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SCORE II
AN
INTERACTIVE NEUTRON EVALUATION SYSTEM

AEC Research and Development Report



ATOMICS INTERNATIONAL

A DIVISION OF NORTH AMERICAN ROCKWELL CORPORATION

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SCORE II
AN
INTERACTIVE NEUTRON EVALUATION SYSTEM

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ABSTRACT

The ability to analyze and evaluate the increasing amount of new neutron cross-section information is a vital part of the effort to design economic nuclear reactors. By application of computer graphics techniques, one may supply the cross-section evaluator with the tools which are necessary. By permitting man-computer interaction through computer graphics, both the rapidity and quality of evaluations will be greatly increased. A brief description of a prototype system, SCORE, is described in this document. Methods tested during the development of this prototype evaluation system have widespread general applications as well.

I. INTRODUCTION

Evaluation of neutron cross-section data for use in nuclear reactor design usually requires major nontechnical efforts, quite often to the exclusion of detailed physics analysis of data. This nontechnical effort consists chiefly of such multistep operations as data compilation, formatting, reformatting, plotting, curve fitting, etc. Since these operations, however necessary, are for the most part time consuming and yield only a minimal amount of physics evaluation, it is of extreme importance that these procedures be fully automated in order that evaluators will be able to meet the more stringent data evaluation requirements of future nuclear reactor design. In addition, the difficulties of conventional neutron cross-section evaluation are being multiplied enormously by the increasing flow of new experimental data, thereby requiring more efficient data evaluation methods.

A brief sketch of a proposed comprehensive evaluation system has been given previously.⁽¹⁾ A schematic diagram of this system is shown in Figure 1. This diagram illustrates the future direction which this automated evaluation project will take. The present project has evolved as part of the national cross-section evaluation effort, ENDF/B,⁽²⁾ and has been designated SCORE (SCISRS Conversion Routine).

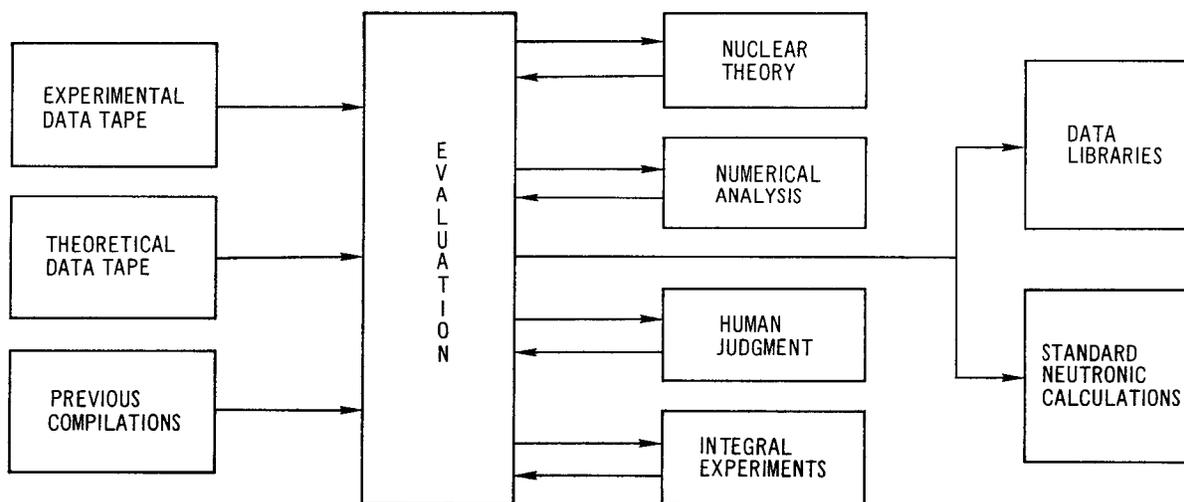


Figure 1. General Flowchart for SCORE

The basic concept which makes an automated cross-section evaluation system feasible is a rapid, yet convenient, conversational mode operating between the evaluator and his computer. In the past, this conversational capability has been absent; but recent developments in operating systems and in auxiliary computer hardware (viz, the cathode-ray-tube console) now provide the conversational mechanism. The SCORE system is designed to make optimum use of the cathode ray tube (CRT) and computer graphics, as both a visual and digital interface between the various components of an evaluation scheme. By using the CRT as an input-output device, the evaluator has a flexible and convenient tool for control of the logical flow of computer operations.

A prototype version of SCORE, which contains only a fraction of the system described in Figure 1, has been completed. The three major problem areas investigated during the development of SCORE include data storage and retrieval, interactive graphics, and numerical data analysis. The results of our investigation have been included in a computational system which is presently operational on I. B. M. equipment only. SCORE was originally developed on the IBM System 360, Model 50 (360-50) at the I. B. M. Scientific Center in Palo Alto, California, as a joint project of Atomics International and International Business Machines Corporation. The program has been executed successfully at several installations, utilizing various combinations of the 360 series computing machines and auxiliary hardware.

SCORE is written in a modular form, permitting an overlay structure which will operate in less than 180,000 bytes of computer memory. A scientific computer, such as the Model 50 or larger, should be used, although execution is marginally possible on a Model 40. One disk drive and two magnetic tape units should be available to the system. A 2250 display unit⁽³⁾ is required by SCORE. This may be a Model 1, 2, or 3, with at least 4096 bytes of buffer storage, a light pen, a character generator, and an alphameric keyboard. Operating System/360, release 11 or higher, with Basic Graphics and FORTRAN Direct Access support is required.

Five major independent segments constitute the current version of SCORE. These segments relate to SCISRS⁽⁴⁾ (a storage system for experimental neutron data) data retrieval, SCISRS data manipulation, ENDF/B⁽²⁾ (a storage system for evaluated neutron data) data retrieval and display, smooth curve representation

of experimental data, and resonance parameter analysis of neutron resonance region cross sections. The overlay structure is based on these five general tasks.

The experimental data retrieval module contains a very fast data-retrieval scheme for SCISRS I data. The data are stored in a series of bulk storage devices of increasing speed. Files of data, one per nuclide, are stored on tape. When required, a file is transferred from tape to a direct-access data set. When a particular request is made (reaction type and energy range), a series of short tables are searched. If the request can be satisfied, an index in the direct-access data set is returned. At this record in the data set, retrieval begins. Details of this storage and retrieval system are given in Section III.

Once the data have been retrieved and displayed, any sequence of several bookkeeping operations may be executed. These include listing, correcting, or deleting of data, as well as various options to modify the presentation of the data display. Evaluated neutron cross-section data may be retrieved, and a smooth data curve will appear as an overlay on the experimental data. The storage and retrieval system for ENDF/B data is described in Section IV.

Considerable emphasis was placed upon methods for choosing a smooth curve to represent a cross section over a given energy region. A method for entering nodal points for the smooth curve was developed. These points may be moved or deleted with other options. Cubic spline or linear curves passing through the nodes can be calculated, as well as the resulting residuals. A least squares cubic spline program⁽⁵⁾ has been incorporated to provide automatic adjustment of the y-coordinate of the nodes. It is possible to fit curves rapidly to experimental data, using the interactive methods in SCORE.

The final segment of SCORE is a resonance region module. A single-level and a Reich-Moore multilevel resonance model have been included. The cross section resulting from either model may be resolution and Doppler broadened for comparison with experimental data. Resonances may be added or parameters changed iteratively on line to improve the fit to the experimental data.

On-line data analysis is economical with this system when a computer with a multipartitioned memory is available. In such a computing complex, the highest priority partition would be devoted to graphics. Because the 2250 executes

display orders autonomously, to provide regeneration of the picture and to allow keyboard input and editing, the main processor is required only when the END or CANCEL keys are struck or when the light pen detects light. Experience, using a 360/50, shows that the central computer is required for only 5 to 10% of the time that the display console is in use. Thus, the normal batch job stream can be run in a lower priority partition with little noticeable degradation in the performance of either operation.

The mechanisms for interaction with SCORE are the display on the 2250, the light sensitive pen, and the alphameric keyboard. The graphic displays are designed to guide the user through a problem. Data entered through the alphameric keyboard appear on the display for verification. The program checks for errors in input data; and, when one is found, allows the user to take corrective measures.

Succeeding sections of this report will describe the methods used in SCORE and give instructions concerning its operation. It should be noted that SCORE is primarily a demonstration system, and lacks many refinements that a production code would have. There are also many more analysis modules which could be added, in order to perform additional evaluation tasks. Testing of this system under realistic evaluation conditions should yield information which would lead to further extensions and improvements.

II. OPERATION OF SCORE

The SCORE system may be operated by an individual working at the console of an IBM-2250 display device. The console may be operated as part of a remote terminal, or directly linked to a large digital computer. However, some modifications to the graphic subroutines would be required for remote terminal operation. This section has the dual purpose of explaining what SCORE can do and of providing a user manual.

No data cards are necessary to operate SCORE, but a set of control cards are required to load the program into the highest priority partition of the computer and to initiate execution.* The experimental cross-section information resides on a series of tapes in a hexadecimal adaption of the SCISRS format. A detailed description of this format, as well as the experimental data storage and retrieval system of SCORE, is given in Section III. The console used by the evaluator to execute SCORE consists of a CRT on which the graphical displays appear, an alphameric keyboard which can be used to communicate with the CRT, and a light-sensitive pen useful for similar communication functions. This equipment is shown in Figure 2.

A. DATA RETRIEVAL AND DISPLAY

At the beginning of each case, an active display appears on the CRT screen. An active display means a display through which an evaluator may transmit information to the system. This active display, with a part of the input data already appearing, is shown in Figure 3. This display permits the evaluator to provide the following identifying information:

- 1) LABORATORY
- 2) EVALUATOR
- 3) DATE
- 4) PROBLEM IDENTIFICATION NUMBER

In addition, the following data required for retrieval of the desired experimental quantities must be supplied:

- 5) ELEMENT ATOMIC NUMBER
- 6) ELEMENT MASS NUMBER

*One data card may be used to specify the desired 2250 buffer size (See Appendix I).

