for finer group structure?

  (-e.g. for low- and high-energy extrapolation)

- Conclusions

  Above comments mainly effect details of flux spectrum

  Not very important for integral fluence and damage

  Future projects should minimize these uncertainties

***** RTN Comparison With and Without Au(n,g) and Shielding *****

**** Au(n,g) Included with Correct Shielding ****************************

AK1= 0.0000 VAK= 0.00000 NORM= 0 RENORM= 4.3086E+03 CHI 2 = 5.193 NORM. CHI2 = 0.472

ODOSIMETRY ACTIVITIES O	MEASURED	+OR- %	BEFORE	DIFF %	AFTER	DIFF %	CHI	REACTION	90 % LIMITS	
1	5.994E+13	5.00	6.394E+13	-6.68	5.958E+13	0.60	-0.148	SC45(N,G)SC46	1.00E-10	5.50E-07
2	9.690E+13	5.00	1.045E+14	-7.86	9.791E+13	-1.04	0.337	C059(N,G)C060	1.00E-10	1.00E-04
3	3.850E+14	5.00	4.025E+14	-4.56	3.849E+14	0.02	0.003	AU197(N,G)AU198	1.00E-10	3.00E-05
4	1.140E+14	15.00	1.218E+14	-6.87	1.249E+14	-9.60	0.151	TI246(N,X)SC46	1.45E+01	1.54E+01
5	1.220E+14	25.00	9.249E+13	24.19	9.484E+13	22.26	0.754	TI247(N,X)SC47	1.45E+01	1.54E+01
6	2.550E+13	5.00	2.324E+13	8.85	2.384E+13	6.52	0.373	TI48(N,P)SC48	1.45E+01	1.54E+01
7	1.163E+14	5.00	1.093E+14	6.03	1.121E+14	3.63	0.225	FE54(N,P)MN54	1.45E+01	1.54E+01
8	1.156E+14	5.00	1.267E+14	-9.63	1.300E+14	-12.44	0.367	NI58(N,P)C058	1.45E+01	1.54E+01
9	5.152E+13	5.00	4.076E+13	20.88	4.181E+13	18.86	2.635	NI60(N,P)C060	1.45E+01	1.54E+01
10	4.143E+13	5.00	4.262E+13	-2.86	4.371E+13	-5.49	0.318	AL27(N,A)NA24	1.45E+01	1.54E+01
11	3.130E+14	5.00	3.076E+14	1.71	3.155E+14	-0.80	-0.020	C059(N,2N)C058	1.45E+01	1.54E+01
12	1.509E+13	10.00	1.375E+13	8.87	1.410E+13	6.54	0.198	NI58(N,2N)NI57	1.45E+01	1.54E+01
	STD. DEV. =			11.65		10.57				
	CHISQ =			33.20		25.55				

**** No Au(n,g) and No Shielding **

AK1= 0.0000 VAK= 0.00000 NORM= 0 RENORM= 3.9640E+03 CHI 2 = 7.963 NORM. CHI2 = 0.796

ODOSIMETRY ACTIVITIES O	MEASURED	+OR- %	BEFORE	DIFF %	AFTER	DIFF %	CHI	REACTION	90 % LIMITS	
1	5.994E+13	5.00	7.660E+13	-27.80	6.043E+13	-0.82	1.502	SC45(N,G)SC46	1.00E-10	5.50E-07
2	9.690E+13	5.00	1.182E+14	-21.98	9.609E+13	0.84	-0.261	C059(N,G)C060	1.00E-10	1.00E-04
3	1.140E+14	15.00	1.121E+14	1.68	1.232E+14	-8.04	-0.035	TI246(N,X)SC46	1.45E+01	1.54E+01
4	1.220E+14	25.00	8.509E+13	30.25	9.348E+13	23.37	0.997	TI247(N,X)SC47	1.45E+01	1.54E+01
5	2.550E+13	5.00	2.138E+13	16.14	2.350E+13	7.83	0.900	TI48(N,P)SC48	1.45E+01	1.54E+01
6	1.163E+14	5.00	1.005E+14	13.55	1.105E+14	4.99	0.731	FE54(N,P)MN54	1.45E+01	1.54E+01
7	1.156E+14	5.00	1.166E+14	-0.86	1.281E+14	-10.86	0.035	NI58(N,P)C058	1.45E+01	1.54E+01
8	5.152E+13	5.00	3.750E+13	27.21	4.122E+13	19.99	4.115	NI60(N,P)C060	1.45E+01	1.54E+01
9	4.143E+13	5.00	3.921E+13	5.37	4.309E+13	-4.01	-0.517	AL27(N,A)NA24	1.45E+01	1.54E+01
10	3.130E+14	5.00	2.830E+14	9.58	3.110E+14	0.63	0.035	C059(N,2N)C058	1.45E+01	1.54E+01
11	1.509E+13	10.00	1.265E+13	16.16	1.390E+13	7.88	0.463	NI58(N,2N)NI57	1.45E+01	1.54E+01
	STD. DEV. =			19.34		11.38				
	CHISQ =			106.54		26.65				

