NEANDC (E) 207 "L"
INDC (FR) 37/L

SYNOPSIS, AN INTERACTIVE NUCLEAR DATA EVALUATION, FILE INTERFACE AND MAINTENANCE SYSTEM

PART I : BASIC CONCEPT

M. COLLIN, A. SCHETT, C. PHILIS

Service de Physique Neutronique et Nucléaire
Centre d'Etudes de Bruyères-le-Châtel
B.P. n° 561
92542 MONTROUGE CEDEX FRANCE

JANVIER 1980

COMMISSARIAT A L'ENERGIE ATOMIQUE
FRANCE

NEANDC (E) 207 "L"
INDC (FR) 37/L

SYNOPSIS, AN INTERACTIVE NUCLEAR DATA EVALUATION, FILE INTERFACE AND MAINTENANCE SYSTEM.

PART I : BASIC CONCEPT

by

M. COLLIN, A. SCHETT*, C. PHILIS

Service de Physique Neutronique et Nucléaire
Centre d'Etudes de Bruyères-le-Châtel
B.P. n° 561
92542 Montrouge Cedex France

*Present address : Résidence F. Leroux, 91400, Orsay, France

JANUARY 1980

CONTENTS

ABSTRACT

Evaluation and utilization of nuclear data now requires handling processing and graphical representation of a huge collection of information.

In order to solve this problem, we have at Bruyères-le-Châtel developed the program system "SYNOPSIS" the basic concept of which is described in this document.

"SYNOPSIS" permits retrieval of available nuclear data stored in various files (ENDF, ENDL, KEDAK, experimental data in NDD - format, and others) in different formats, creation of an inter-face file in a common format, simultaneous graphical representation of data sets in this file, modification and maintenance of those files and provides a man-computer interactive tool, which facilitates greatly evaluation work. It makes extensive use of conversional mode, direct access storage device and of the capability of a light-pen-sensitive-display station.

A detailed description of the various phases and applications of the system "SYNOPSIS" will be published in Part II of this document.

I - INTRODUCTION

Progress in nuclear research and needs of the nuclear industry caused a production of a vast amount of experimental, calculated and evaluated nuclear data. Since 1970, experimental nuclear data are compiled in a world-wide basis and exchanged between the following four international nuclear data centres :

- National Nuclear Data Centre, NNDC, Brookhaven, USA
- NEA Data Bank, Saclay, France
- IAEA Nuclear Data Section, Vienna, Austria
- Nuclear Data Centre, Obninsk (Kaluga Region) USSR

II - GENERAL CHARACTERISTICS OF THE SYSTEM

The present system has been designed with a view to optimal use of the storage and access capabilities of the SEMS- computer MITRA-125.

A) - Overall Data

Language : FORTAN-IV

Computer : MITRA-125

Permanent storage requirement :

- 2 disk-storage (1 for master-file, 1 for sort work-files),
- 1 magnetic tape unit,
- 1 console display station,
- 1 light-pen sensitive display station,
- 1 plotter,
- 1 printer.

Experimental and calculated data provide the basic information for establishing recommended data sets stored in the so-called evaluated data files. In order to systematize the storage of all the data, formats have been developed. For the exchange of experimental data between the 4 centres the so-called Exchange-Format |1|, X-4 (also known as SCISRS II) is used.

The evaluated data are essentially stored in the following formats :

- ENDF- - (Evaluated Nuclear Data File) format |2|
- KEDAK- (Kerndatenbibliothek, Karlsruhe) format |3|
- UKNDL- (United Kingdom Nuclear Data Library) format |4|

In order to obtain an overall view of the knowledge of a given nuclear reaction probability, experimental and evaluated data files have in principle, to be scanned for pertinent information and its representation has to be standardized to enable comparison of data sets from different origins. Given the large volume of the files ($\sim 10^6$ data points in the evaluated data files) and the various formats used, a satisfactory solution to such a frequently arising problem can only be found with the help of fast data processors,

direct access storage devices and an interactive graph-display station. Attempts to solve this problem have been made by means of the system SCORE II |5|, which can treat experimental data in the SCIRS - I - format|6| (in use until 1970) and evaluated data in the ENDF-format. Our approach differs from SCORE - II essentially in that we link our system to evaluated data on ENDF- and KEDAK- format and to experimental data via the NDD |7|format. The latter, which basically reflects the philosophy of SCISRS - I - and ECSIL |8| format considerably simplifies processing of experimental data, since, contrary to the X-4 format, the data are represented in standardized form, i.e., variables of a given function are in fixed units, they are stored in fixed fields on a record. In addition, contrary to what one might expect, a direct link to the KEDAK-file seems to us to be more efficient than to access it via the ENDF-format |9|.

The system "SYNOPSIS" presented in this paper permits firstly a fast and convenient access to the available experimental, calculated and evaluated nuclear reaction data and a simultaneous graphical representation of any reaction probability retrieved from the various files. Secondly, it provides a tool for modifying and maintaining files.

In order to cover all essential evaluated nuclear reaction data, we stored the following files on a direct access device in their original format :

- The Evaluated Nuclear Data File, ENDF (ENDF- format).
- The LLL (Lawrence Livermore Laboratory) Evaluated Nuclear Data Library, ENDL (ENDF- format) |10|.
- The Kerndatenbibliothek, Karlsruhe, KEDAK (KEDAK- format).
- The ENDFBRC- file (in ENDF- format).

The UKNDL can be accessed via the ENDF/A- file where this library is represented in the ENDF- format. The experimental data (in NDD- format) of a particular function to be investigated are kept on magnetic tape exactly as they are received from the DATA BANK or, if necessary for a quicker search, put onto direct access device. A particular function to be studied can be retrieved from those files by supplying its attributes : Isotope, reaction, energy range, files, to the program operating on conversional mode. An inter-face file in common format is then created from which a function can selectively (choosing there data sets desired) and repetitively be called up for a graphical representation by using a light-pen sensitive display station. Having found iteratively a convenient scale, selected data sets, and eventually modified them, the definitive picture can optionally be put on disk from there it can be spooled onto the plotter. The interface-file can evidently also be used as input for programs treating the data numerically (interpretation, interpolation, etc.).