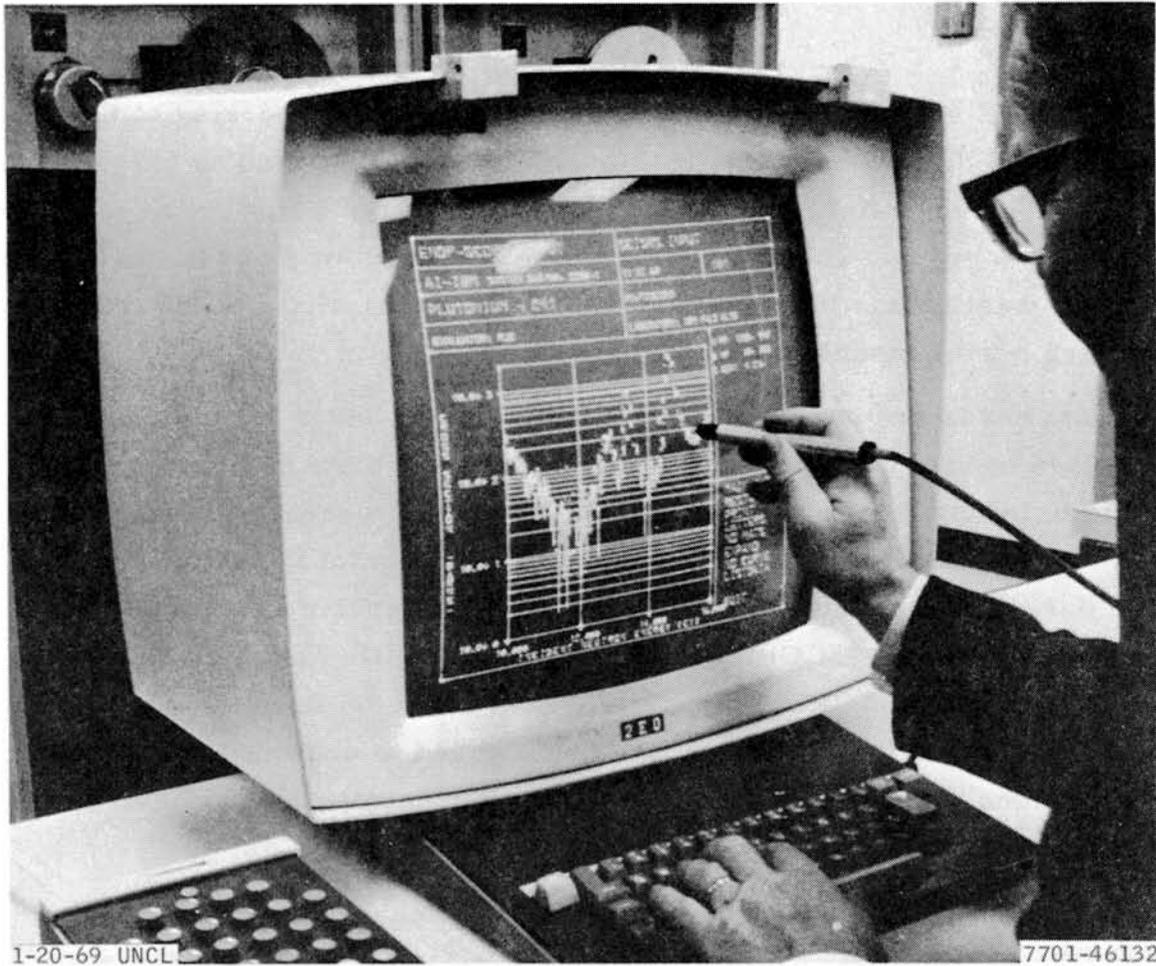


Figure 2. An IBM-2250 Console

Figure 3.
Initial Display With Some Case
Data Inserted

LABORATORY:	A.I. - I.B.M.
EVALUATOR:	C.L. DUNFORD
DATE:	OCTOBER 31, 1948
PROBLEM I.D.:	1
ELEMENT:	11
MASS NUMBER:	23
REACTION:	NA
MINIMUM ENERGY (MEV):	2_
MAXIMUM ENERGY (MEV):	
LEVEL ENERGY (MEV):	

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- 7) REACTION TYPE
- 8) MINIMUM ENERGY
- 9) MAXIMUM ENERGY
- 10) LEVEL ENERGY

Items 5, 6, and 7 follow the SCISRS⁽⁴⁾ nomenclature, with the natural element (a mixture of isotopes) mass number given as 000. Table 1 lists the SCISRS files available on the sample tape. Table 2 lists the reaction types that are presently recognized by SCORE, their symbols, and the reactions requiring a level energy. All energies are supplied in Mev. In the case where an angular distribution is requested, SCORE will retrieve the first angular distribution available between the specified energy limits. In the case of an inelastic interaction, an excited level energy may be required.

TABLE 1
SCISRS DATA AVAILABLE ON THE SAMPLE TAPE

Element/Isotope	Atomic Number	Mass Number
Sodium	11	023
Iron	26	000
Iron-54	26	054
Lithium	3	000
Lithium-7	3	007
Plutonium-241	94	241

A short line, called a cursor, may be seen in Figure 3 (following the "2" on line 8). The cursor indicates the position at which a character, entered through the keyboard, will appear on the screen. This cursor may be moved to any position in the active area of the display by a key on the keyboard. Thus, there is complete freedom to enter or correct any input data on the screen. When all required data have been correctly specified, the evaluator strikes the "END" key, which will cause the program to continue execution.

Using the data supplied through the first display, SCORE retrieves the requested experimental data from the SCISRS library. Details of the storage and retrieval system are given in Section III. If the requested isotope or element is not currently residing in the direct-access data set on the disk, a table is searched

TABLE 2
REACTION TYPES RECOGNIZED BY SCORE

SCORE and SCISRS Symbol	ENDF/B		Reaction
	File No. MF	Reaction No. MT	
NA	3	107	n, alpha
ND	3	104	n, deuteron
NF	3	18	n, fission
NG	3	102	n, gamma
NH	3	106	n, He ³
NP	3	103	n, proton
NT	3	105	n, triton
NNG	3	4	(n, n' γ)
N2N	3	16	(n, 2n)
N3N	3	17	(n, 3n)
SEL	3	2	(n, n)
SIN	5	4	(n, n') (requires level energy)
TOT	3	1	Total cross section
DEL	4	2	Differential elastic scattering
DIN	4	4	Differential inelastic scattering (requires level energy)
DIT	-	-	Differential elastic and inelastic scattering

to find its location by tape, and the file on that tape. The program then checks to see whether the tape is mounted. If the correct tape is not mounted, a message appears on the 360-50 console, telling the operator to mount the tape. When the correct tape is mounted, the requested isotope or element is loaded into the direct-access data set, the required data retrieved, and SCORE is ready to proceed.

If the isotope or reaction type is not allowed, or no data are available for the reaction type or energy range specified, an error message (Figure 4) appears. Any one of three options (CONTINUE, RESTART, or TERMINATE) may be selected by a light-pen detect on the appropriate characters on the screen. The first two options (CONTINUE and RESTART) return to the first display (Figure 3), so that the evaluator may modify the input parameters. The TERMINATE option ends the job.

* REACTION TYPE NAT IS NOT ACCEPTABLE. TRY AGAIN.

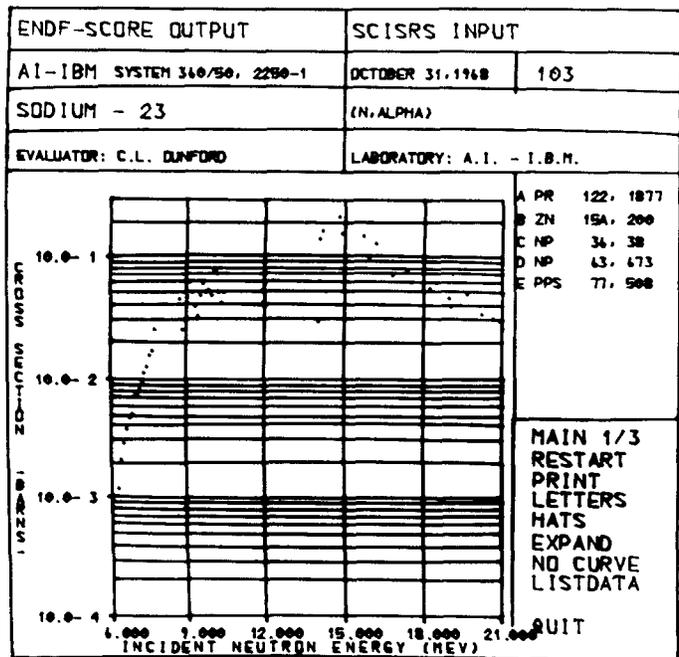
Figure 4.
Error Message

CONTINUE
RESTART
TERMINATE

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Figure 5.
Basic Data Display