******** RTN Flux Comparison With and Without Au(n,g) and Shielding *****

**** Au(n,g) and Neutron Self-Shielding Included ****

GROUP	ENERGY,low	FLUX	FLUENCE	SDEV,%
TOTAL		3.952E+14	3.952E+14 +/-	4.35
	1.000E-10	1.161E-12	1.161E+12 +/-	4.00
	5.500E-07	2.267E+12	2.267E+12 +/-	8.56
	1.275E-03	1.623E+12	1.623E+12 +/-	13.84
	1.000E-01	1.053E+12	1.053E+12 +/-	17.30
	5.000E-01	6.776E+11	6.776E+11 +/-	19.41
	1.000E+00	2.406E+12	2.406E+12 +/-	14.22
	5.000E+00	5.595E+11	5.595E+11 +/-	11.43
	1.000E+01	2.729E+11	2.729E+11 +/-	7.71
	1.200E+01	3.775E+11	3.775E+11 +/-	6.69
	1.400E+01	3.848E+14	3.848E+14 +/-	4.43

RELATIVE COVARIANCES(10X10)

1000	-194	-11	-1	1	31	144	294	335	353
1000	87	0	0	6	28	58	66	70	
1000	317	28	2	0	1	1	1		
1000	565	164	15	2	1	0			
1000	639	139	37	20	5				
1000	640	309	202	87					
1000	799	634	404						
1000	964	832							
1000	949								
1000									

***** No Au(n,g) and No Self-Shielding **********

GROUP	ENERGY.low	FLUX	FLUENCE	SDEV,%
TOTAL		3.889E+14	3.889E+14 +/-	4.44
	1.000E-10	8.990E+11	8.990E+11 +/-	4.42
	5.500E-07	2.071E+12	2.071E+12 +/-	10.07
	1.275E-03	1.493E+12	1.493E+12 +/-	13.84
	1.000E-01	9.691E+11	9.691E+11 +/-	17.30
	5.000E-01	6.247E+11	6.247E+11 +/-	19.41
	1.000E+00	2.260E+12	2.260E+12 +/-	14.21
	5.000E+00	5.534E+11	5.534E+11 +/-	11.45
	1.000E+01	2.768E+11	2.768E+11 +/-	7.81
	1.200E+01	3.827E+11	3.827E+11 +/-	6.81
	1.400E+01	3.794E+14	3.794E+14 +/-	4.52

RELATIVE COVARIANCES(10X10)

1000	-149	-10	-1	1	34	153	310	352	369
1000	79	0	0	2	10	20	23	24	
1000	317	28	2	0	0	0	0		
1000	565	163	14	2	1	0			
1000	636	138	37	20	5				
1000	642	310	203	89					
1000	800	637	412						
1000	965	837							
1000	951								
1000									