The system "SYNOPIS" can easily be linked to any future nuclear data file on condition that functions are represented in standardized form.

B) - Flowchart Summary

A detailed representation is given in Figure II/1 .

III - MASTER FILE : STORAGE AND ACCESS PROCEDURE

A) - File Configuration

The storage method must optimize

1 - The amount of disk to be used
2 - Access speed of each reaction
3 - Introduction of new versions
4 - Elimination of old data

Evaluated data is supplied to us on cards, each of which contains 6 pieces of data. In order to be able to store 6 real or 12 integer numbers, the "main file" structure must be 6 x 4 = 24 bytes.

In order to store more than 32767 cards on our 16 bit computer one must use 2 words (block address and internal address) to specify its location.

The size of the block is determined from 2 criteria :

1) no loss of space on the disk
2) the limit on the number of blocks in the file, or the number of cards in each block is to be 32767.

During the storage of evaluated data, a reaction index is created which gives the address in the "main file" of the first card of each section.

A quick access method is the dichotomic reading of the reaction index in the order Z,A, MF, MT, library version number. One reads the middle line of the index to determine if the reaction is located in the first or second half, and then one chooses the centre of the appropriate half and chooses the appropriate quarter etc...

We estimate that after fifteen such readings a record can be read inside a data set as large as 8 times ENDF/B.IV.

The index 0 file, containing only Z,A, library, and version number allows one to detect isomers or duplicates.

If some data are to be eliminated, we replace Z by Z + 30000 in the appropriate index file forbidding access to them and deleting them in the next copy of the disk.

A re-entry file containing the address of the first free record of each main and index files (after the storage of each tape) allows to go on storing in sequence or erasing one or several of the last tapes.

Using both index 1 file in original order and the sorted one, we can extract a nuclide without calling each section. We reach the first section (MF = 1, MT = 451) by dichotomic access (as described above).

The record of index 1 concerning the first section contains the address of original index 1 access for the same section. This allows one to call this reaction and in sequence all the others as they had been stored.

Of course it is possible to build a partial tape reaching each asked section.

Index 2 file is planed to contain the address of each sub-section of KEDAK files MF = 4 and 5 to reach the tabulated data directly for a given section and a given incident energy particle. Thus, we avoid enlarging index 1 file with rarely used data.

a) - level-0-index

This index is a sequential file and contains the following data per logical record :

Byte	Content
1 - 2	Z, element number
3 - 4	A, mass number
5 - 6	ACC, accession number to reach level-1-index block
7 - 8	SACC, subacession number pointing to the record within this block.

(we store MAT to allow access by translation MAT → Z,A).

LRECL = 8 bytes

b) - level-1-index

This index is accessed directly from level-0-index and contains the following data per record unit :

Byte	Content
1 - 2	Z, element number
3 - 4	A, mass number
5 - 6	MF, file number
7 - 8	MT, reaction number
9 - 10	F, file number
11 - 12	VN, version number
13 - 14	D, date of update
15 - 16	NP, number of values in a data set
17 - 18	ACC , accession number to reach a block of the main file
19 - 20	SACC, subaccession number pointing to the record within this block
21 - 22	ACCX2, accession number to reach a block within the level-2-index
23 - 24	SACCX2, subaccession number pointing to the record within this block
25 - 28	EMIN, minimum energy of incident particle
29 - 32	EMAX, maximum energy of incident particle

One logical record consists of eight record units, i.e, 8* 32 bytes, which fills exactly one sector (= 256 octets).

Once again, this sorting hierarchy has been chosen, in order to minimize retrieval time. A sample of level-1-index is listed in Appendix IIb.

NB - bytes 25 to 32 are used, in the case of MF-1, MT = 451, to store index 1 access number and sub access number. This allows a sequential reading of index 1 after a dichotomic access on sorted one.

c - level-2-index

This index is accessed directly from level-1-index. It contains only information for functions with more than one independent variable and if the corresponding tables are big. This is, for example, true for tabulated angular distributions as given in KEDAK. The Legendre polynomial representation of such distributions as given in ENDF, e.g., is compact and, therefore, the tables are small. In the case of angular distributions of particles elastically scattered, there are i tables of the form $f(E_i, \cos\theta)$, i.e., one table

f(cos θ) for each E_i. In general, a function of more than one independent variable is represented in the form f(X) the other variables being constant. In practise, a function $f(X_1, X_2, X_3)$ is general enough for the representation of reaction probability distributions. In order to avoid time consuming searches in the main file for a specific table $f(E_i, \cos \theta)$, e.g., the variables remaining constant for a table are stored in the main file.

The format of a record unit is defined as follows :

byte	Content
1 - 4	X_1, incident energy
5 - 8	X_2, level energy
9 - 12	free
13 - 14	ACC, accession number for reaching a block within the main file
15 - 16	SACC, subaccession number pointing to the record within this block.

For economising disk-space, we put 16 record units together on one logical record, i.e., LRECL = 256 bytes (= 1 sector).

d) - main file

The main file contains the huge amount of data. The numeric values are in tabulated - parameterized, - or polynomial coefficients representation. This file is directly accessed via the level-indexes. Non integer values are stored in floating point - (4 bytes/value) and integer values are stored in 2 fixed points - (2x2 bytes/Value) representation. A record unit contains 6 values and 64 record units form one logical record, i.e., LRECL = 1536 bytes.

