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PROCESSING OF EVALUATED NEUTRON DATA FILES IN ENDF FORMAT ON PERSONAL COMPUTERS

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Abstract

A computer code package – FDMXPC – has been developed for processing evaluated data files in ENDF format. The earlier version of this package is supplemented with modules performing calculations using Reich-Moore and Adler-Adler resonance parameters. The processing of evaluated neutron data files by personal computers requires special programming considerations outlined in this report. The scope of the FDMXPC program system is demonstrated by means of numerical examples.

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1. Introduction

The recently released basic evaluated data files such as ENDF-6 [1], represent the neutron interaction cross-sections in a very sophisticated parametrized form. Calculation of any functionals of cross-sections requires considerable computional efforts. Therefore the effective processing codes for these files are implemented on large mainframe computers. Nevertheless, unless large group constant libraries are to be produced, even medium sized personal computers can be used for many processing purposes. Moreover, the PC's are cheap and readily available.

In this report a PC program package for processing evaluated neutron data files is presented. The author has spent over twenty years dealing with nuclear data processing and his troublesome experiences with underdeveloped computing environments have prompted him to elaborate a method of processing utilizing modest computing resources. The first generation of such programs - represented by FEDGROUP-2 [2] and FEDGROUP-3 [3]- required a memory space no more than 200kbyte and the CPU time required in one run could be reduced by the possibility of piece-wise processing in energy space. In this way the problem arising from frequent system failure could be eliminated.

The FEDGROUP versions produce infinite dilution group-averaged and self-shielded constants, and elastic and inelastic transfer matrices for thermal reactor calculation.

The recently developed program systems FEDMIX [4] and FDMXPC [5] do not calculate transfer matrices but calculate transmission and self-indication functionals even for mixtures of elements. The FDMXPC is a program developed directly for personal computers on the basis of FEDMIX which was originally designed for mainframes but the good tradition of the modest use of computing resources has facilitated its implementation on PC-s with Intel 286/386 processors under the Microsoft DOS. The newest version of FDMXPC has been extended to use ENDF-6 format and to process resonance data specified either by Reich-Moore parameters or by Adler-Adler parameters.

In the following the method of resource sparing nuclear data processing is to be reviewed. Some demonstrative calculations are presented in order to show the possible range of applications.

The algorithms applied in the code and the detailed program manual are given in Ref.[5]. Here only the new developments connected with the processing of the ENDF-6 library are given.

2. Method of resource sparing processing

Flexible usage of computer memory can be assured with the dynamic space allocation for such large arrays for which dimension can be problem dependent. In this way, the length of one large dynamic array will determine a great part of the memory allocation and many restrictions can be eliminated.

Effective data exchange can be achieved by buffering the I/O operations on FORTRAN level. The file underlying the I/O operations is regarded as a large contiguous data field broken into equal records. The length of the buffer is the same as the length of such record and contains one of them fixed by a record pointer. A data pointer specifies the place of the data item on the file to be input/output. A real I/O operation occurs only if the data pointer points outside the record in the buffer. In this case the content of the buffer is changed to that which is actually needed.

The card-image data file has to be preprocessed to get a file – called RFOD – suitable for the above I/O procedure. RFOD has a special structure. It is divided into data directories and bulk data. The data directories contain control numbers and pointer offsets which facilitate the pointer handling of bulk data. When data are processed by the main part of the program system the corresponding data directories are written into the memory and data retrieval can be organized optimally.

The output file – called SFGK – for the processed constants is organized in a similar way but it is a cumulation of output data sets rather than a division into directories and bulk data parts. Each output data set begins with label 'BEGN' and with integer type control information, and the whole file finishes with the label 'END '. The result of a subsequent calculation may continue the SFGK file. Group constant libraries and any other applications are connected with the SFGK file and the programs accomplishing these connections are the postprocessors.