******** TAN REAL84 Be(d,n) 16 MeV **********

AK1= 0.0000 VAK= 0.00000 NORM= 0 RENORM= 3.2711E-08 CHI 2 = 9.556 NORM. CHI2 = 0.562

O	MEASURED	+OR- %	BEFORE	DIFF %	AFTER	DIFF %	CHI	REACTION	90 % LIMITS	
1	2.690E+07	3.00	2.644E+07	1.71	2.731E+07	-1.54	-0.095	AL27(N,A)NA24	6.70E+00	1.40E+01
2	3.810E+07	3.00	3.587E+07	5.85	3.401E+07	10.73	0.381	AU197(N,G)AU198	1.10E+01	5.00E+00
3	4.070E+08	3.00	3.935E+08	3.31	3.932E+08	3.39	0.143	NI58(N,P)CO58	3.30E+00	1.20E+01
4	1.110E+06	3.00	1.031E+06	7.16	1.081E+06	2.61	0.111	NI58(N,2N)NI57	1.30E+01	1.80E+01
5	5.350E+07	5.00	4.869E+07	8.99	4.991E+07	6.71	0.330	NI60(N,P)CO60	6.00E+00	1.30E+01
6	1.180E+08	3.00	1.116E+08	5.38	1.135E+08	3.77	0.124	TI46(N,P)SC46	4.50E+00	1.30E+01
7	7.650E+07	10.00	8.078E+07	-5.60	8.084E+07	-5.67	0.129	TI47(N,P)SC47	2.90E+00	1.20E+01
8	1.130E+07	10.00	1.039E+07	8.04	1.075E+07	4.90	0.172	TI48(N,P)SC48	6.70E+00	1.50E+01
9	2.770E+06	3.00	2.726E+06	1.59	2.614E+06	5.64	0.159	SC45(N,G)SC46	6.60E-02	9.00E+00
10	2.740E+07	3.00	2.506E+07	8.56	2.578E+07	5.90	1.661	FE56(N,P)MN56	6.00E+00	1.40E+01
11	3.780E+06	3.00	3.904E+06	-3.27	3.704E+06	2.01	-0.090	CO59(N,G)CO60	1.90E-01	8.20E+00
12	5.650E+06	7.00	5.157E+06	8.72	5.328E+06	5.70	0.563	CO59(N,A)MN56	6.70E+00	1.50E+01
13	3.290E+08	3.00	3.170E+08	3.65	3.170E+08	3.66	0.422	FE54(N,P)MN54	3.30E+00	1.20E+01
14	4.090E+07	3.00	4.044E+07	1.12	4.234E+07	-3.53	-0.019	CO59(N,2N)CO58	1.10E+01	1.70E+01
15	2.670E+08	3.00	2.762E+08	-3.46	2.687E+08	-0.64	0.013	IN115(N,N')IN115	1.40E+00	1.00E+01
16	1.400E+09	3.00	1.571E+09	-12.24	1.538E+09	-9.84	4.023	U235(N,FISSION)	7.20E-01	1.20E+01
17	6.660E+08	3.00	6.951E+08	-4.37	6.898E+08	-3.57	0.570	U238(N,FISSION)	1.80E+00	1.30E+01
18	3.100E+07	3.00	3.521E+07	-13.58	3.285E+07	-5.98	0.960	U238(N,G)U239	1.60E-01	5.50E+00
	STD. DEV. =			7.06		5.56				

SUMMARY OF BROAD-GROUP FLUXES,FLUENCES,AND UNCERTAINTIES

GROUP ENERGY,low	FLUX	FLUENCE	SDEV,%
TOTAL	1.108E+09	1.108E+09 +/-	2.42
1.000E-10	8.154E-02	8.154E-02 +/-	30.41
5.500E-07	1.458E+02	1.458E+02 +/-	25.04
1.000E-04	3.514E+06	3.514E+06 +/-	19.13
1.100E-01	2.765E+07	2.765E+07 +/-	17.91
5.000E-01	7.773E+07	7.773E+07 +/-	7.98
1.000E+00	1.444E+08	1.444E+08 +/-	6.24
2.000E+00	2.936E+08	2.936E+08 +/-	4.73
5.000E+00	4.218E+08	4.218E+08 +/-	2.93
1.000E+01	1.274E+08	1.274E+08 +/-	3.32
1.500E+01	1.220E+07	1.220E+07 +/-	4.79

RELATIVE COVARIANCES(10X10)

1000	1000	1000	1000	45	-545	-257	10	74	40
1000	1000	1000	45	-545	-257	10	74	40	
1000	1000	45	-545	-257	10	74	40		
1000	45	-545	-257	10	74	40			
1000	575	-109	-184	56	102				
1000	501	-87	-129	-20					
1000	495	-278	-329						
1000	374	-60							
1000	840								
1000									

APPENDIX 2.

ANALYSIS OF SOME INPUT COVARIANCE MATRICES OF THE REAL84 EXERCISE

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Introduction

The covariance matrices of some input data for the REAL84 exercise have been analysed. Some characteristic results are presented here in Tables 1 to 4. The effective rank of the matrices was determined using the definitions given in Section 3.2. The following data sets have been investigated:

- covariance matrices derived for the same reaction cross section of the IRDF85 in case of different neutron spectra using the distributed UNC33 code,

- covariance matrices of different reaction cross sections of the IRDF85 derived for the same spectrum using the distributed UNC33 code,

- input spectrum covariance and correlation matrices for all the REAL84 tasks.