The choice of this logical record length results from the upper limit of the accession number (2 bytes), the amount of information to be stored and the size of a sector (= 256 bytes). A logical record of the main file, therefore, fills 6 sectors on one disk.

IV - INTERFACE OF DATA FILES

The central performance of the present system is the interface of the various nuclear reaction data files, by means of which a function stored in various files and represented in different formats can be directly compared either optically or numerically and easily treated further.

A) - Retrieval and Conversion to Common Working Format

The interface-file is generated via the retrieval and conversion phases. The retrieval is made in a conversional manner using a console-displaysstation. Specifying the characteristics of the function to be investigated, i.e., the element number, the mass number, the reaction code, type of representation of the function (integrated cross-section, angular distribution, energy distribution, etc.) defined by the File Number MF, the energy range of the incident particle and eventually parameters in the level-2-index, then the reaction probability is selected from the data files desired.

If the function is not given in tabulated form (resonance parameters, Legendre polynomial representation, etc.) tabulation is performed.

The following files can be accessed :

a) All files stored in the master-file.

b) Experimental data in NDD- format structures received from the NEA-DATA BANK at Saclay.

c) Any specific data set (calculated, e.g.) in ENDF- format.

d) Data of an experiment in a well defined format (not yet stored in the experimental data file of the NEA-DATA BANK).

In order to be able to display simultaneously tables of a function retrieved from different files they have first to be represented in an unique format. For this purpose a common working format (CWF) has been

developed on the basis of the following principles :

a) Reaction codes and units used are the same as those in the ENDF- format.

b) Conversion from the different files to CWF should be kept to a minimum.

c) Variables are stored in fixed fields of a record.

d) The information unit is a record.

e) Functions with up to 4 independent variables $f(X_1, X_2, X_3, X_4)$ can be represented.

Representation of a function retrieved from the various files in the CWF offers the following advantages :

a) All data sets are represented in the same format.

b) This permits repeated treatment (graphical display, plots, modification, integration, interpolation, etc.) of data sets without repeating time consuming retrievals from the voluminous master file, and conversions. Such repetitions are in practice necessary.

c) The file can easily be resorted. An adequate sorting order permits a saving in execution time.

A schematic view of the retrieval and conversion procedure is given in FIGURE IV/1.

B) - Definition of the CWF

We wish to point out that the information unit of the CWF is a record with a fixed format and length.

The record format is defined as follows :

col(1) - col(4) : Z, element number

col(5) - col(8) : A, mass number

col(9) - col(12) : MF, file number (type of function) (see Appendix I.a)

col(13) - col(16) : MT, reaction code (see Appendix I.b)

col(17) - col(30) : Code for reference (see Appendix I.c)

col(31) - col(32) : Version of file or year of publication (see Appendix I.c)

col(33) - col(36) : Reference system - (1 indicates LAB.
2 " C.M.)
+ 2 number of data set.

col(37) - col(56) : $f(X_1, X_2, X_3, X_4)$ represented in floating point (4 octets/value)

LRECL = 56 bytes.

An example of a function represented in the CWF is given in Appendix III.b.

The following functions cover the common nuclear reaction probabilities :

a) $f(X_1, X_2) = \sigma$, $X_1 = E$, $X_2 = \Delta\sigma$

σ ..... cross-section

E ..... incident particle energy

$\Delta\sigma$ ..... uncertainty on σ

b) $f(X_1, X_2, X_3) = \frac{\partial \sigma}{\partial \theta}$, $X_1 = E$, $X_2 = \Delta \frac{\partial \sigma}{\partial \theta}$, $X_3 = \cos \theta$

$\frac{\partial \sigma}{\partial \theta}$ ..... angular distribution

c) $f(X_1, X_2, X_3) = \frac{\partial \sigma}{\partial E'}$, $X_1 = E$, $X_2 = \Delta \frac{\partial \sigma}{\partial E'}$, $X_3 = E'$

$\frac{\partial \sigma}{\partial E'}$ ..... energy distribution

E' ..... energy of outgoing particle

d) $f(X_1, X_2, X_3, X_4) = \frac{\partial^2 \sigma}{\partial E' \partial \theta}$, $X_1 = E$, $X_2 = \Delta \frac{\partial^2 \sigma}{\partial E' \partial \theta}$

$X_3 = \cos \theta$, $X_4 = E'$

$\frac{\partial^2 \sigma}{\partial E' \partial \theta}$ ..... energy, angular distribution

For these functions the units used in the various files are given in table IV/1.

C - Usages of the Interface-File

Once a function to be investigated is selected from the various files and converted into CWF, the values can easily be displayed graphically or numerically, modified, interpolated, averaged, etc.

a) - Graphical display of a function

Evaluated, experimental and calculated data sets in CWF can be displayed simultaneously. Data tables, range of variable and linear or logarithmic scale can be chosen. The graph-display station VG 2100, which we use, also permits the representation of data sets in 4 different colours (red, orange, yellow, green). Considering only the two dimensional representation one meets in practice the following important cases as sketched in FIGURES IV/2 - 6.

The images are superimposed. Using the interactive features of the light-pen-sensitive-display-station, cross-section can easily be normalised. This facilitates comparison of shape of cross-sections, which is particularly helpful when applied to experimental data, since they are usually normalised to different values and cover an energy range piecewise as shown schematically in figure IV/7.

Having obtained by means of the interactive features of the light-pen sensitive display station a satisfactory representation of the function under study, the picture can be kept on disk and from there spooled onto a plotter.

b) - Modification of the interface-file

Modification of the content of a file can conveniently be performed by making use of the possibilities offered by the light-pen sensitive display station VG - 2100. As for the interface-file a particular need to change numerical values might occur.

c) - Other possible treatment of data in the interface-file

Data in the CWF can conveniently be used for further treatments such as averages, renormalisation, summation of partial cross-sections, consistency checks, interpolation, derivational recommended values, etc.