The above described programming philosophy is equally used in the mainframe and PC versions of the program system. The programs – written in standard FORTRAN-77 – differ only in their outer shell which must conformed with the actual operational system. An important deviation of PC versions, however, is in the handling of original nuclear data. As magnetic tape devices are not typical of PC configurations the nuclear data are to be stored on floppy or hard disc media. On such media it is recommended that each material file be stored separately. For long term storage the data can be archived by means of any well-known compressing utility of the PC world (e.g. PKARC or PKZIP of Golden Software). Judging from our experience the dimension of a compressed

Table 1. Length of some material files (in bytes) in different representations

Isotope	Library	MAT	Total	Reduced	Compressed	RFOD
Fe-56	ENDF-6	2631	1351040	219186	64374	60120
U-235	JENDL-3	3924	881680	111776	29173	36578
U-235	ENDF-6	9228	1235120	374278	107233	125986
U-238	JENDL-3	3926	783520	148584	35695	52104
U-238	ENDF-6	9237	615600	227386	45781	76152
Pu-239	JENDL-3	3943	805840	102500	26788	28056
Pu-239	ENDF-6	9437	978960	188108	50434	48096

data file is about one fourth that of the original one. This means, for example, that the whole ENDF-6 library can be held on 10 floppies, 1.2Mbyte each! Moreover, if we are to work only within the scope of FDMXPC then no other data but MF=1,MT=451, - MF=2,MT=151, - MF=3,MT=1,2,16,18,102 are required where MF and MT are the file type and data type number, respectively. The corresponding reduced subset requires even less storage.

In Table 1. the dimension of some original data sets and that of the reduced subset and its compressed dimension are presented. The dimension of the corresponding RFOD (this file is used directly in the processing) is also given.

The production of subsets from the original ENDF tapes may be accomplished either by a standard ENDF utility or the service program EVDATS supplied with the FDMXPC package.

3. Examples of calculations and hints regarding computing time

In the following the range of applications is overviewed by presenting some interesting results of calculations. All calculations were performed on an IBM compatible AT having the following specification

Processor	Intel 386
Coprocessor	Intel 387
Frequency	33MHz
Memory RAM	4Mbyte

The executable modules were prepared by means of the Silicon Valley Software compiler and linker. This allowed us to use memory extended over the

640kbyte thereby avoiding the DOS restriction. Most of the calculations, however, could be performed with modules prepared with the Microsoft FORTRAN 5.0 compiler and the Microsoft Linker not using the extended memory facility. The computing time was about 20-50% more in the latter case.

a) Let us consider a transmission measurement of U-235 on a spectrometer with the following parameters:

base length: 50m, channel width $2\mu s$, neutron impulse decay time:$1.6\mu s$, length of neutron impulse: $3.2\mu s$. The transmission as a function of energy between 10 and 20 eV (corresponding to channels 583-416) are calculated from ENDF-6 (MAT=9228, Reich-Moore parameters) as well as from JENDL-3 data (MAT=3924, single level Breit-Wigner parameters). The results for a sample of 0.005 atom/barn thickness are compared in Figs. 1-3 where the first is the case of no Doppler broadening and no instrumental resolution, the second is instrumental resolution and no Doppler broadening, and the third is instrumental