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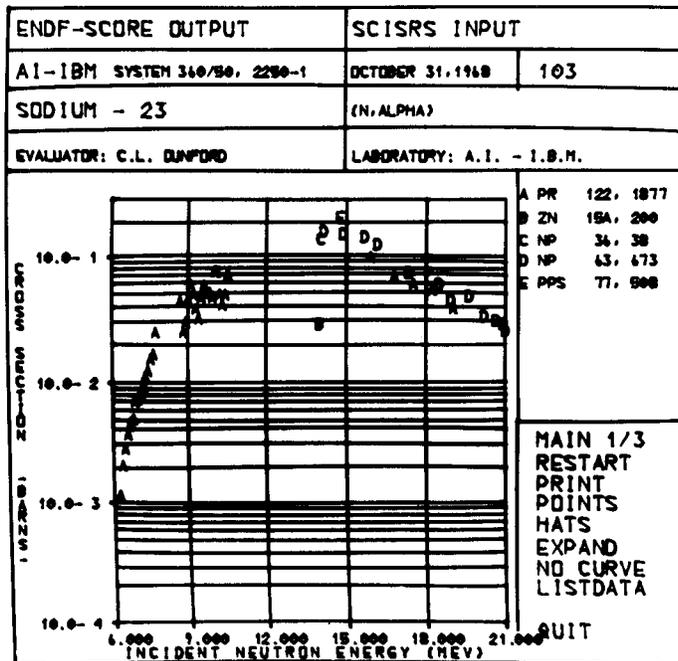
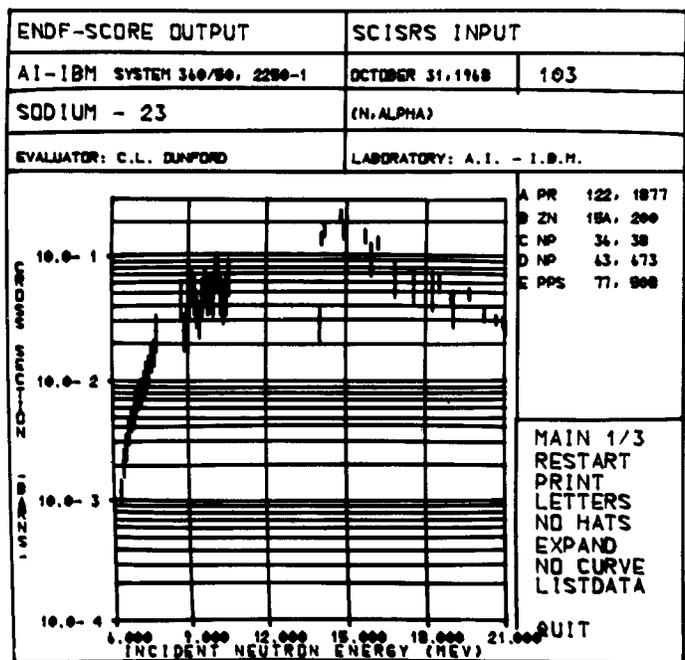


Figure 6.
Basic Data Display With Characters

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Figure 7.
Basic Data Display Points and Error Bars



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When the requested data have been retrieved, the program chooses a set of grid parameters (e.g., axis limits) from the limits of the retrieved data according to a simple algorithm. Then the data display is generated as shown in Figure 5. Experimental cross-section information is displayed in the lower portion of the display (9 by 9 in.). Data are represented by points on the display. The upper portion of the display consists of identifying information. In the right center of the display are the data references, up to a maximum of ten. More details concerning these short reference identifiers may be found in Reference 6. If more than ten references have been retrieved, each subsequent set of ten references may be displayed when a light-pen detect occurs in that area.

The lower right-hand side is also light-pen sensitive, and consists of up to ten key words or options. A light-pen detect on a word will initiate a program option.

Three sets of options are available for controlling the flow of the program. The first key word in each option set provides an identifier for each option set. These key words are MAIN 1/3, MAIN 2/3, and MAIN 3/3, for the first through the third option sets, respectively. If the light pen selects one of these identifiers, another option set will appear on the screen. Thus, if MAIN 1/3 is selected, the option list headed by MAIN 2/3 will appear; selection of MAIN 2/3 brings in the option list headed by MAIN 3/3; and selection of MAIN 3/3 returns to the MAIN 1/3 option set.

The list identified as MAIN 1/3 contains eight additional light pen switches (see Figure 5). These are RESTART, PRINT, LETTERS, HATS, EXPAND, NO CURVE, LIST DATA, and QUIT.

- 1) RESTART — By selecting this option, the user causes the program to return to the initial display, so that a different set of experimental data may be retrieved and displayed.
- 2) PRINT — A detailed set of printed output, describing the current display, is produced when this option is selected.
- 3) LETTERS — It is possible to display the data points as alphabetic characters (Figure 6). In that way, individual data points can be related to the source through the reference list in the right center of the display. When this option is chosen, the points are transformed

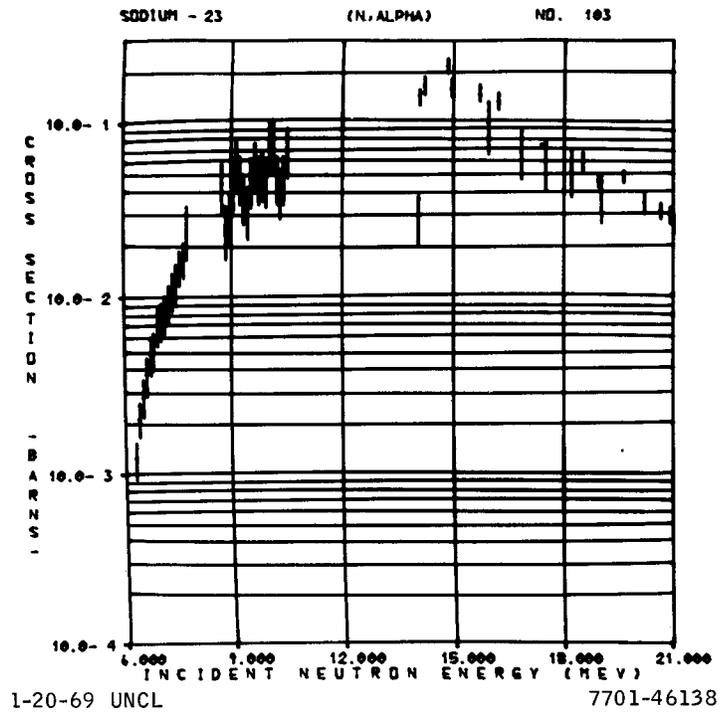


Figure 8.
Expanded Data Display

SODIUM - 23 (N,ALPHA) NO. 103

ENERGY (MEV)	SIGMA (BARN S)	ENERGY (MEV)	SIGMA (BARN S)
6.30000E 00	1.20000E-03	8.70000E 00	4.50000E-02
6.40000E 00	2.10000E-03	8.80000E 00	2.50000E-02
6.50000E 00	2.80000E-03	8.90000E 00	3.00000E-02
6.60000E 00	3.70000E-03	9.00000E 00	4.60000E-02
6.70000E 00	4.80000E-03	9.10000E 00	6.00000E-02
6.80000E 00	5.10000E-03	9.20000E 00	5.00000E-02
6.90000E 00	7.00000E-03	9.30000E 00	3.90000E-02
7.00000E 00	7.50000E-03	9.40000E 00	3.20000E-02
7.10000E 00	8.20000E-03	9.50000E 00	4.80000E-02
7.20000E 00	9.30000E-03	9.60000E 00	5.90000E-02
7.30000E 00	1.10000E-02	9.70000E 00	5.00000E-02
7.40000E 00	1.23000E-02	9.80000E 00	5.20000E-02
7.50000E 00	1.51000E-02	9.90000E 00	4.80000E-02
7.60000E 00	1.68000E-02	1.00000E 01	7.71111E-02
7.70000E 00	2.50000E-02	1.01000E 01	7.71111E-02

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Figure 9.
Data List Option

to letters, and the word POINTS appears in the place of LETTERS. If one desires to return to a point display, the word POINTS is selected.

- 4) HATS – Experimental data errors may be displayed when the HATS option is chosen (Figure 7). The words NO HATS replace the word HATS, and the error is represented as a vertical line in the y (cross section) direction. The error bars may be removed by selecting NO HATS.
- 5) EXPAND – The EXPAND option creates a 12 by 12 in. display of the data (Figure 8). In this case, only a brief identifying title appears at top of the screen, instead of the references and light pen options appearing on the standard display. Depressing the "END" key on the alphanumeric keyboard restores the standard display.
- 6) NO CURVE – Any smooth curves overlaying the experimental data are removed when the light switch is activated.
- 7) LIST DATA – This option causes the experimental data in the current display to be listed on the 2250 (Figure 9). The list consists of two pairs of two columns. The adjacent columns contain x-y coordinate pairs. A maximum of 30 points may be displayed at one time, so a paging mechanism has been included. Each time the "END" key is depressed, a new set of 30 points appears, until the entire set has been displayed. A return to the basic display is effected by either completing the paging of data or by depressing the "CANCEL" key.
- 8) QUIT – This light switch causes the job to terminate.

The second option list, headed by MAIN 2/3, contains nine additional options (Figure 10). Some of these options are repeats from the first list, and are included in this second list for convenience. The new options are:

- 1) REPLOT – This option allows the user to modify the data display by changing the axis limits, number of grid lines, axis units, or mode of display (log or linear). The upper portion of the display (Figure 11) gives the extremes for the data which were previously displayed. The remainder of the display gives the current status of all the grid parameters. The user may proceed to modify any of these parameters. The

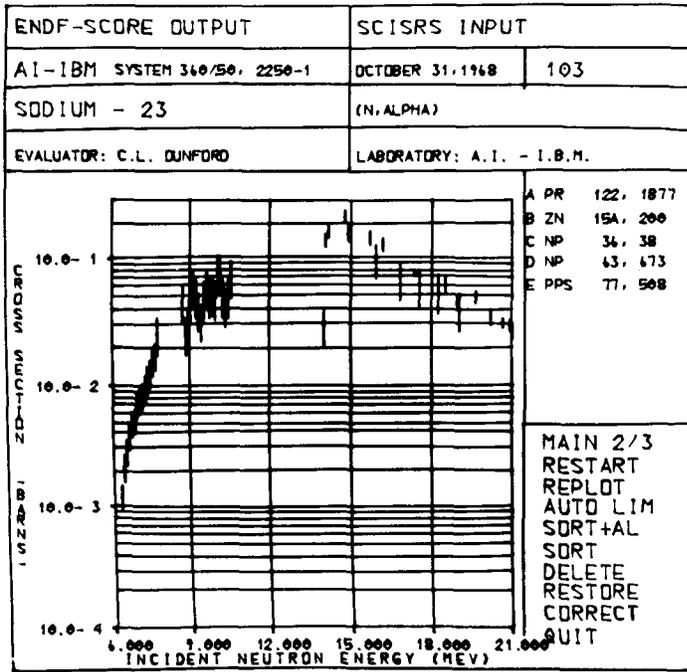


Figure 10.
Basic Display With
MAIN 2/3 Options

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11 023 NA 6.30000E 00 TO 2.10000E 01 MEV.
SIGMA MIN = 9.12000E-04 SIGMA MAX = 2.44200E-01

X-AXIS: LOG LIN Y-AXIS: LOG LIN

UNITS

X-AXIS MEV KEV EV LAB CM

Y-AXIS B MB B/ST MB/ST

X-MIN 6.0E 00 X-MAX 2.1E 01

Y-MIN 1.0E-04 Y-MAX 3.0E-01

DELTA X 3.0E 00 DELTA Y 8.6E-02

Figure 11.
Replot Option
Display

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axis units are also chosen in a similar manner. There are three options for the energy axis (MEV, KEV, or EV), or two choices for angular data [LAB or CM (center-of-mass)]. The y-axis may be in barns (B) or millibarns (MB) for cross sections, or barns/steradian (B/ST) or millibarns/steradian (MB/ST) for angular data.