Besides, being a unique and easily treatable format, this file offers the considerable advantage of furnishing complete information on the knowledge of a reaction probability.

A schematic view of possible utilization of the inter-face file is given in FIGURE IV/8.

V - MASTER-FILE MODIFICATION AND UPDATE PROCEDURE

The evaluated data files such as ENDF/B, ENDL remain in principle unchanged and are replaced each time a new version is released. It might, however, happen that parts of it have to be modified. Moreover, data set additions to the ENDF BRC- file will be frequent.

A) - Modification of Data

For practical reasons we distinguish those modifications which leave the storage area of data to be changed invariable, and those which vary. In the former case, the data are retrieved, altered by means of a display station and can then be put onto the original area of the disk. In this case the only change in the level-1-index is the data of update. No index generation is required.

If, however, a modification of data results in a change of the original storage space, then the corresponding data set has to be entirely generated and added to the existing file in the course of an update of the master file.

B) - Update of the Master File

As the replacement of a data set will seldom occur, we can limit ourselves to cumulative updates, i.e., data sets are simply added to the file, but no data are deleted. This permits a direct utilization of modules of the master file generation procedure already described in Chapter III.C.

VI - CONCLUSIONS

Given the vast amount of nuclear data now available, the use of modern computer techniques became indispensable for an efficient utilization and evaluation of these data.

In this context, the program system "SYNOPSIS" has been developed in order to provide users of nuclear data with a fast and convenient tool which permits time saving access to available experimental, calculated and evaluated data ; a pointwise representation of the nuclear reaction functions to be studied in a common format ; a simultaneous graphical display of data sets either by scope or plotter ; interactive modification of data and generation of recommended sets representing a function pointwise - in parameterized - or functional form.

"SYNOPSIS" therefore provides rapid information on the availability of data of a given nuclear reaction, the agreement of the various data sets, the systematic behaviour and represents a performant tool for data evaluation.

The present system is open-ended for the addition of modules for any specific data treatment and possible linkage to peripheral files, e.g., a requestor-file.

BIBLIOGRAPHY

[1] EXFOR, Exchange Format for Nuclear Data, description and up-to-date tables of codes used available from the Data Centres.

[2] GARBER D., DUNFORD C.L., PERLSTEIN S., Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF - 102, (Oct. 1975)

[3] WOLL D., Card Image Format of the Karlsruhe Evaluated Nuclear Data File - KEDAK (1968)

[4] PARKER K., The Aldermaston Nuclear Data Library, AWRE 0-70/63 (1963)

[5] DUNFORD C.L., BERLAND R.F., HUBNER R.S., CREASY R.J., SCORE II, an Interactive Neutron Evaluation System, AI - AEC - 12757 (1969)

[6] FRIEDMAN J.M., PLATT M., SCISRS, Sigma Center Information Storage and Retrieved System, BNL 883 (T-357) (1964)

[7] SCHETT A., Description of the NEUDADA Format, Internal Report of the NEA-DATA BANK, Centre d'Etudes Nucléaires de Saclay, France

[8] CULLEN D.E., HILL K.L., HOWERTON R.J., PERKINS S.T., ECSIL, A System for Storage, Retrieval, and Display of Experimental Neutron Data, UCRL-50400, Vol. 1 Rev. 2 (1974)

[9] STEIN E., The KEDAK Program Compendium Part VI, Mechanized Transfer of Nuclear Data from ENDF/B to KEDAK and vice-versa, KFK-2387/VI (1978)

[10] HOWERTON R.J., The LLL Evaluated Nuclear Data Library (ENDL) : Translation of ENDL Neutron Induced Interaction Data into the ENDF/B Format, UCRL-50400, Vol. 15, Part C (1976)