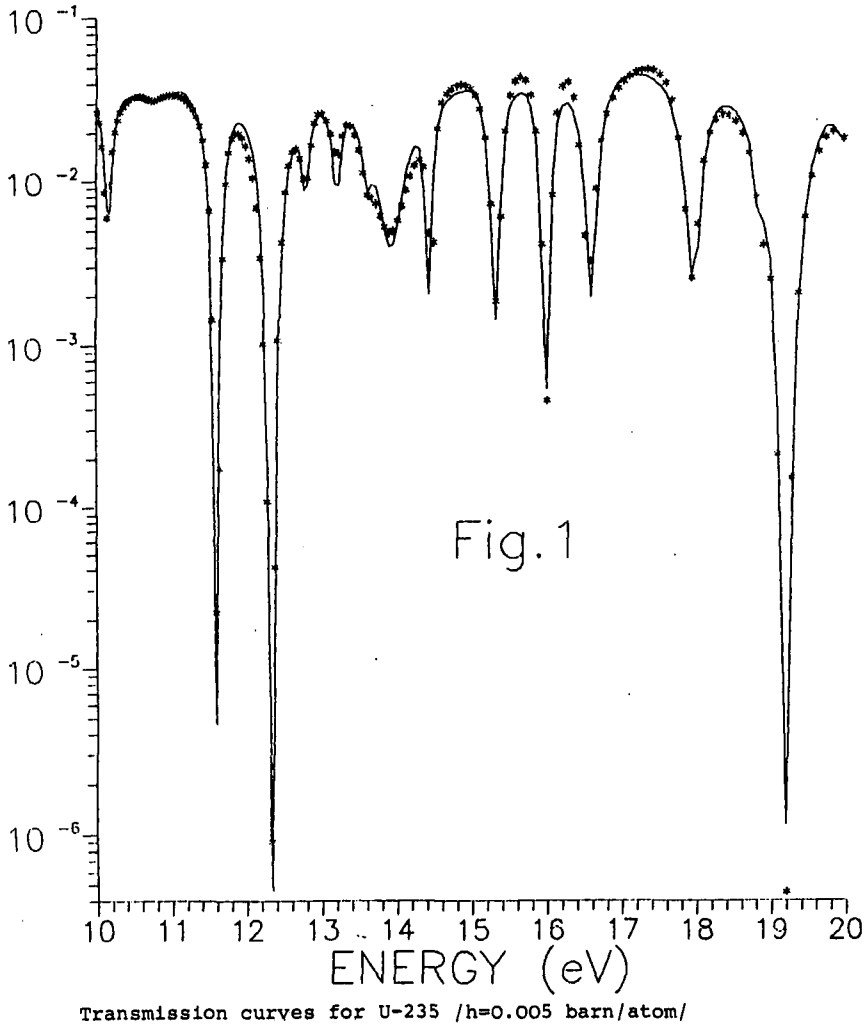


Fig. 1

Transmission curves for U-235 /h=0.005 barn/atom/
solid line: calculated from JENDL-3 data /SLBW formalism/
dots: calculated from ENDF-6 data /Reich-Moore formalism/
no instrumental resolution and Doppler broadening taken into account