The final three lines of Figure 11 allow the user to design a display grid. The minimum and maximum of the x- and y-axis are supplied. In the case of log plotting, 0.0 or a negative value may not be requested for that axis. The minimum is reset by SCORE to the nearest lower decade when log plotting is requested. The quantities DELTA X and DELTA Y are grid units which specify the separation between grid lines for linear plotting. For log plotting, these values are ignored and set internally. In all cases, the values must be specified in the same units given in the upper two lines of the display, not in the chosen axis units.

When all required data have been specified, the "END" key is depressed, causing the program to continue. If an error was made in specifying the units for either axis, an error message, in the format of Figure 3, appears with the three options: CONTINUE, RESTART, or TERMINATE. If CONTINUE is chosen, the previous display appears and the error can be corrected.

- 2) AUTO LIM – If the user wishes to let the program automatically reset the grid parameters, this option may be selected. A built-in grid parameter selection algorithm is used.
- 3) SORT + AL – When this option is chosen, the display in Figure 12 appears. By using this display, various subsets of the experimental data may be selected for display. The subsets are created through restrictions on reference and energy range (or angle cosine range). The uppermost two lines give the data extremes. The references are listed in the same format as in the basic data display. The references are light-pen sensitive; so that, when more than ten references have been retrieved, a light-pen detect moves the next ten (or less) into the display. Successive detects continue to move new references into the

11 023 NA 6.30000E 00 TO 2.10000E 01 MEV.
 SIGMA MIN = 9.12000E-04 SIGMA MAX = 1.86000E 02

A	PR	122,	1877	
B	ZI	15A,	200	
C	NP	36,	38	
D	NP	63,	673	∩
E	PPS	77,	508	

Figure 12.
Sort Option

REFERENCE: A D E
 ENERGY 6.30000E 00 TO 2.10000E 01 MEV.

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display until all references have been displayed. Then a detect re-
 cycles by bringing in the first ten references again.

If the user wishes to add or delete all data for a reference or ref-
 erences from the data to be displayed, then the identifying alphabetic
 character for each desired reference must be typed in the area of the
 screen to the right of the word REFERENCE. If no change in refer-
 ences from the previous specification is desired, then that area is left
 blank. The default condition is that all references retrieved will be
 plotted, and this condition exists until the evaluator has made a change
 in the list of references from which data will be displayed, using this
 option. Each light-pen detect on the reference list (see previous para-
 graph) clears the area to the right of the word REFERENCE, and
 stores the characters which were entered from the keyboard. Finally,
 the energy limits of the data, or (in the case of angular distributions)
 the angular limits desired, are entered into the bottom line through
 the keyboard.

When all data are entered, striking the "END" key initiates the
 final data sort and causes the program to automatically reset the grid
 parameters. If there are no data within the restricted limits, an error

message (similar to Figure 4) appears. The options, RESTART and TERMINATE, have the same meaning as before. The CONTINUE option returns to the display in Figure 12 and allows the evaluator to correct the error or errors.

- 4) SORT – This option is the same as the previous one, except that the grid parameters are not automatically reset.
- 5) DELETE – Individual data points may be deleted from the data display by using this option. The graphical display expands from 9 by 9 in. to 12 by 12 in., and the data points are made sensitive to a selection by the light pen. Data points selected by the light pen disappear from the display. If a point has been deleted incorrectly, it may be restored by depressing the "CANCEL" key. It is recommended that data points be plotted as alphabetic characters before this option is used, in order to provide a larger target for the light pen. A return to normal operation is effected by depressing the "END" key.
- 6) RESTORE – All data points which have been deleted from the display by using the DELETE option will be returned to the display when this option is selected.
- 7) CORRECT – If any of the data in a display are incorrect, action may be taken to correct this data. The light pen is used to select the CORRECT option. Immediately, the graphical part of the display is expanded to full-screen size, and the data points are made sensitive to detection by the light pen. Each data point which the evaluator wishes to modify is successively detected with the light pen. Each point, as chosen, disappears from the screen and is stored for future use. If a point has been detected and deleted from the display, it may be restored by striking the "CANCEL" key, providing that no other succeeding point has been detected and deleted.

When the evaluator has completed selection of the incorrect data, he strikes the "END" key. The display shown in Figure 13 appears on the screen. In addition to the identifying information, there are four columns of data displayed. The left two columns are the incorrect values of the x and y coordinates, respectively. The right two columns

Figure 13.
Correction
Option

LIGHT PEN DATA TIMES 1.00 -03 PLUS 0.00 +00			
INCORRECT DATA		CORRECTED DATA	
ENERGY (MEV)	SIGMA (BARN)	ENERGY (MEV)	SIGMA (BARN)
1.48100E 01	1.64000E 02	1.48100E 01	1.64000E-01
1.56700E 01	1.53000E 02	1.56700E 01	1.53000E-01
1.61800E 01	1.34000E 02	1.61800E 01	1.34000E-01
1.73300E 01	7.55000E 01	1.73300E 01	7.55000E-02
1.84100E 01	6.00000E 01	1.84100E 01	6.00000E-02
1.81200E 01	4.56000E 01	1.81200E 01	4.56000E-02
1.96100E 01	4.90000E 01	1.96100E 01	4.90000E-02
2.01900E 01	3.40000E 01	2.01900E 01	3.40000E 01
2.06300E 01	3.07000E 01	2.06300E 01	3.07000E 01
2.09000E 01	2.90000E 01	2.09000E 01	2.90000E 01
2.10000E 01	2.55000E 01	2.10000E 01	2.55000E 01

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are initially duplicates of the left-hand pair of columns. Any changes made in the data by the evaluator appear in these columns.

Data may be corrected in either of two ways: (1) The display contains two locations (TIMES and PLUS) into which multiplicative and additive factors can be entered from the keyboard. This linear transformation can then be applied to any piece of data in the right-hand pair of columns by detecting the datum with the light pen. (2) Alternately, the cursor may be placed at any character position in the right-hand columns and a new character entered in that position from the keyboard.

The display will hold only 15 data points at one time. If more than 15 data points are to be corrected, then successive displays are required. Each succeeding display is reached by striking the "END" key. If all points in the correction array have been displayed, the "END" key is used to return to continue execution of SCORE.

The final option list, headed by MAIN 3/3 (Figure 14), contains four new options, ENDF/B, DATA FIT, RES CALC, and E SHIFT:

- 1) ENDF/B – If this option is chosen, any available evaluated data from ENDF/B which satisfies the description of the experimental data set will appear as a smooth curve overlaying the experimental data (Figure 15). The storage and retrieval system for ENDF/B is described in Section IV.
- 2) DATA FIT – This option allows an evaluator to fit smooth curves to experimental data. This option is described in more detail in Section II-B.
- 3) RES CALC – Analysis of resonance region cross sections can be made when this option is chosen. A detailed description of this option is given in Section II-C.
- 4) E SHIFT – The energy coordinate for a given set of data points can be transformed according to

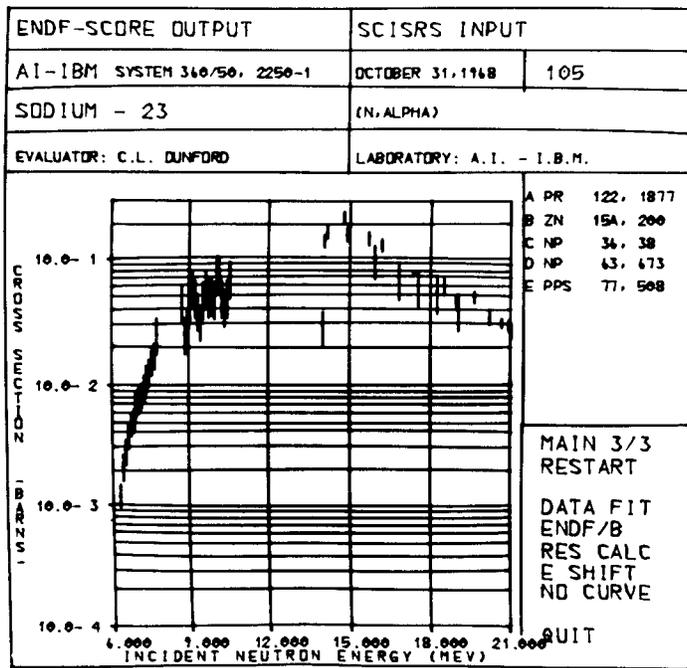
$$E_c = C_1 \left(\sqrt{1/E} + C_2 \right)^{-2}$$

When the option is chosen, a display (Figure 16) appears in which the user may enter a letter selecting a reference and values of C_1 and C_2 . When the "END" key is depressed, the display disappears, the data are transformed, and then the display reappears so that additional transformations may be made. The "CANCEL" key will return from this option.

B. DATA FITTING OPTIONS

One of the most frequent operations performed by an evaluator is the reduction of a set of scattered experimental data to a single, smooth, evaluated curve. A graphics interactive system, such as SCORE, provides an ideal mechanism for producing evaluated data curves which are parametrized for easy storage.