Correlation matrices of the FE54P reaction

The covariance information is given as a 8*8 relative covariance matrix in the File 33 of the IRDF85. The effective rank using the 98% definition is less than 8 in all cases, ie part of information has been lost during the data processing. Nevertheless, the computers will insert extra information the amount of which depends on the single/double precision arithmetic processors. The rank of the problem-dependent correlation matrices is less than the number of non-zero cross section groups, ie these matrices are singular, therefore there is no possibility to perform simultaneous adjustment of the neutron spectrum and the cross section. (The characteristic data are given in Table 1.)

Correlation matrices of the CFR cross sections

Depending on the threshold energy, generally the same problems arise, as it has been mentioned in the previous paragraph. Probably due to the relatively high threshold energies of the Al-reactions, the treatment of their covariance matrices does not mean any problem. (The importance of these small size covariance matrices lain out of scope of this analysis.) (See Table 2.)

Table 1.

	IRDF85	ANO	ANO	PS2	U35	CFR
Number of spectrum groups	-	55	16	37	24	26
Number of x-section groups	8	38	16	18	16	11
Number of positive eigenvalues	8	22	12	12	11	8
Number of zero eigenvalues	0	3	2	1	2	2
Number of negative eigenvalues	0	13	2	5	3	1
Effective rank using single precision arithmetic	8	14	10	12	10	7
Effective rank using double precision arithmetic	8	14	10	12	10	8
Number of eigenvalues to the 98% of the trace	8	6	6	7	6	5

Table 2.

	AL27P	AL27A	C059G	AU197G	U235F	FE54P
Number of groups	5	4	26	26	26	11
Number of positive eigenvalues	5	4	13	13	18	8
Number of zero eigenvalues	0	0	8	8	0	2
Number of negative eigenvalues	0	0	5	5	6	1
Effective rank using single precision arithmetic	5	4	15	16	25	7
Effective rank using double precision arithmetic	5	4	15	16	25	8
Number of eigenvalues to the 98% of the trace	5	4	10	8	9	5

Table 3.

(Covariance matrices)

	ANO	ANO	PS1	PS2	RTN	TAN	U35	CFR
Number of groups	55	16	37	37	60	39	24	26
Number of positive eigenvalues	33	16	37	37	49	29	12	20
Number of zero eigenvalues	5	0	0	0	0	0	0	0
Number of negative eigenvalues	17	0	0	0	11	10	12	6
Effective rank using single precision arithmetic	14	14	29	31	1	32	15	22
Effective rank using double precision arithmetic	15	16	37	37	25	38	23	26

Table 4.

(Correlation matrices)

	ANO	ANO	PS1	PS2	RTN	TAN	U35	CFR
Number of groups	55	16	37	37	60	39	24	26
Number of positive eigenvalues	34	16	37	37	40	25	13	20
Number of zero eigenvalues	2	0	0	0	0	0	0	0
Number of negative eigenvalues	19	0	0	0	20	14	11	6
Effective rank using single precision arithmetic	15	16	37	37	60	39	22	26
Effective rank using double precision arithmetic	15	16	37	37	60	39	24	26
Number of eigenvalues to the 98% of the trace	7	9	14	14	12	6	2	6

Input spectrum covariance/correlation matrices

The covariance matrices of the ANO, PS1, PS2 and RTN spectra are positive definite or positive semidefinite, depending on the computer accuracy, while the ones of TAN, U35 and CFR spectra have negative eigenvalues, as well. The number of the zero and negative eigenvalues remains practically unaltered during the covariance ==> correlation matrix transformation, but the effective rank can be increased using this conversion. This case the unfolding procedure cannot insert new, not-physically based relations among the group fluxes of the spectra investigated. Nevertheless, the quality of the original matrices is not sufficient. (The numerical data on the covariance and correlation matrices are given in Tables 3 and 4, respectively.)

APPENDIX 3.

ON THE COMPARISON OF THE NEUTRON SPECTRUM ADJUSTMENT METHODS NAMED STAY'SL AND EAGLE

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In the following remark we shall produce a comparison of the methods STAY'SL [1] and EAGLE (=Elaborated Adjustment by Generalized Least-squares Estimate; a code under development at the Technical University Budapest). We give also some methods to accelerate EAGLE.