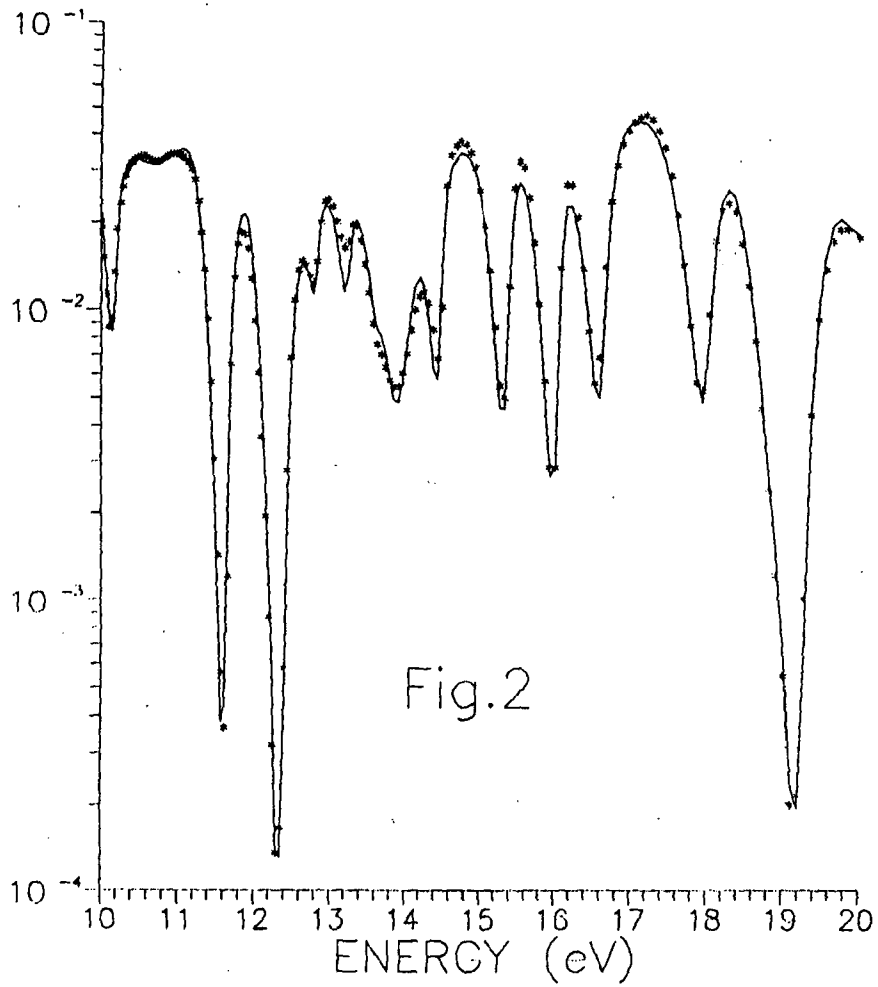


Fig.2

The same as the Fig.1 but intrumental resolution is accounted

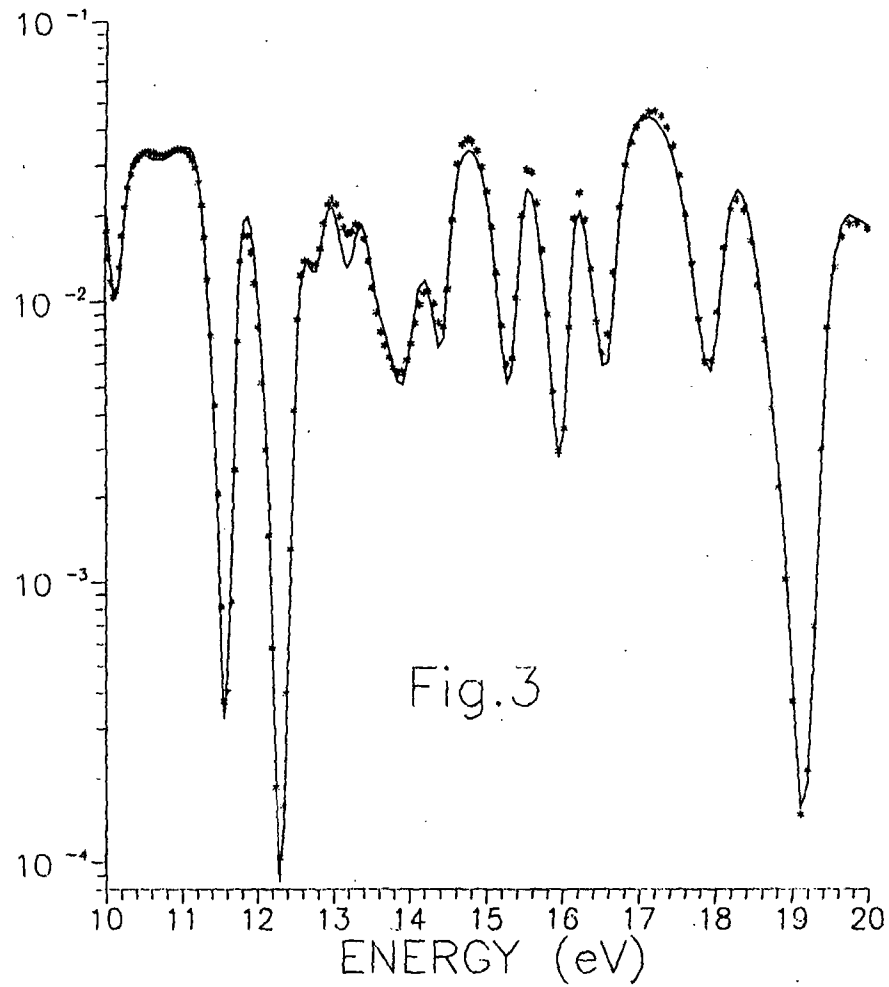


Fig.3

The same as Fig.2 but the Doppler broadening is also accounted

resolution and Doppler broadening. In the case of Doppler broadening the computing time is extremely large for the material with Reich-Moore parameter in spite of the fact that $D = 2.0$ was taken (see formula (1) below).

In Figs. 1-3 solid lines belong to data MAT=3924 of JENDL-3 while dots belong to MAT=9228 of ENDF-6. Computing times:

Fig.1: MAT=3924 - 0.3min, MAT=9228 -1.5min.

Fig.2: MAT=3924 - 0.7min., MAT=9228 - 14min.