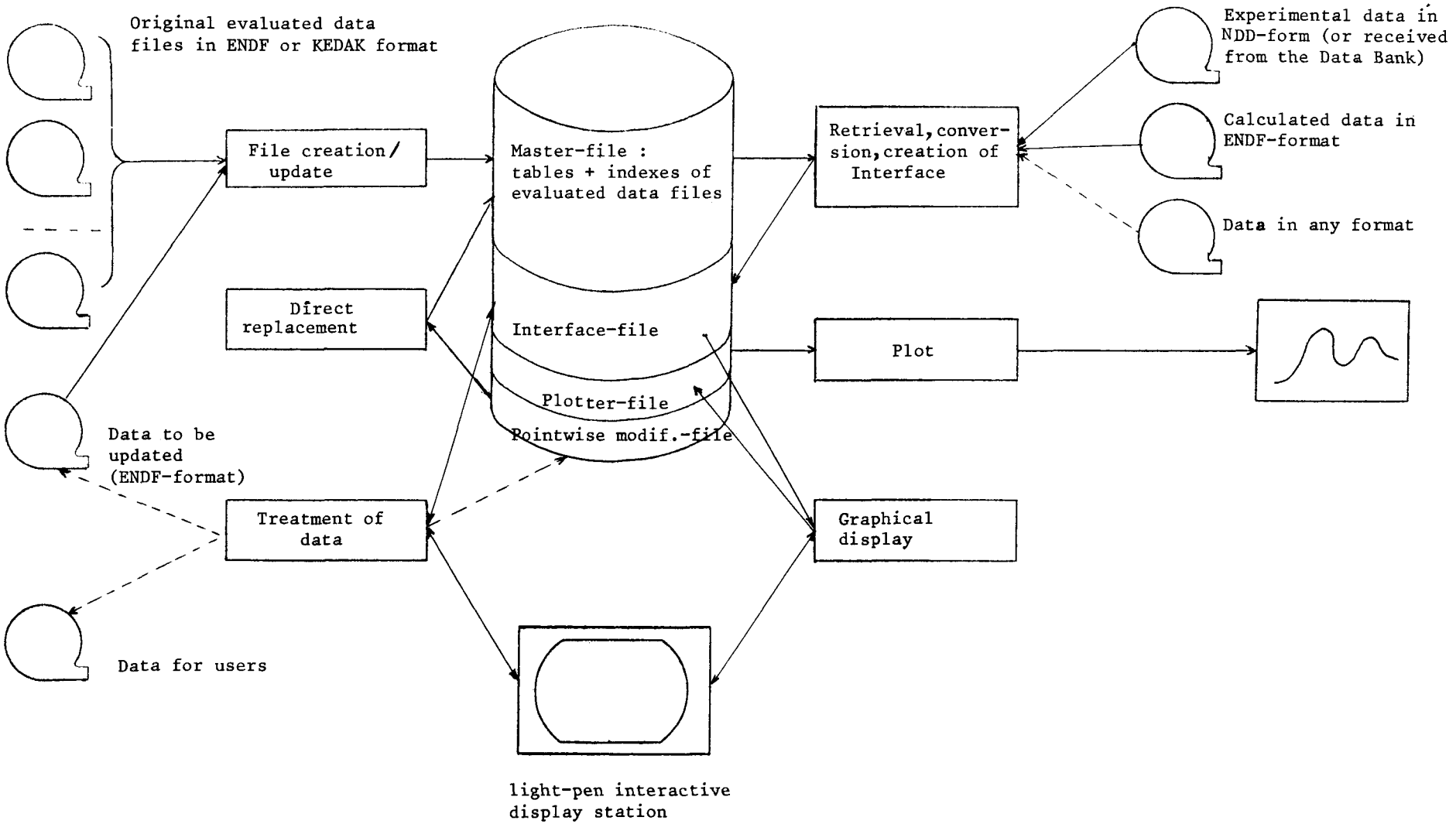

FIGURE II/1 : FLOWCHART SUMMARY

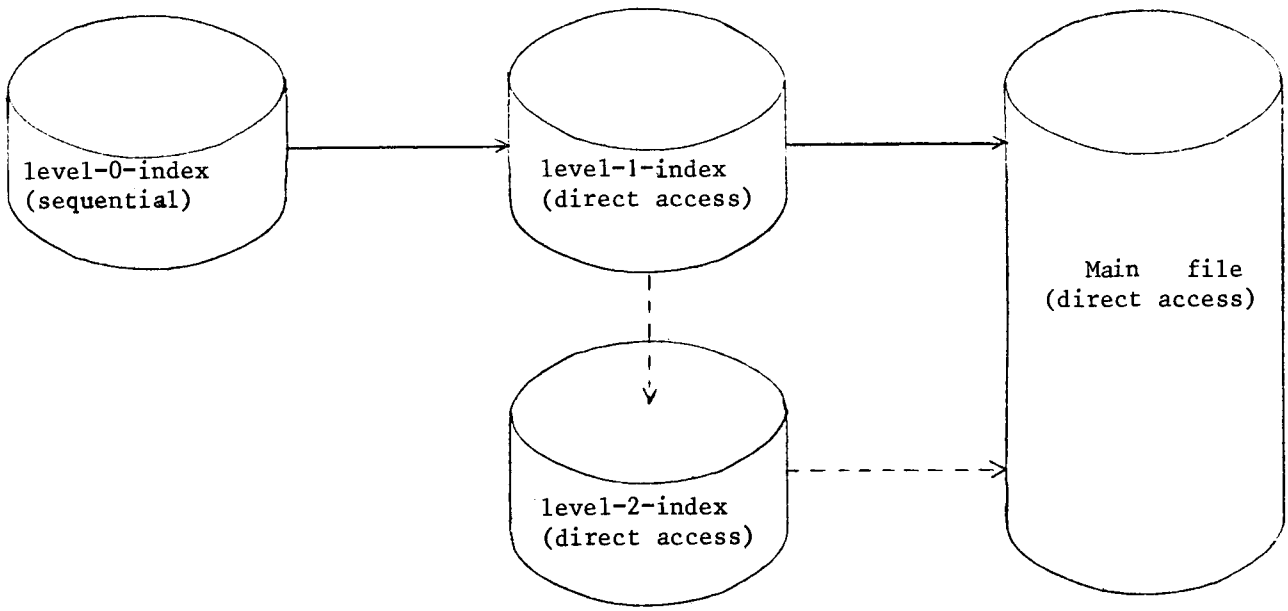

FIGURE III/1 : CONFIGURATION OF MASTER FILE

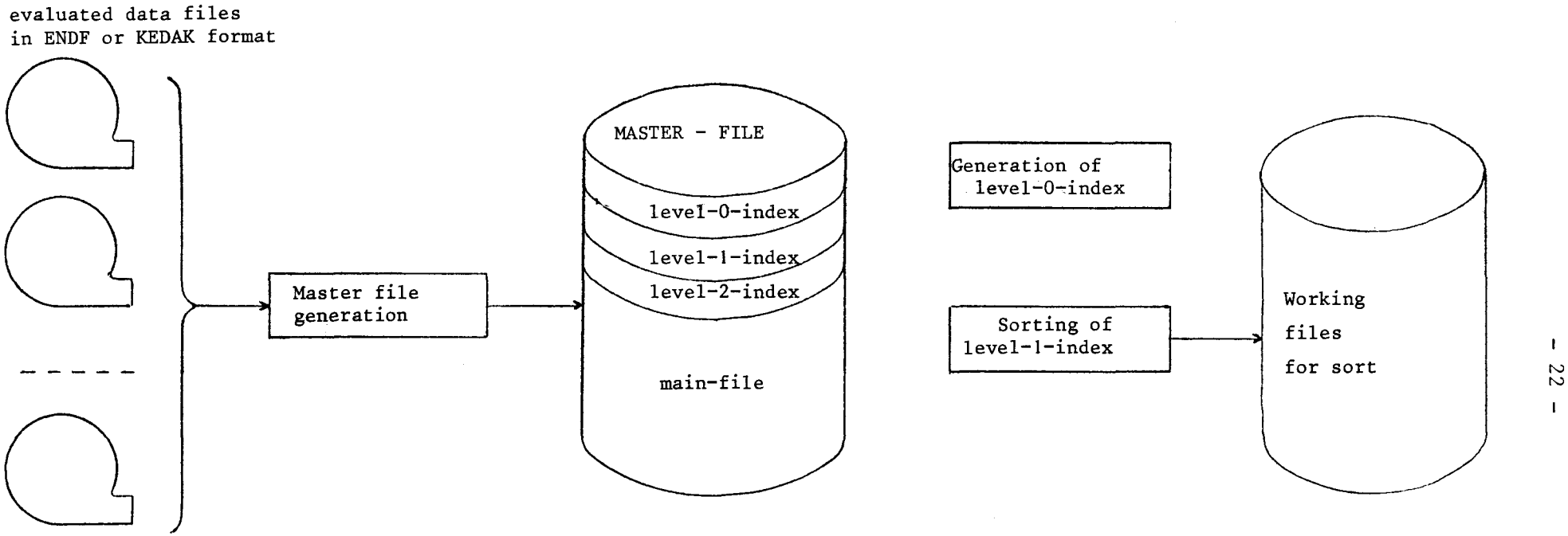

FIGURE III/2 : MASTER FILE GENERATION