We introduce the following notations:

saturation activities (reaction rates) of detectors: $\underline{a} = \begin{pmatrix} a_1 \\ \cdot \\ \cdot \\ \cdot \\ a_n \end{pmatrix}$

covariance matrix of them (n*n): cov($\underline{a}$)

detector cross sections: $\underline{\underline{\sigma}} = \begin{pmatrix} \sigma_{11} \dots \sigma_{1n} \\ \cdot \quad\quad \cdot \\ \cdot \quad\quad \cdot \\ \cdot \quad\quad \cdot \\ \sigma_{m1} \dots \sigma_{mn} \end{pmatrix}$

(so σ_{kl} is the cross section of l-th detector for K-th group)

neutron spectrum: $\underline{\Psi} = \begin{pmatrix} \Psi_1 \\ \cdot \\ \cdot \\ \cdot \\ \Psi_m \end{pmatrix}$

In a non-realistic case, one would solve the following system of linear equations, and the whole adjustment procedure would be unnecessary:

$$a_i = \sum_{j=1}^{m} \sigma_{ji}\, \Psi_j \qquad (i=1,\dots,n)$$

This cannot be made because of the following two problems:

- $n < m$
- uncertainties in $\underline{\underline{G}}$ (and $\underline{a}$)

The following questions naturally arise:

- How add new information to ensure the uniqueness of solution?
- How to treat the approximations of the (numerical) model?

In case of STAY'SL the following assumptions have been made:

(1) $$\Delta_{\underline{a}} = \underline{\underline{G}} \begin{bmatrix} \Delta\underline{\psi} \\ \Delta\underline{\Sigma} \end{bmatrix}$$

where:

$$\underline{\Sigma}^T = \left(\sigma_{11} \ldots \sigma_{m1} \ldots \sigma_{1k} \ldots \sigma_{mk} \ldots \sigma_{1n} \ldots \sigma_{mn}\right)^T$$

and $\underline{\underline{G}}$ is the (fixed) sensitivity matrix, whose elements are partial derivatives of the type

$$\frac{\partial a_i}{\partial \psi_j} \quad \text{and} \quad \frac{\partial a_i}{\partial \sigma_{kl}}.$$

This assumption causes no problems when only little adjustment is necessary, but this is not the situation in many real cases.

(2) $\underline{a}$, $\underline{\Sigma}$, and $\underline{\psi}$ are uncorrelated.

Based on these assumptions, the algorithm of the STAY'SL is the following.

Using the assumption of multidimensional linear normal distribution, and Bayesian hypothesis, the function

$$\chi^2 = \begin{bmatrix} \underline{\psi} - \underline{\psi}' \\ \underline{\Sigma} - \underline{\Sigma}' \\ \underline{a} - \underline{a}' \end{bmatrix}^T \begin{bmatrix} \mathrm{cov}(\underline{\psi}) & 0 & 0 \\ 0 & \mathrm{cov}(\underline{\Sigma}) & 0 \\ 0 & 0 & \mathrm{cov}(\underline{a}) \end{bmatrix}^{-1} \begin{bmatrix} \underline{\psi} - \underline{\psi}' \\ \underline{\Sigma} - \underline{\Sigma}' \\ \underline{a} - \underline{a}' \end{bmatrix}$$

is to be minimalized with condition

$$\underline{a} - \underline{a}' = \underline{\underline{G}} \begin{bmatrix} \underline{\psi} - \underline{\psi}' \\ \underline{\Sigma} - \underline{\Sigma}' \end{bmatrix}$$

The solution $\begin{bmatrix} \underline{\psi}' \\ \underline{\Sigma}' \end{bmatrix}$ can be computed using the next formula:

$$\begin{bmatrix} \underline{\psi} - \underline{\psi}' \\ \underline{\Sigma} - \underline{\Sigma}' \end{bmatrix} = \begin{bmatrix} \mathrm{cov}(\underline{\psi}) & 0 \\ 0 & \mathrm{cov}(\underline{\Sigma}) \end{bmatrix} \underline{\underline{G}}^T \left[\underline{\underline{G}} \begin{bmatrix} \mathrm{cov}(\underline{\psi}) & 0 \\ 0 & \mathrm{cov}(\underline{\Sigma}) \end{bmatrix} \underline{\underline{G}}^T + \mathrm{cov}(\underline{a}) \right]^{-1} (\underline{a} - \underline{a}')$$

where:

$$a_j = \sum_{i=1}^{m} \Psi_i \sigma_{ij} \qquad (j=1,\ldots,n)$$

After it, we approximate $\mathrm{cov}\begin{bmatrix}\underline{\Psi}'\\ \underline{\Sigma}'\end{bmatrix}$ on the following way:

$$\mathrm{cov}\begin{bmatrix}\underline{\Psi}'\\ \underline{\Sigma}'\end{bmatrix} = \mathrm{cov}\begin{bmatrix}\underline{\Psi}\\ \underline{\Sigma}\end{bmatrix} - \mathrm{cov}\begin{bmatrix}\underline{\Psi}\\ \underline{\Sigma}\end{bmatrix}\underline{\underline{G}}^T\left[\underline{\underline{G}}.\mathrm{cov}\begin{bmatrix}\underline{\Psi}\\ \underline{\Sigma}\end{bmatrix}\underline{\underline{G}} + \mathrm{cov}(a)\right]^{-1}.\underline{\underline{G}}.\mathrm{cov}\begin{bmatrix}\underline{\Psi}\\ \underline{\Sigma}\end{bmatrix}$$

In other case, when $\underline{\Psi}$ and $\underline{\Sigma}$ are correlated, so

$$K = \mathrm{cov}\begin{bmatrix}\underline{\Psi}\\ \underline{\Sigma}\end{bmatrix} \neq \begin{bmatrix}\mathrm{cov}(\Psi) & 0\\ 0 & \mathrm{cov}(\underline{\Sigma})\end{bmatrix}$$

we have the approximation

$$\mathrm{cov}\begin{bmatrix}\underline{\Psi}'\\ \underline{\Sigma}'\end{bmatrix} = \underline{\underline{K}} - \underline{\underline{K}}.\underline{\underline{G}}^T\left[\underline{\underline{G}}.\underline{\underline{K}}.\underline{\underline{G}}^T + \mathrm{cov}(a)\right]^{-1}.\underline{\underline{G}}.\underline{\underline{K}}$$

In case of EAGLE, we minimize

$$\chi^2 = \left[f\,\underline{\underline{\sigma}}\,\underline{\underline{F}}\,\underline{\Psi} - \underline{a}\right]^T \mathrm{cov}(\underline{a})^{-1}\left[f\,\underline{\underline{\sigma}}\,\underline{\underline{F}}\,\underline{\Psi} - \underline{a}\right] + \left[(\underline{\underline{F}}-\underline{\underline{I}})\,\underline{\Psi}\right]^T \mathrm{cov}(\underline{\Psi})^{-1}\left[(\underline{\underline{F}}-\underline{\underline{I}})\,\underline{\Psi}\right]$$

where

$$F = \begin{bmatrix}F_{11} & 0 & 0 & \ldots & 0\\ 0 & F_{22} & 0 & \ldots & 0\\ 0 & 0 & F_{33} & \ldots & 0\\ \ldots & \ldots & \ldots & \ldots & \ldots\\ 0 & 0 & 0 & \ldots & F_{mm}\end{bmatrix}$$ unKnown diagonal matrix,

f = scalar unKnown,

and the output spectrum is: $\underline{\Psi}' = f.\underline{\underline{F}}.\underline{\Psi}$

The additional assumption

$$\sum_{j=1}^{m} \Psi_j = \sum_{j=1}^{m} F_{jj}\,\Psi_j$$

is necessary to ensure the uniqueness of f.

So, no any linearity as in case of STAY'SL is assumed.

Being the problem far from linear, and the number of dimensions (m+1) is too large, in the original algorithm of the EAGLE a special iteration procedure named FLEXPO (on the base of [2]) was used.

The method FLEXPO (Flexible Polyeder) works on the following way. Let us pick the starting vectors

$$\underline{y}_1 , \underline{y}_2 , \dots , \underline{y}_{m+1} \in R^{m+1}$$

compute the χ^2 values and assume

$$\chi^2(\underline{y}_1) \geq \chi^2(\underline{y}_2) \geq \dots \geq \chi^2(\underline{y}_{m+1})$$

After it, we compute the vector

$$\underline{s} = \frac{\underline{y}_2 + \underline{y}_3 + \dots + \underline{y}_{m+1}}{m},$$

and the vectors

$$\underline{P}_1 = \underline{s} + (\underline{s} - \underline{y}_1)$$

$$\underline{P}_2 = \underline{s} + 2(\underline{s} - \underline{y}_1)$$

$$\underline{P}_{1/2} = \underline{s} + \frac{1}{2}(\underline{s} - \underline{y}_1)$$

Computing $\chi^2(\underline{P}_1)$ we check whether $\chi^2(\underline{P}_1) < \chi^2(\underline{y}_1)$. If this is valid, let $\underline{y}_1 = \underline{P}_1$, and restart the procedure. If this is not the situation, we check whether $\chi^2(\underline{P}_2) < \chi^2(\underline{y}_1)$. If this is valid, let $\underline{y}_1 = \underline{P}_2$, and restart. If neither this is the situation, we check whether $\chi^2(\underline{P}_{1/2}) < \chi^2(\underline{y}_1)$. If this is valid, let $\underline{y}_1 = \underline{P}_{1/2}$, and restart.