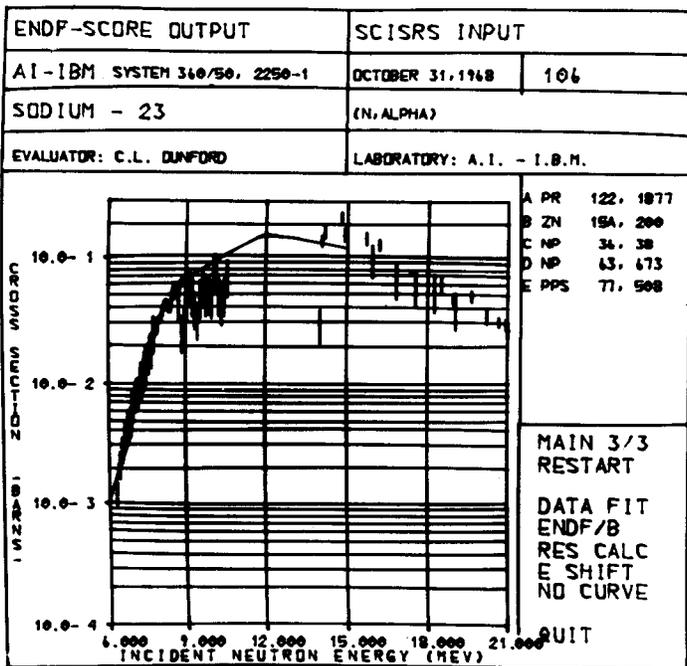
It is important to emphasize that the production of a smooth data curve does not constitute an evaluation, but is the end product of an evaluation. The evaluator must use other information, such as the original documentation, to aid in



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Figure 14.
Basic Display With MAIN 3/3
Options



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Figure 15. Overlay of Evaluated Data

$$EC = C1*(SQRT(1/E) + C2)**-2$$

REFERENCE : H

C1(DIMENSIONLESS) : .95

C2(SQRT(1/EV))-: 1.2_

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Figure 16. Energy Shift Option

the selection of an evaluated curve. SCORE has been designed to provide the evaluator with the tools necessary to develop an evaluated curve, in much the same manner as he does it now, with the addition of several numerical aids and a large reduction in response time to an evaluator's query.

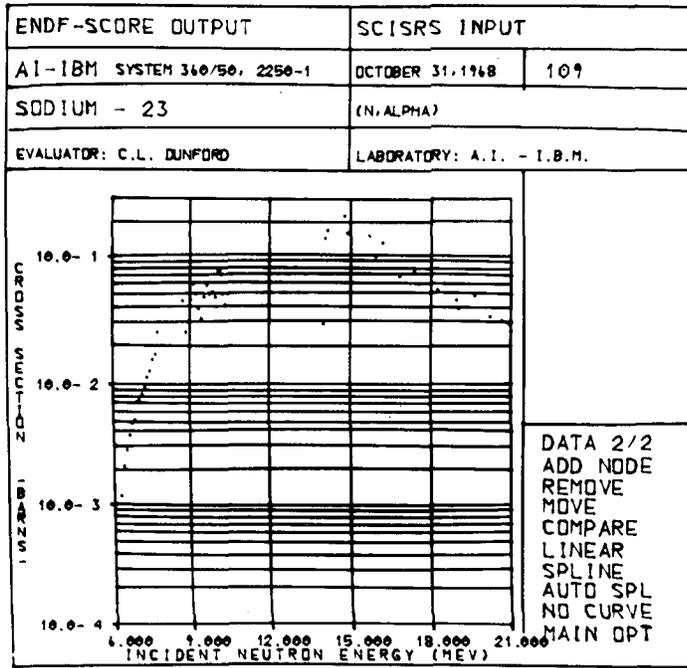
Our approach to the production of evaluated data curves in SCORE is through the use of piecewise analytical curves. These curves are uniquely defined by a set of parameters for collection of points, called nodes, and a prescription for interpolation between nodes. The prescriptions that are presently available for interpolation between nodes are linear curves and cubic spline curves.

The evaluator may prepare a set of experimental data for evaluation, using the SCORE options described in Section II-A. He may have selected the data from only one or two references, deleted obviously erroneous data points, corrected or renormalized other points, and selected the space (log-log, lin-log, etc.) in which the data will be evaluated.

Selection of the DATA FIT option with the light pen causes the program to begin execution of the data-fitting module. Two possible sets of option lists may be activated during the data-fitting procedure. The first list is headed by a light pen switch, DATA 1/2. When this button is selected, the list headed by DATA 2/2 appears. The list DATA 1/2 is returned by selection of DATA 2/2 with the light pen.

The list headed by DATA 2/2 (Figure 17) contains all the options necessary to produce a smooth data curve. First, it is necessary to supply nodes for the data curves. For this purpose, three switches (Items 1 through 3) are available. The options are:

- 1) ADD NODE – By selection of this switch, the evaluator may add nodes to the screen. The expanded data (Figure 18) display and a tracking pattern, consisting of a point surrounded by three concentric circles, appear. Motion of this tracking pattern is initiated and terminated by detection of light on the screen by the light pen. The pattern moves toward any light detected on the screen, with a velocity related to the distance between the detected point and the center of the tracking pattern. Thus, fine positioning of the tracking pattern may be accomplished by using the concentric rings of the tracking pattern. Movement is terminated with the next light pen activation, and restarted with the succeeding detect.

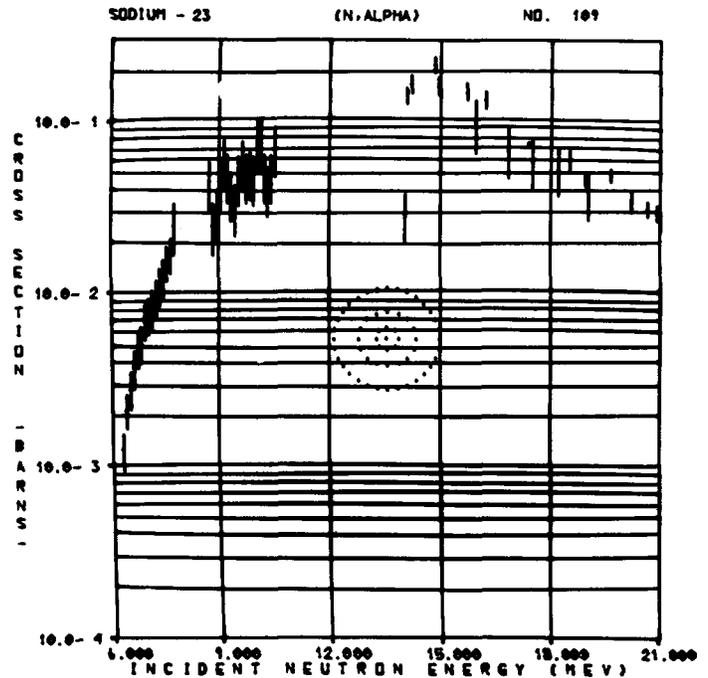


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Figure 17.
 Data Display With DATA 2/2
 Options

Figure 18.
 Tracking Pattern for Nodal
 Placement



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When the center of the tracking pattern is properly positioned, the "END" key is depressed. This action causes the coordinates of the center of the tracking pattern to be stored, and a small asterisk appears on the screen to represent the node. The tracking pattern also reappears, so that additional nodes may be entered. When all nodes which the evaluator feels are necessary to adequately describe the experimental data have been entered, the "CANCEL" key will return control from the ADD NODE option.

- 2) REMOVE – One may wish to remove some nodes from the display. When this option is chosen, the large graphical display appears. The nodes are sensitive to detection by the light pen, and a node may be removed from both the display and storage when it is selected. When the evaluator has completed this task, the "CANCEL" key will return to the standard display.
- 3) MOVE – The MOVE option is a logical combination of ADD and REMOVE. The selection of this option causes the expanded display to appear, and the nodes to become light-pen sensitive. Selection of a point causes the asterisk to be replaced by the tracking pattern. The tracking pattern may be moved as described in the ADD option. Depression of the "END" key reenters the node at its new location. When the evaluator has completed this option, he can exit by means of the "CANCEL" key.
- 4) LINEAR – A piecewise linear curve is passed through the nodes in the display (Figure 19). A value of CHI:

$$X = \sqrt{\frac{1}{N} \sum_{i=1}^N \left(\frac{\sigma_{\text{Calculated}} - \sigma_{\text{Experimental}}}{\Delta\sigma_{\text{Experimental}}} \right)_i^2}$$

is calculated, using all data points displayed, and appears in the right center of the screen.

- 5) SPLINE – When this light pen switch is selected, a cubic spline curve is passed through the nodes displayed (Figure 19). A value of CHI is calculated so that the evaluator may have a numerical measure of the goodness of fit of a particular curve.

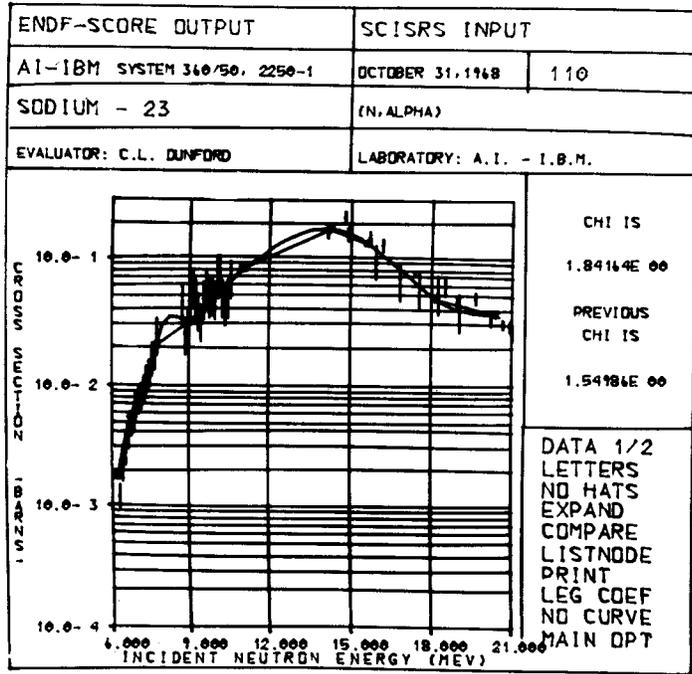


Figure 19.
Linear and Spline Curve
Data Fits

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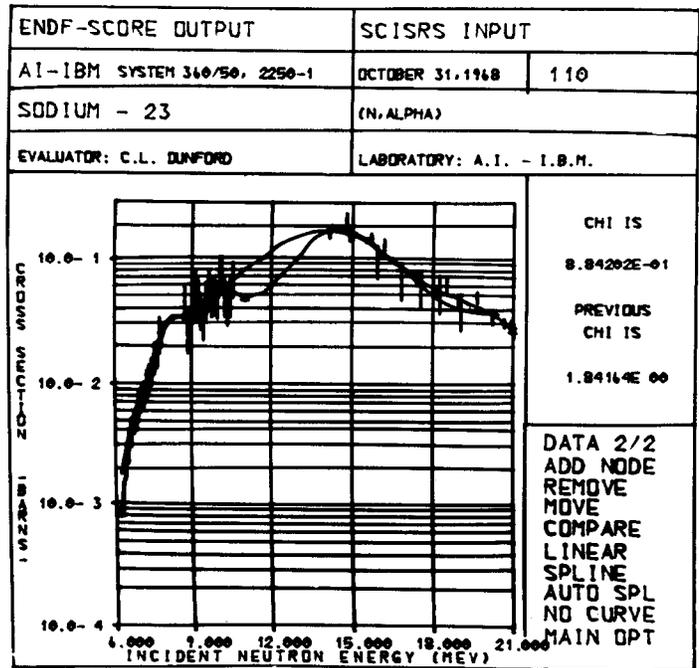