Fig.3: MAT=3924 - 1.2min., MAT=9228 - 480min.

b) Calculating the cold, total shielded ($\sigma_0 = 0.0, T = 0.0K^o$) Bondarenko's factors for MAT=9228 and MAT=3924 in the energy range 100.eV-1000.eV (17-15 groups of the Bondarenko system, the group boundaries are 100., 215., 465., and 1000eV). In this range cross-sections are given for MAT=9228 of ENDF-6 by Reich-Moore resolved parameters, and for MAT=3924 of JENDL-3 by unresolved resonance parameters. In the latter case the method of stochastic ladders is used and the f-factors have been calculated by formula (2.4) of [5]. Table 2 shows the results with the corresponding computing times.

Table 2. Bondarenko's factors (cold and total shielded)

group/MAT	f_s	f_γ	f_f	computing time (min)
15 3924	0.9647	0.6741	0.7804	21
9228	0.9615	0.5556	0.5648	81
16 3924	0.9630	0.7630	0.6420	10
9228	0.9419	0.5338	0.4134	29
17 3924	0.9560	0.7490	0.6151	5
9228	0.9495	0.4819	0.3656	21

c) Stochastic fluctuation of infinite diluted group averaged cross-sections calculated from the average parameters given for U-238 in the JENDL-3 file MAT=3926. Results are compared with those of Hauser-Feshbach (H-F) averaging.

The averaging interval is 9.5keV-10keV.

Table 3.

case	σ_t	σ_s	σ_γ	computing time (min)
average from 50 ladders	14.46	13.76	0.703	0.5
stat.error %	7.3	7.4	10.0	
H-F average	14.52	13.80	0.720	0.3

d) Transmission probability in unresolved region and its stochastic fluctuation. The same material and energy interval are taken as in c). Group averaged transmission is calculated for three samples using a stochastic resonance ladder generated from the specified distribution. Statistical average and error of transmission probabilities are calculated as an average from 6 stochastic series. Results are given in Table 4.

Table 4.

case	0.001	0.005	0.01	computing time (min)
from one ladder	0.985	0.931	0.872	3
average from 6 ladders	0.986	0.934	0.877	16
stat.error %	0.1	0.4	0.6	

Note: Comparing the errors in Table 3 with those in Table 4 it can be seen that the fluctuation error of transmissions is significantly lower than that of the infinite diluted averages. Thanks to this fact one may hope that the self-shielding calculated by means of the statistical ladder method, has no large statistical inaccuracy.

e) In Fig.4 the cold cross-sections of U-233 (ENDF-6, MAT=9222) in the range 6-18eV are drawn as they could be seen from a hundred meter time-of-flight basis. The resonance cross-sections of this material are specified by Adler-Adler parameters.

The computer time required for this calculation was negligible: only 30sec.