The above was the so-called normal step. If no one of these conditions fulfilled, ie

$$\chi^2(\underline{P}_1) \geq \chi^2(\underline{y}_1)$$

and

$$\chi^2(\underline{P}_2) \geq \chi^2(\underline{y}_1)$$

and

$$\chi^2(\underline{P}_{1/2}) \geq \chi^2(\underline{y}_1)$$

then we compute the new starting vectors:

$$\underline{y}_i = \frac{1}{2}(\underline{y}_i + \underline{y}_{m+1}) \qquad (i=1,\dots,m)$$

and restart. The latter is called as contraction step.

The rate of convergence of this method was very poor in numerical experiments. A rather complicated probability argument (not discussed here in detail) shows, that in the case there is not necessary any contraction step, the number of necessary iteration steps is far from large, it is about d times square root of m, where d is the distance from starting vector to optimal (ie to the minimum of the function).

Typically, the spectrum shape modification factors are

$$0.8 \leqslant F_{ii} \leqslant 1.2$$

and the normalization factor is

$$0.8 \leqslant f \leqslant 1.2$$

so the distance can be

$$d = \mathrm{sqrt}\left[(1-f)^2 + \sum_{i=1}^{m} (F_{ii} - 1)^2\right] \leqslant 0.2*\mathrm{sqrt}(m+1)$$

We have d=1.2 for the realistic case m=35. The following table shows the number of necessary iteration steps in the mean.

d=	m=20	m=30	m=50	m=100
1	4	5	7	10
1.2	5	6	8	12
1.4	6	7	9	14
1.6	7	8	11	16
1.8	8	9	12	18
2	8	10	14	20

Nevertheless, we have to perform in the more realistic cases many contraction steps, as well. In these cases the model gives in the mean

$$\text{No. of iterations} = d*\frac{2^m}{\mathrm{sqrt}(m)}$$

and the numbers of the following table far too big to use even the fastest computers.

d=	m=20	m=30	m=50
1	234E3	196E6	159E12
1.2	280E3	235E6	190E12
1.4	327E3	274E6	222E12
1.6	374E3	313E6	254E12
1.8	421E3	352E6	286E12
2	468E3	391E6	318E12

So, we have developed a method for the iteration, which approximates the function χ^2 on a whole line, and computes the minimum on this line. The problem to bes solved is the following. Given

$$\underline{x} \in R^{m+1} , \underline{v} \in R^{m+1} , \underline{v} \neq 0$$

We must give a formula for

$$G(t) \equiv \chi^2(\underline{x} + t.\underline{v})$$

Here one can show easily that

$$F_{ti} = \frac{c_0^{(i)} + c_1^{(i)} t}{c_2 + c_3 t} \qquad (i=1,\ldots,m)$$

Here the denominators are the same. Also we have

$$f = c_4 + c_5 t.$$

A rather lenghty but elementary computation shows that

$$G(t) = g_0 + g_1 t + g_2 t^2 + \frac{g_3 + g_4 t}{t^2 + g_5 t + g_6}$$

Here $g_0,\ldots,g_6$ are unKnowns. Income $|t|$ large:

$$G(t) \approx g_0 + g_1 t + g_2 t^2$$

So, choosing $|t_0|$, $|t_1|$, and $|t_2|$ large, we have the equations:

$$G(t_0) = g_0 + g_1 t_0 + g_2 t_0^2$$

$$G(t_1) = g_0 + g_1 t_1 + g_2 t_1^2$$

$$G(t_2) = g_0 + g_1 t_2 + g_2 t_2^2$$

From this, g_0, g_1, and g_2 can be computed easily. Computing $G(t_3)$, $G(t_4)$, $G(t_5)$, and $G(t_6)$, where $t_0,\ldots,t_6$ are different, we have

$$\begin{aligned} G(t_i)(t_i^2 + g_5 t_i + g_6) = {} & g_0(t_i^2 + g_5 t_i + g_6) + \\ & + g_1(t_i^2 + g_5 t_i + g_6)t_i + \\ & + g_2(t_i^2 + g_5 t_i + g_6)t_i^2 + \\ & + g_3 + g_4 t_i \end{aligned} \qquad (i=3,4,5,6)$$

which is a system of linear equations to g_3, g_4, g_5, and g_6.