Figure 20.
Results of a Least Squares
Spline Fit

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- 6) AUTO SPL – A least squares spline program, developed by Powell⁽⁷⁾ and by Horsley and Parker,⁽⁵⁾ has been added to SCORE. When this option is chosen, the y-coordinates (cross section) of the nodes are automatically adjusted to obtain a minimum X^2 , based on having N nodes with fixed x-coordinates (Figure 20). If this option is chosen, and then followed by the regular SPLINE option, slightly different curves will result, because of different conditions imposed at the end point of the curve.
- 7) COMPARE – This option allows the user to display the current fitted curve, as well as the most recent previous curve, for comparison purposes (Figure 19). The CHI value for both curves is displayed in the right-hand center box. In order to remove the overlaid curve, COMPARE should be selected again.
- 8) NO CURVE – All curves are deleted from the display when this option is chosen.
- 9) MAIN OPT – Selection of this option terminates the data fitting, and returns to the main program.

The other set of options, headed DATA 1/2 (Figure 21), relates primarily to data manipulation. There are three options which are the same as those in DATA 2/2, and will not be repeated here. The new options are:

- 1) LETTERS – The meaning of this option is the same as previously described. When it is chosen, the references replace the CHI values in the right center box.
- 2) LIST NODE – The data nodes are displayed, and may be modified in the same manner as the data in the CORRECT option.
- 3) PRINT – The print option will cause the data pertinent to the current data evaluation to be recorded on the printer.
- 4) LEG COEF – Legendre coefficients may be calculated for an angular distribution only (Figure 22). The order of the fit is 9. A curve generated from these coefficients is overlaid on the screen to permit evaluation of the goodness of the fit. The Legendre coefficients are displayed in the right center box.

Figure 21.
Data Display With
DATA 1/2 Options

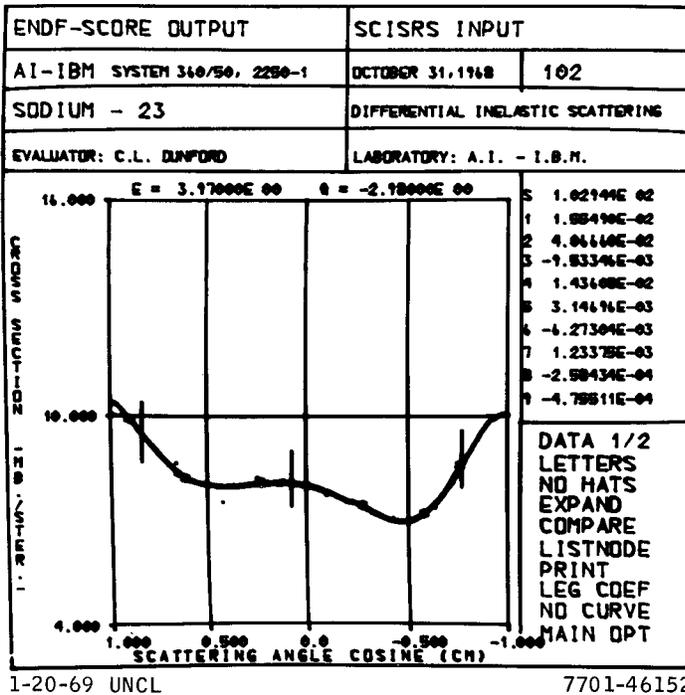
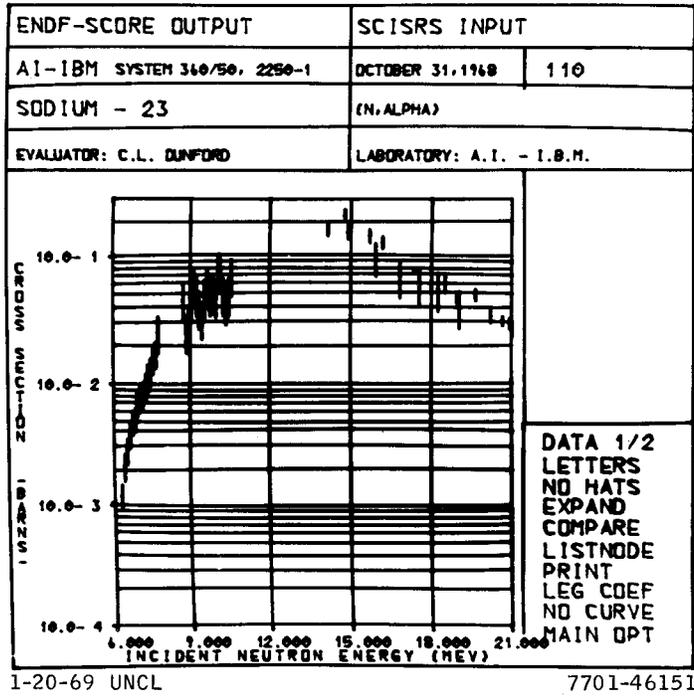


Figure 22.
Legendre Fit to an
Angular Distribution

This completes a brief description of the activities which are presently available when the user wishes to fit a smooth curve through a set of experimental data points.

C. RESONANCE OPTION

One of the areas of application of SCORE which shows tremendous potential is that of resonance cross-section analysis. This analysis requires an iterative procedure which can be carried out efficiently through interactive computer graphics. With the cooperation of M. S. Moore of Idaho Nuclear and N. Marshall of Phillips Petroleum, a module for the analysis of resonance cross sections has been included in SCORE.

This module is activated when the RES CALC light pen switch is selected. The resonance calculation option has three option lists, headed by RES 1/3, RES 2/3, and RES 3/3 (Figure 23). Option list RES 1/3 contains only options which have been explained previously.

The option list headed by RES 2/3 contains two options for calculating a resonance line shape. This line shape is both resolution and Doppler broadened. A value of CHI is calculated, using a spline curve interpolation to get the cross-section value at experimental energy values between points on the calculated curve. Four cross sections may be calculated (total, scatter, capture, or fission), depending on the nature of the experimental data being displayed.

- 1) S-LEVEL – A sum of single-level Breit-Wigner reaction amplitudes, using resonance parameters stored in a data set on a disk, is used to calculate a line shape (Figure 24). Since the data set is designed for a two-channel multilevel formalism, the fission width for the single level is the absolute value of the sum of the two channel widths.
- 2) M-LEVEL – A Reich-Moore two-fission-channel multilevel formula is used to generate the Doppler- and resolution-broadened line shape (Figure 25). As before, a CHI value is calculated to help determine the "goodness" of the fit.

The option list, RES 3/3, contains options for modifying resonance parameters and the experimental parameters, such as flight path and temperature.

SCISRS INPUT	
OCTOBER 31, 1968	101
(N.FISSION)	
LABORATORY: A.I. - I.B.M.	
RES 1/3 LETTERS HATS EXPAND	
COMPARE PRINT	
NO CURVE MAIN OPT	

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ENDF-SCORE OUTPUT		SCISRS INPUT	
AI-IBM SYSTEM 360/50, 2250-1		OCTOBER 31, 1968	101
PLUTONIUM - 241		(N.FISSION)	
EVALUATOR: C.L. DUNFORD		LABORATORY: A.I. - I.B.M.	
RES 2/3		S-LEVEL M-LEVEL	
COMPARE EXPAND		NO CURVE MAIN OPT	

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b. RES 2/3

ENDF-SCORE OUTPUT		SCISRS INPUT	
AI-IBM SYSTEM 360/50, 2250-1		OCTOBER 31, 1968	101
PLUTONIUM - 241		(N.FISSION)	
EVALUATOR: C.L. DUNFORD		LABORATORY: A.I. - I.B.M.	
RES 3/3		EXP COND	
LOAD RES STORE RES ADD RES MOD RES		MAIN OPT	

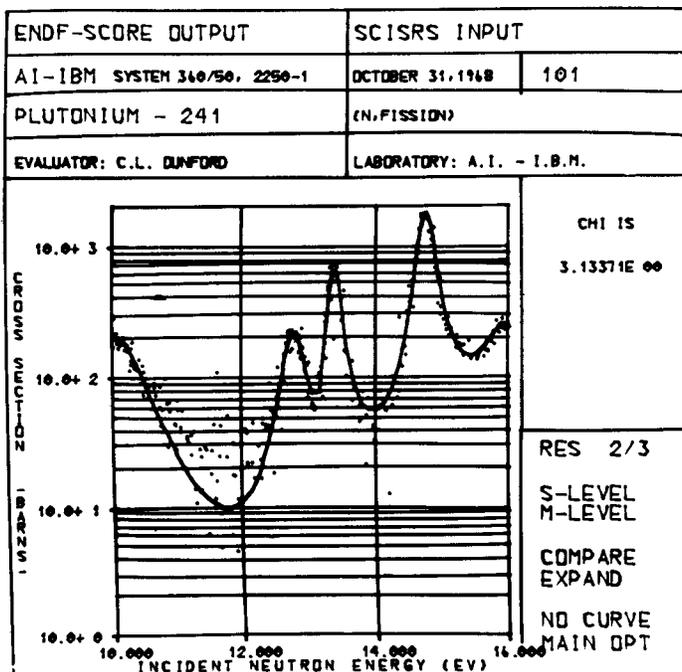
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c. RES 3/3