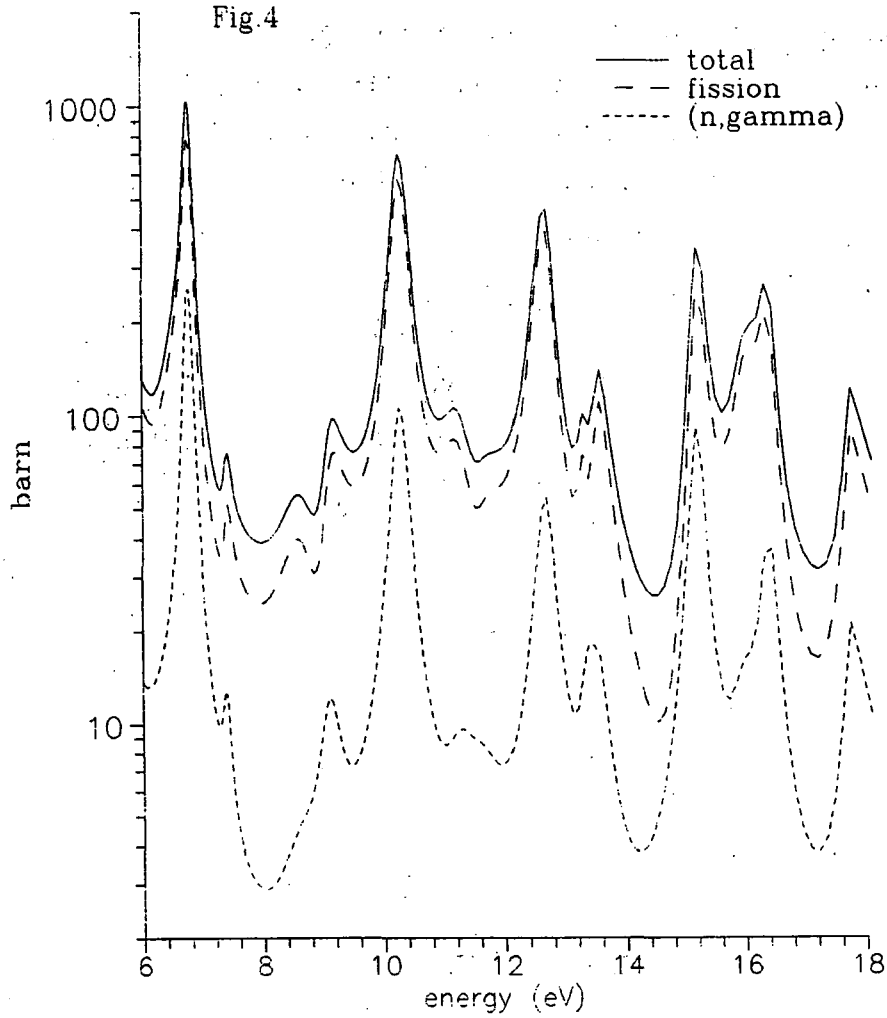
On the basis of the above calculations one may form an opinion of the computing time requirements. Generally, the following hints may help one to estimate the computing time in certain cases.

a) In the resolved resonance region the computing time depends on the total number of resonances and is approximately proportional to the length of the energy interval used for averaging if this length is far more than the average level distance. In the case of a new material file it is a good tip to make a trial calculation in a short energy interval (corresponding to about once or twice times the average distance between resonances).

b) In unresolved resonance region the H-F averaging requires negligible time. However if stochastic ladders are used then the same consideration is valid as in the resolved case.

c) In the case of SLBW representation the calculation for a temperature higher than 0.0 requires practically no excess time. For the MLBW case the

Fig.4



Cross-section curves for U-233; ENDF-6 data - Adler-Adler formalism /T=0°K/

computing time will be about twice more. In the case of Reich-Moore parameters the increase of computing time is very large depending on the accuracy requirement. Normally, we can count on a factor ten.

References

[1] P. F. Rose, C. L. Dunford, ENDF-102 Data Formats and Procedures for Evaluated Nuclear Data File, ENDF, March 1990

[2] P. Vértes, FEDGROUP – A Program System for Producing Group Constants from Evaluated Nuclear Data of Files Disseminated by IAEA, INDC(HUN)-13/l+Sp., 1976

[3] P. Vértes, FEDGROUP-3 – A Program System for Processing Evaluated Nuclear Data in ENDF/B, KEDAK or UKNDL Format to Constants to be used in Reactor Physics Calculation, KFKI-1981-34, 1981

[4] P. Vértes, FEDMIX: Neutron Transmission Functions and Lumped Averaged Cross-Sections from Standardized Evaluated Neutron Data, Computer Physics Communications 56 (1989) 199-229

[5] P. Vértes, Calculation of Transmission and other Functionals from Evaluated Data in ENDF Format by means of Personal Computers, KFKI-1991-10/G

Appendix

Changes in FDMXPC due to its extension to the ENDF-6 files

The extension of the FDMXPC program system to the files in ENDF-6 formats and using Reich-Moore and Adler-Adler parametrization in the resolved resonance region has required a tremendous change in the RFOD representation of data and in the processing modules.

The changes were performed only in the MS and SVS versions. It has not been of any worth to revise the RM version: because of the restriction of dimensioned variables to 64Kbyte length, many applications may fail if this compiler is used. The new possibilities of Microsoft FORTRAN 5.0 have resulted in almost all modules and user shells of the FDMXPC program system being independent of whether a Microsoft or SVS compiler is used.