The minimal value of G can be computed using the five-degree polynomial equation

$$G'(t).(t^2 + g_5 t + g_6)^2 = 0$$

The above method can be applied vor one $\underline{v}$ direction, after it, from the minimum point, we can swithch to an other, and so on.

The cost of one such step is (mainly) the cost of 7 χ^2 evaluations. So, the switching to FLEXPO from this method would be

useful not before

$$\frac{\text{step with the above method}}{7} < \frac{\text{FLEXPO vertex to be used}}{\text{sqrt}(m)}$$

We remark here, that in the case, when FLEXPO verices are small, the following modification of FLEXPO would be preferable.

We have starting vectors

$$\underline{y}_1, \ldots, \underline{y}_{m+1} \in R^{m+1}$$

and we assume again

$$\chi^2(\underline{y}_1) \geq \chi^2(\underline{y}_2) \geq \ldots \geq \chi^2(\underline{y}_{m+1})$$

Then we can write

$$\underline{\text{grad}} \cdot (\underline{y}_i - \underline{y}_{m+1}) = \chi^2(\underline{y}_i) - \chi^2(\underline{y}_{m+1}) \qquad (i=1,\ldots,m)$$

where $\underline{\text{grad}}$ is an approximation of the gradient vector at the point $\underline{y}_{m+1}$. So, we restart with

$$\underline{y}_1 = \underline{y}_{m+1} - t.\underline{\text{grad}}$$

for some t step value.

We hope that with these new methods, the necessary computer time for EAGLE shall decrease by magnitudes. Some probability reasonings show, that in the case of realistic problems, this accelerated EAGLE shall need computer time only 20 times more than STAY'SL.

To approximate the out-in and out-out covariances, we have

$$\text{cov}[(f.\underline{\underline{F}}.\underline{\Psi})_k, \Psi_i] = \sum_{p=1}^{p=1} \frac{\partial (f.\underline{\underline{F}}.\underline{\Psi})_k}{\partial \Psi_i} \text{cov}(\Psi_p, \Psi_i)$$

This is exact up to the third order.

The formula

$$\text{cov}[(f.\underline{\underline{F}}.\underline{\Psi})_k, (f.\underline{\underline{F}}.\underline{\Psi})_i] =$$

$$= \sum_{p=1}^{m} \sum_{q=1}^{m} \frac{\partial (f.\underline{\underline{F}}.\underline{\Psi})_k}{\partial \Psi_p} \text{cov}(\Psi_p, \Psi_q) \frac{\partial (f.\underline{\underline{F}}.\underline{\Psi})_i}{\partial \Psi_q}$$

is exact up to the third order.

References:

[1] F. G. Perey: Least squares dosimetry unfolding. The program STAY'SL. Report ORNL/TM-6062; ENDF-254. Oak Ridge National Laboratory, Oak Ridge, TN, 1977.

[2] L. Ugray: Determination of the unconditional local minimum of a multivariate function by the flexible polyeder method (in Hungarian). ESZK TájéKoztató, 12 (1974), Budapest, p. 108-116.

COMPARISON OF CODES STAY'SL AND EAGLE

STAY'SL	EAGLE
1) $\Delta \underline{a} = \underline{\underline{G}} \begin{bmatrix} \Delta \underline{\Psi} \\ \Delta \underline{\underline{\Sigma}} \end{bmatrix}$	1) No linearity assumption
2) $\underline{\underline{G}}, \underline{\Psi}, \underline{a}$ uncorrelated	2) $\underline{\Psi}$ and $\underline{a}$ uncorrelated. (If correlated, the method has a little modification.)
3) One step computation	3) Long computations (seems to 20 times longer, than STAY'SL).
4) cov($\underline{\Psi}'$) uncertain	4) More certain formulas for cov($\underline{\Psi}'$)
5) Normalization and adjustment made in two steps.	5) Normalization and adjustment made in one step.
6) STAY'SL may give negative spectrum	6) EAGLE can give only positive spectrum

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