Figure 23. Three Option Lists for Resonance Theory Calculation

Figure 25.
Multilevel Calculation
for Pu-241



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TARGET TEMPERATURE (KELVIN):	_3.00000E 02
FLIGHT PATH (METERS):	1.05600E 01
BURST WIDTH (MICROSECONDS):	3.00000E-01
CHANNEL WIDTH (MICROSECONDS):	2.50000E-01
DETECTOR THICKNESS (INCHES):	0.0
SAMPLE THICKNESS**-1 (BARN/ATOM):	5.00000E 03
POTENTIAL SCATTERING (BARN):	1.00000E-04
ATOMIC WEIGHT (AMU,C-12):	2.41000E 02

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Figure 26.
Experiment Parameter
Modification Display

RESONANCE ENERGY (EV): 1.2+01
 REDUCED NEUTRON WIDTH (EV): .003
 CAPTURE WIDTH (EV): .023_
 FIRST FISSION WIDTH (EV):
 SECOND FISSION WIDTH (EV):
 G FACTOR:
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Figure 27.
Add Resonance Option

PLUTONIUM - 241		(N,FISSION)	NO. 101
LIGHT PEN DATA TIMES _		PLUS	
THOSE MODIFIED		RESONANCES	
ENERGY	ENERGY	ENERGY	ENERGY
(EV)	(EV)	(EV)	(EV)
	4.58000E 00	4.27500E 00	4.58000E 00
		5.91000E 00	6.91500E 00
		8.58500E 00	9.48000E 00
	0.0	1.01100E 01	1.20000E 01
		1.27700E 01	1.33800E 01
		1.47300E 01	1.60100E 01
1.66900E 01		1.64800E 01	1.77800E 01
		2.06300E 01	2.28600E 01
		2.39600E 01	2.63400E 01
		2.87500E 01	2.93500E 01
		3.08800E 01	3.49000E 01

Figure 28.
Modify Resonance
Option

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- 1) EXP COND – A sample set of parameters, necessary for calculating Doppler and resolution broadening, is stored and may be used as a default condition. However, these parameters relate to a particular Pu-241 experiment. If the user chooses this option, a display appears in which the parameters and their values are listed (Figure 26). By positioning the cursor and entering new values from the keyboard, any parameter may be changed. This option may be terminated with the "END" key.
- 2) LOAD RES – This option transfers the resonance parameters from the data set to the computer. This operation is performed automatically when the RES CALC option is executed for the first time. This option is most useful when many parameter changes have been made and the user wishes to return to some intermediate point in the evaluation.
- 3) STORE RES – If some intermediate point is reached in the evaluation, such that the evaluator might wish to return to that point, the current resonance parameters may be stored in the data set on the disk, replacing old parameters. Thus, by using the LOAD RES option, the evaluator can return to some intermediate point in the evaluation.
- 4) ADD RES – New resonances may be added to the parameter arrays when this option is selected. A display appears (Figure 27), and the resonance parameters are entered in the usual way. When each new resonance has been completely specified, the "END" key may be used to record the new parameters. The "CANCEL" key is used to return when all new resonances have been specified.
- 5) MOD RES – If the evaluator wishes to modify the parameters for any resonance, this option may be used. A display appears, in which the resonance energy of all resonances is listed (Figure 28). The parameters for a particular resonance appear after the resonance energy is selected with the light pen as in Figure 27. Any parameters may be modified from the keyboard. If the resonance energy is set to zero, that resonance is eliminated. The "END" key returns to Figure 28, and further resonances may be selected for changes. When all changes are complete, the "CANCEL" key will terminate the option.

III. SCISRS DATA STORAGE AND RETRIEVAL

A. METHOD

The evaluator requests a particular isotope, reaction type, energy range, and level energy (if applicable) by entering data in the initial display (Figure 3). The problem then is to retrieve the requested information in the most efficient manner, in order to minimize the time during which the evaluator must wait before continuing with SCORE.

The retrieval scheme chosen uses both tape and disk storage. All the available experimental cross-section data for an isotope or a natural element are stored as a hexadecimal sequential data file on one of several multifile magnetic tapes. The tapes are prepared by program SAP (Appendix V), and are referred to as SAP tapes. In addition to experimental data, each file contains identification information and two tables which describe the contents of the file.

When a new isotope is requested by the evaluator, a table is searched to find the tape and file containing that isotope. If the correct tape is not mounted, a message will be printed on the computer operator's typewriter, giving him tape mounting instructions. When the correct tape is mounted, the file handling features of OS/360⁽⁸⁾ are used to position the tape to the correct data file. This file is copied into a direct-access data set on a disk, so that the direct-access feature of FORTRAN-IV may be used.

In order to retrieve the requested data with the reaction type and energy range restrictions imposed by the evaluator, two tables, which catalog the data file as to reaction types and energy regions, are searched. The result of that search is a record number which is used to initiate a sequential search in the direct-access data set. Since an entry is made in the energy region table for every 250th data point for each reaction type, the sequential search is started within 250 data points (5 records on the disk) of the requested data. The advantage of this method over a purely sequential search through a data file containing tens of thousands of records is obvious.

If the desired isotope already resides in the direct-access data set, all subsequent requests for different reaction types, energy ranges, etc., for this

isotope are retrieved from this data set, using the methods described in the previous paragraph. The cross-section information for an isotope remains in the direct-access data set until another isotope is requested.

A description of the SAP tape layout, along with the SAP program description, are given in Appendix V. The following sections describe in detail the direct-access data set and the search procedure.

B. DIRECT-ACCESS DATA SET

The direct-access data set is an intermediate storage area on an IBM direct-access device which receives the data for the requested isotope as it is copied from the appropriate SAP tape and file. The block size on the tape was chosen so that SCORE would read a block from the tape into core and then write the entire block as a record which filled a full track on the 2311 disk. This is repeated until the end-of-file on tape is sensed and all the information has been written onto the disk.

Each data point on the SAP tape consists of a 16-word record. The block size of 56 for the SAP tape was chosen, because this is the maximum number of 16-word records which may be collapsed into one record to fill a single track on the 2311 disk. This is important, since transmission time to or from the disk can be greatly reduced by writing or reading an entire track at a time. The collapsing of the 56 records into one record for the disk are done in core by using a doubly dimensioned array, 16 by 56.

The direct-access data set is formatted, written, and read by using the direct-access input-output statements in FORTRAN-IV. Once this data set is created, it should be kept, since the initial formatting of a direct-access data set may take several minutes and requires operation of the SAP program.

The following statement defines the direct-access data set:

```
DEFINE FILE 17 (500, 896, U, IV)
```

Data set Reference Number 17 refers to 500 records; each record has a maximum of 896 words, and the record is to be read or written without formal control. This data set will hold almost 28,000 SCISRS data points. It requires 500 tracks, or one-fourth of a 2311 disk pack.

Only the SCORE subroutines DIRECT and RECORD (Appendix I) reference this data set. These subroutines must therefore be compiled with a FORTRAN compiler supporting direct-access I/O.

C. SEARCH PROCEDURE

If the isotope requested is not in the direct-access data set, a table is searched to find the corresponding tape and file number. This table and a table of tape identifiers are stored on disk, and are read by SCORE at the beginning of execution. This table contains the isotope identification number ($Z*1000 + A$), the tape and file number, along with the previous (now obsolete) tape and file number, stored as one word, and the date of entry (see Appendix V). The tape number is used as an index in the table of tape identifiers to obtain the desired tape identifier.

The tape identifier is then used to make certain that the correct SAP tape is mounted. The file number (NF) is used to compute a data set reference number ($NF + 20$) which has an associated data definition (DD) card defining the ($NF + 1$) file on the tape (see Appendix II). By assigning each file a different data set reference number, OS/360 will do all the tape positioning; the one set of DD cards will work for all the SAP tapes, if a nonlabeled tape is used. However, no tape may have more than one label and six data files, because ENDF material files start on logical unit 28.

Once the tape is positioned, 56 records (one block) at a time are read into core and then written as one record into the direct-access data set. This continues until the end-of-file is sensed. The last four words read from tape contain control information:

- 1) ISAVE contains the starting record number of the table of reaction types.
- 2) KU contains the number of pairs in the table of reaction types.
- 3) KE contains the number of pairs in the table of energy points.
- 4) NRS contains the number of records in the file (896-word records).

These control parameters are in core, and are used to read the table of reaction types and the table of energy points from the direct-access data set into core.

The direct-access data set is always checked first, to see whether it already contains the requested isotope. When a file is copied into this data set, the isotope identification number and the total number of records (NRS) are written into the dummy-word area of the first disk record. This record is read and the identification checked. If it is not the desired isotope, the program proceeds as described previously. If it is the desired isotope, NRS is used in a direct-access read to obtain the control information (ISAVE, KU, and KE). This control information is then used to read the tables from the direct-access data set into core. In either case, once the tables are in core, they will be used until another isotope is requested.

After the tables are established in core, a search is made in the table of reaction types for the requested reaction. If a match occurs, the associated index is used to locate the initial point in the energy table for beginning the search for the requested minimum energy. When the minimum energy is less than an energy point in the table, or the last entry for this reaction type has been checked, the record number for the previous energy table entry is used in a direct-access read to begin a sequential search for the desired energy range. This starting point will be within 250 data points (5 disk records) of the requested data.

If there are less than 500 data points for the requested reaction in the requested energy range, these data points are stored in core. All subsequent selection of a restricted subset of this data (by reference or energy range), using the SORT option described in Section II, is done from this in-core data set. However, if more than 500 data points exist which satisfy the initial request, only the first 500 are retrieved and stored in core. Any subsequent request, using the SORT option, retrieves the first 500 points satisfying the restricted data requirements from the direct-access data set.