The Lahey compiler was also tried, however, the modules have not been fully tested.

a) Change in the RFOD representation of resonance parameters. The resolved and unresolved parameters are merged into one RFOD set with type number NTN=5253 and with the following data heading:

NTF=11, NL=2+NFN*8, NW=3, NFN=number of parameter groups,
one parameter group:

EL=lower energy boundaries for the parameter group,

EH=upper energy boundaries for the parameter group,

ISC=number of isotope (if the material is a natural element),

$$NDAT = \begin{cases} \textit{number of resonances} & \text{for SLBW, MLBW or Reich-Moore parameters} \\ \textit{number of resonances for given } l & \text{for Adler-Adler parameters} \\ \textit{number of series of resonances} & \\ \textit{twice the energy values} & \text{if data represents energy dependent scattering length} \end{cases}$$

NAC= data set pointer,

NFC=10*NAPS+NRO (see p.2.6 of [1])

IA=100*LFW+10*LRU+LRF (see p. 2.5 and 2.6 of [1])

$$IF = \begin{cases} -1 & \text{if data represents energy dependent scattering length} \\ LRX\ flag\ see\ p.2.9\ of\ [1] & \text{for SLBW and MLBW resonances} \\ NLSC\ see\ p.2.11\ of\ [1] & \text{for Reich-Moore resonances} \\ 10 * L + NX\ see\ p.2.12\ of\ [1] & \text{for Adler-Adler resonances} \\ LSSF\ see\ p.2.39\ of\ [1] & \text{for unresolved resonances} \end{cases}$$

bulk data:

resolved resonance parameters:

AB=isotope abundance

AW=reduced mass

RR=scattering length

repeated for each resonance:

E_r=resonance energy

AL=orbital momentum

AJ=spin of the compound nucleus

g_j=statistical factor

for SLBW and MLBW resonances:

Γ= total width

Γ_n=neutron width

Γ_γ=radiation width

Γ_f=fission width

for Reich-Moore resonances:

Γ_n=neutron width

Γ_γ=radiation width

Γ_{f_a}=fission width in the first channel

Γ_{f_b}=fission width in the second channel

unresolved resonance parameters

AB=isotope abundance

RIS=spin of the target in the ground state

RR=scattering length

repeated for each series:

AL=orbital momentum

AJ=spin of the compound nucleus

$AMUX$=degree of freedom for competitive reaction

$AMUN$=degree of freedom for elastic neutron emission

$AMUG$=degree of freedom for (n,γ) reaction

$AMUF$=degree of freedom for fission reaction

AW=reduced mass

NE=number of energies for which average parameters are given
for each energy value:
E= energy
D=average distance
Γ_x=competitive width
Γ_n=average reduced neutron width
Γ_γ=average radiation width
Γ_f=average fission width

b) In the case of cold cross-sections (no Doppler broadening) the multilevel Breit-Wigner formalism is used according to recommendation D.1.2 of [1], i.e. the elastic cross-section is calculated directly from the scattering matrix element thereby highly reducing the computing time for the unbroadened case.

c) The Reich-Moore cross-sections are calculated from formulae (1)-(8) of D.1.3 of [1] making use of the complex arithmetic which is very effective in the FORTRAN language. The matrix inversion is accomplished by the direct calculation of determinant and cofactors.

The cross-sections are Doppler broadened by the numerical evaluation of the integrals

$$\sigma(E) = \frac{1}{\Delta\sqrt{\pi}} \int_{-\infty}^{+\infty} dE' e^{\frac{-(E'-E)^2}{\Delta^2}} \sqrt{\frac{E'}{E}} \sigma(E')$$

$$\approx \frac{1}{\Delta\sqrt{\pi}} \int_{-D\Delta}^{D\Delta} dE' e^{\frac{-(E'-E)^2}{\Delta^2}} \sqrt{\frac{E'}{E}} \sigma(E')$$

where $\Delta = \sqrt{\frac{kTE}{A}}$ is the Doppler width, T – temperature in Kelvin, k – the Boltzmann constant, A – reduced mass, D is input specified in the namelist PARM under the name *DM*..(D=3 taken as default.)

The numerical integration is performed by means of the Romberg halving method widely applied in the code.