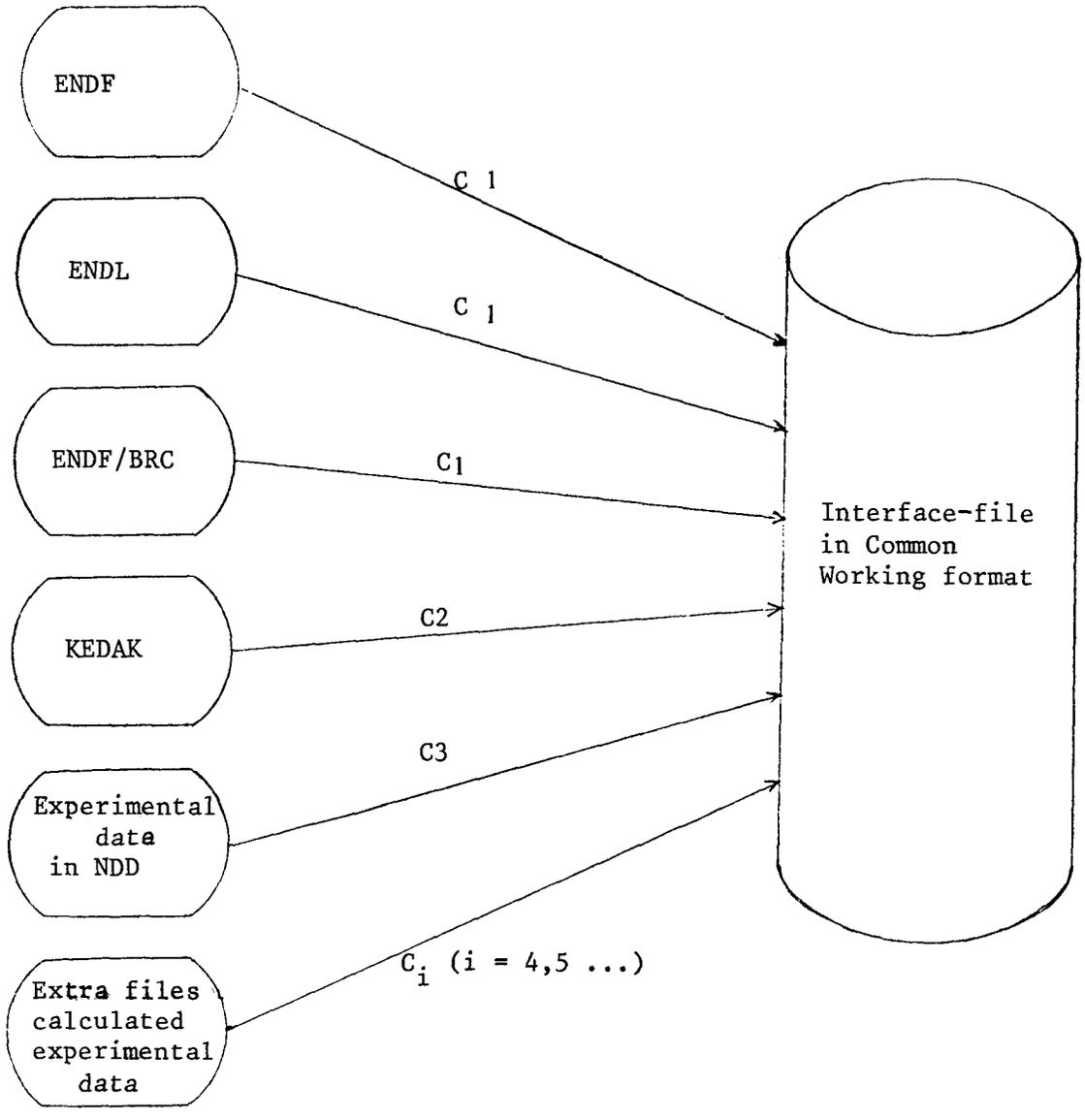

FIGURE IV/1 : SCHEMATIC VIEW OF THE CREATION OF THE INTERFACE-FILE

Ci indicates the conversion routine required for conversion from the format i in the imput to the CWF

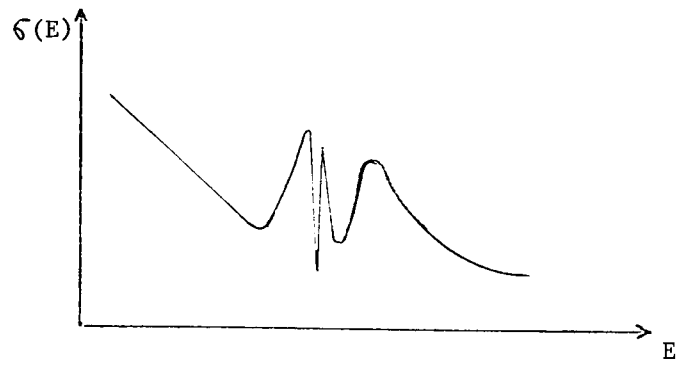

FIGURE IV/2

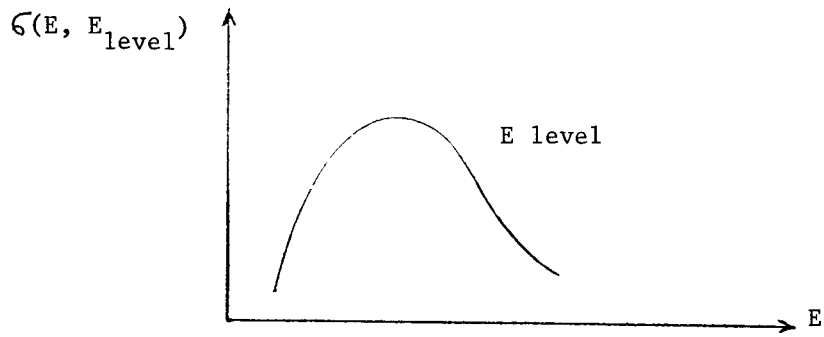

FIGURE IV/3

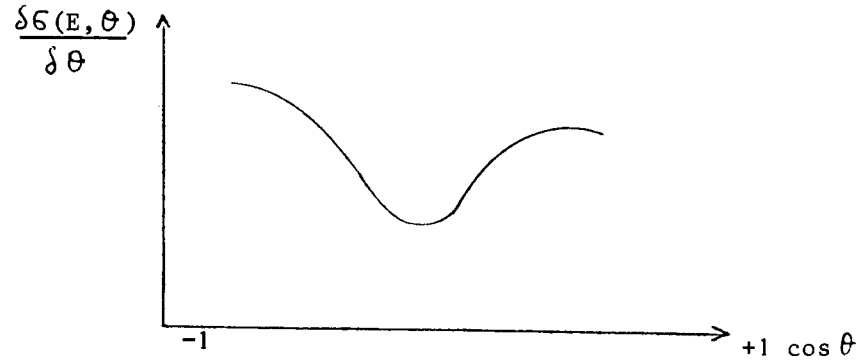

FIGURE IV/4

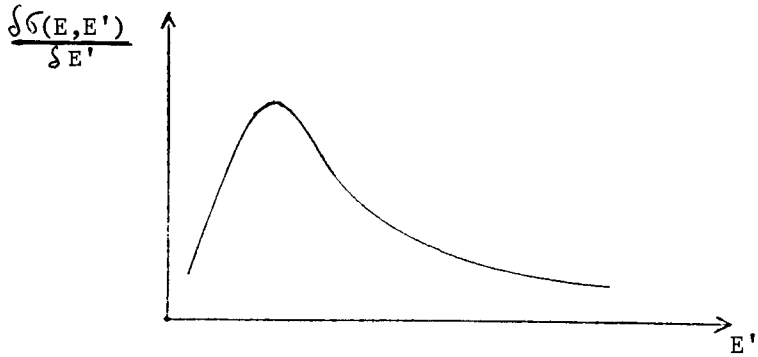

FIGURE IV/5

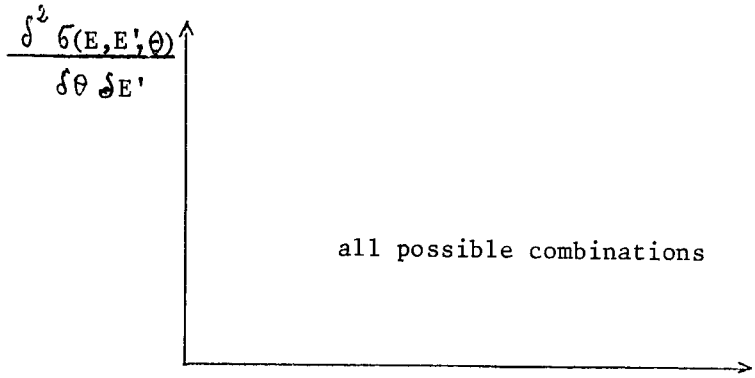

FIGURE IV/6

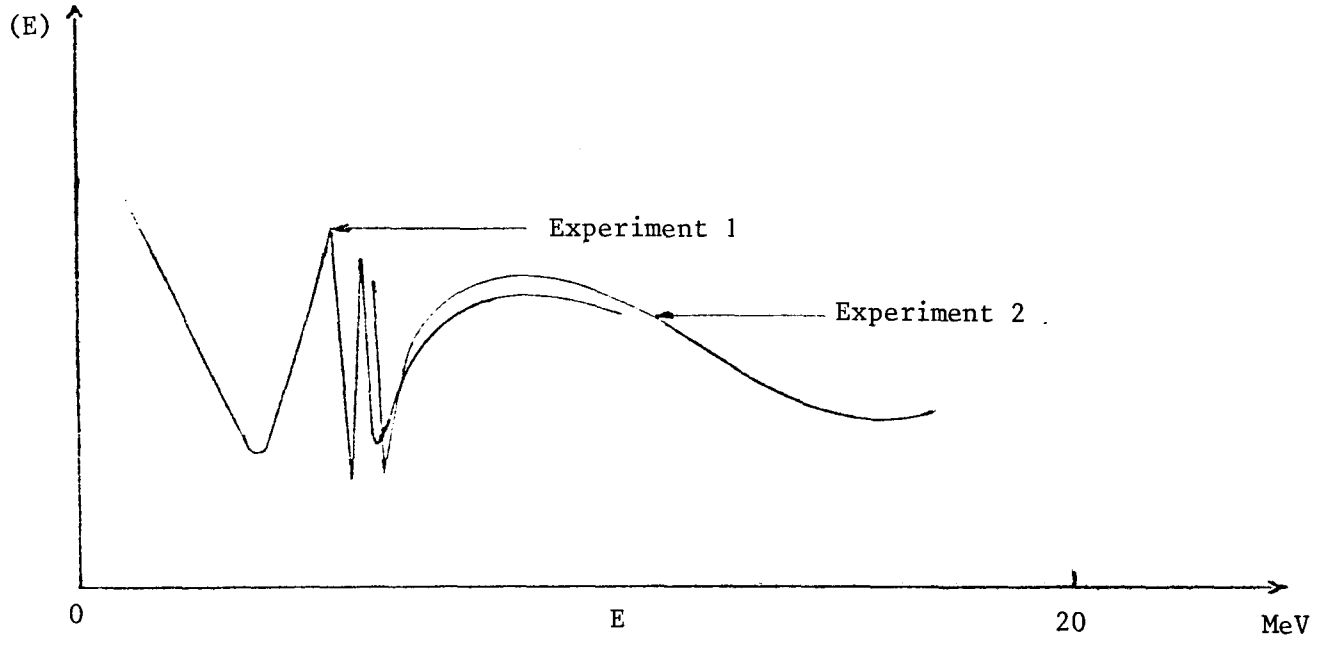

FIGURE IV/7 : COVERAGE OF THE ENERGY RANGE FROM 0 TO 20 MeV
BY DIFFERENT EXPERIMENTS

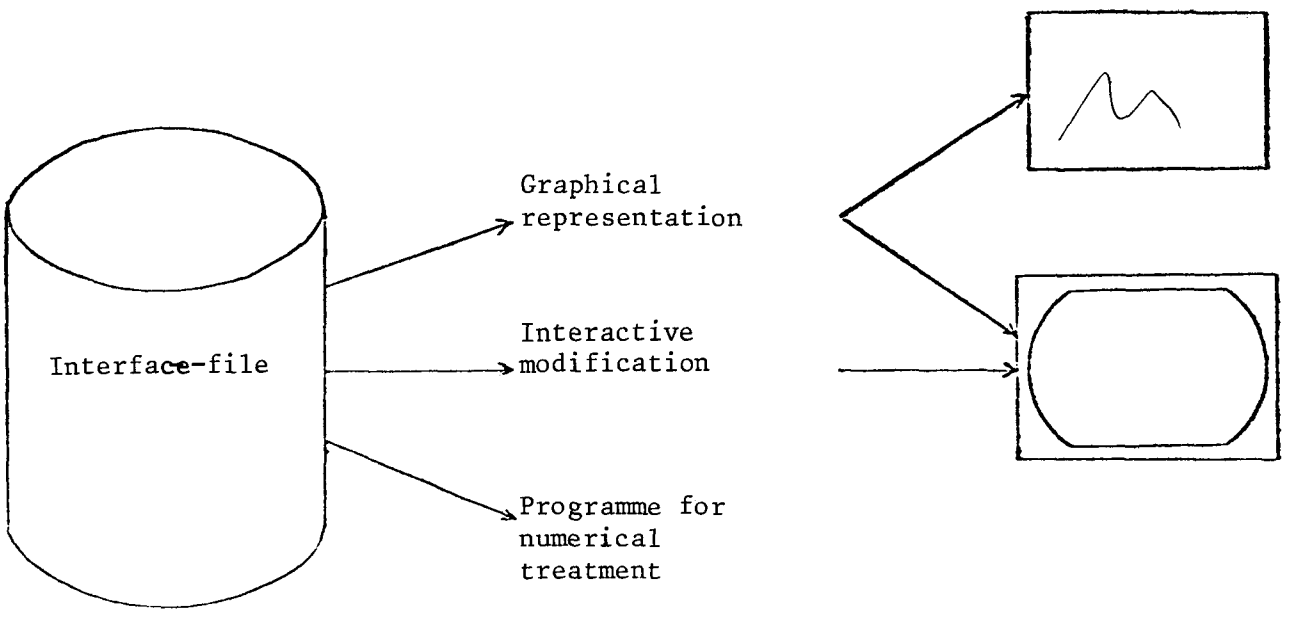

FIGURE IV/8 : UTILIZATION OF THE INTERFACE-FILE

	Access	Record Unit (bytes)	LRECL(1) (bytes)	BLKL(2) (bytes)	Storage Requirement (bytes)
level-0-index	sequential	8	256	256	10^3
level-1-index	direct access	32	256	256	10^6
level-2-index	" "	16	256	256	10^5
Main File	" "	24	1536	1536	4.10^7

(1) Record length
(2) Block length

Table III/1 : Characteristics of the master file.

Variable / File	E	σ	$\frac{\partial \sigma}{\partial \theta}$	$\frac{\partial \sigma}{\partial E'}$	$\frac{\partial^2 \sigma}{\partial E' \partial \theta}$	θ	E'	Δ
ENDF	eV	b	b/sr	b/eV	b/sr.ev	cos θ	eV	as function
ENDL	eV	b	b/sr	b/eV	b/sr.eV	cos θ	eV	"
KEDAK	eV	b	b/sr	b/eV	b/sr.eV	cos θ	eV	"
Exp. data in NDD	MeV	b	mb/sr	b/MeV	mb/sr.MeV	cos θ	MeV	" or %

Table IV/1 : Units used in files