IV. ENDF/B STORAGE AND RETRIEVAL

A. METHOD

After the evaluator has requested and displayed a particular isotope, reaction type, energy range, and level energy (if applicable), he may select the ENDF/B option. Depending upon the SCORE reaction symbol (Table 2), smooth data of File 3,^{*} angular distributions of File 4, or inelastic discrete level data of File 5 are overlaid on the display. The latter two files contain probability distributions which are combined with File 3 smooth data before being displayed. The requested information must be retrieved in the most efficient manner, in order to minimize the time during which the evaluator must wait before continuing with SCORE.

The retrieval scheme is similar to that used for the SCISRS data. Both tape and disk storage are used. Selected data for a material on an ENDF/B EBCDIC tape⁽²⁾ are stored as a hexadecimal sequential data file on one of several multifile magnetic tapes. The tapes are prepared by program SCOFF (Appendix VI), and are referred to as SCOFF tapes. In addition to the data, each file contains identification information and a file contents directory, which consists of several tables describing the contents of the file. All records of a material file contain 900 floating point words.

When the ENDF/B option is selected for a new material, a table is searched to find the SCOFF tape and file containing that material. If the correct tape is not mounted, a message will be printed on the computer operator's typewriter, giving him tape mounting instructions. When the correct tape is mounted, the file handling features of OS/360⁽⁸⁾ are used to position the tape to the correct data file. This file is copied into a direct-access data set on a disk, so that the direct-access feature of FORTRAN IV may be used. All records written on the disk contain 900 words.

In order to retrieve the requested data from the disk with the reaction type and energy range restrictions imposed by the evaluator, the file contents directory, which catalogs the data as to reaction types and energy regions, is searched.

*These data files are used in the sense of Reference 2, and should not be confused with data sets on tape or disk.

The result of that search is a record number which is used to bring into core, by direct-access means, the appropriate 900-word record in which the desired data resides; in addition, a word number is obtained which is the index of the beginning of the desired data within the 900-word record. Thus, time-consuming sequential searches through the data file are eliminated.

If the desired material already resides in the direct-access data set, all subsequent requests for different reaction types, energy ranges, etc., for this material are retrieved from this data set, using the methods described in the previous paragraph. A material remains in the direct-access data set until a different material is requested.

A description of the SCOFF tape layout, along with the SCOFF program description, are given in Appendix VI. Not all of the data on a SCOFF tape can be used by SCORE. Only ENDF/B File 3 (smooth cross sections), File 4 (angular distributions), and File 5 Subsection 3 (secondary energy distributions for discrete levels) may be used by SCORE, subject to the reaction types available, as given in Table 2.

The following sections describe in detail the direct-access data set and the search procedure.

B. DIRECT-ACCESS DATA SET

The direct-access data set is an intermediate storage area on an IBM direct-access device onto which the requested material is copied from the appropriate SCOFF tape and file. The block size on the tape was chosen so that SCORE would read a block from the tape into core, and then write the entire block as a record which fills a full track on the 2311 disk. This is repeated until the end-of-file on the tape is sensed, and all the information has been written onto the disk.

Transmission to or from the disk is done with 900-word records, each of which fills a single track on the 2311 disk. Reading or writing an entire track at a time greatly reduces the transmission time. When SCORE reads a record from the disk, the data are stored in core in a singly dimensioned array of 900.

The direct-access data set is formatted, written, and read by using the direct-access input-output statements in FORTRAN IV. Once this data set is

created, it should be kept, since the initial formatting of a direct-access data set may take several minutes, and it may be created only by using the SCOFF program.

The following statement defines the direct-access data set:

```
DEFINE FILE 16 (40, 900, U, IX)
```

Data set Reference Number 16 refers to 40 records; each record has a maximum of 900 words, and the record is to be read or written without format control. The 40th record is reserved for the material correspondence and tape requirements tables, which are updated each time program SCOFF adds a material to the SCOFF tapes (see Appendix VI). The remaining space, Records 1 through 39, will hold 35,100 words of ENDF/B data. This should be enough space for normal ENDF/B usage; however, if the maximum dimensions allowed in the ENDF/B specifications were used, this would not be enough space. One of the materials with the largest amount of data on the current ENDF/B tapes is iron (ENDF/B Tape 115, MAT = 1020); this material requires 19,800 words on the disk.

Only subroutine RETREV (Appendix I) references this direct-access data set. It is the only subroutine that must be compiled with a FORTRAN compiler which supports direct-access statements.

C. SEARCH PROCEDURE

If the material requested is not in the direct-access data set, the material correspondence and tape requirements tables are searched to find the corresponding tape and file number and the tape identifier. These tables are stored on the disk in Record 40 of data set Reference Number 16, and are read by SCORE at the beginning of execution.

The material correspondence table contains the material identification number ($Z*1000 + A$), the ENDF/B material identification (MAT), the total number of 900-word records, the tape and file number, along with the previous (now obsolete) tape and file number, stored as one word, and the date of entry (see Appendix VI). The tape number is the index of the tape identifier entry in the tape requirements table.

The tape identifier is then used to make certain that the correct SCOFF tape is mounted. The file number (NF) is used to compute a data set reference number (NF + 27) which has an associated data definition (DD) card defining the (NF + 1) file on a nonlabeled tape (see Appendix II). By assigning each file a different data set reference number, OS/360 will do all the tape positioning; the one set of DD cards will work for all the SCOFF tapes, if the tape is nonlabeled. The maximum number of material files per tape is the maximum allowable DD cards in a system (usually 32) minus 27.

Once the tape is positioned, one record (900 words) at a time is read into core, and then written as one record into the direct-access data set. This continues until the end-of-file is sensed. The last five words read from tape contain control information.

- 1) ISAVE contains the starting record and word numbers of Table 1* of the file contents directory.
- 2) KU1 contains the starting record and word numbers of Table 2* of the file contents directory.
- 3) KU2 contains the starting record and word numbers of Table 3* of the file contents directory.
- 4) KU3 contains the starting record and word numbers of ISAVE.
- 5) NREC is the total number of 900-word records in the file.

These control parameters are in core, and are used to read Tables 1, 2, and 3 from the direct-access data set into core.

The direct-access data set is always checked first, to see whether it already contains the requested material. The 17th and 18th words of the first 900-word direct-access record contain the material identification numbers, the atomic number, and the mass number. The first record is read and the identification checked. If it is not the desired material, the program proceeds as described previously. If it is the desired material, NREC is obtained from the material correspondence table, and is used in a direct-access read of the final 900-word record to obtain the control information. These data are then used to read

*These tables catalogue the data as to reaction types and energy regions, as well as provide other descriptive parameters.

the three tables of the file contents directory from the direct-access data set into core. In either case, once the tables are in core, they will be used until another material is requested.

After the three tables are established in core, the SCORE reaction symbol is used to obtain the corresponding ENDF/B file and reaction number, which are packed into one word. This is used to search Table 1, in order to obtain the Table 1 and Table 2 indices for the requested reaction. If ENDF/B File 4 or File 5 data are required, Table 1 is also searched to obtain the Table 1 and Table 2 indices for the required File 3 data. Further processing of the data depends upon the ENDF/B file in which the data resides. Since only File 3, File 4, and File 5 (Subsection 3) data can be processed by SCORE at this time, there are only three methods of retrieval to be described – one for each of these files.

1. File 3 – Smooth Cross Sections

The Table 2 index is used to examine the energy ranges that are available. The Table 2 index is modified to correspond to the available energy range in which the desired energy range begins. This new index is used to obtain the 900-word direct-access record number and appropriate word number from Table 2. The direct-access record is then read into core, using a 900-word array.

Starting with the known word number, the energy - cross-section pairs in the desired energy range are transferred to the array which will eventually be displayed. If the desired information is continued in the next 900-word direct-access record, this next record is read into core, and the transfer is continued. If the energy boundaries of the desired energy range are not included in the ENDF/B data, the cross sections at these boundaries are found by interpolation, using the ENDF/B interpolation scheme which is included in Table 2. If data in the desired energy range are not available, a message is displayed with this comment.

2. File 4 – Secondary Angular Distributions

Using the Table 2 index for the required File 3 smooth cross-section data, the cross section for the energy at which the secondary angular distribution is desired is found, using the File 3 method of retrieval. If the desired energy is

not included in the energy - cross-section pairs, the cross section is interpolated to that energy, using the ENDF/B interpolation scheme.

If the angular distribution data are given as Legendre coefficients, the Table 2 index is used to examine the energy ranges that are available. The Table 2 index is modified to correspond to the available energy range in which the desired energy lies. If no appropriate energy range is available, a message is displayed with this comment. This new index is used to obtain the 900-word direct-access record number and appropriate word number from Table 2. The direct-access record is then read into core, using a 900-word array. Starting with the known word number, the energies are examined until a match with the desired energy is found or until energies which bracket the desired energy are found. The coefficients are transferred to special arrays; and interpolation to the desired energy, if required, is done, using the ENDF/B interpolation scheme. The angular distribution is then evaluated at 101 points, equally spaced on the interval -1.0 to $+1.0$; the distribution is multiplied by the File 3 cross section, and the units are converted to millibarns per steradian. The results are stored in the array that eventually will be displayed.

If the angular distribution data are given as a tabulation, the Table 2 index is used to examine the energies that are available. The Table 2 index is modified to correspond to a match with the desired energy or to correspond to energies which bracket the desired energy. If no appropriate energies are found, a message is displayed with this comment. This new index is used to obtain the 900-word direct-access record number and appropriate word number from Table 2. The direct-access record is then read into core, using a 900-word array. Starting with the known word number, the angular distributions are transferred to special arrays. If the desired energy is available, further interpolation is not required; however, if the desired energy is not available, interpolation to the desired energy for each value of the angular distribution must be done. In order to carry out this interpolation, the two angular distributions at energies which bracket the desired energy must have the same cosine of the scattering angle (μ) grid. If the μ grid is not the same for each angular distribution, the larger grid (the one with more μ values) is selected. The angular distribution which has the smaller grid is then interpolated to the larger grid, using the ENDF/B μ interpolation scheme given in Table 2. Next, the interpolation of

each value of the angular distribution to the desired energy is done, using the ENDF/B energy interpolation scheme given in Table 2. The resulting angular distribution resides in the array which eventually will be displayed. The distribution is multiplied by the File 3 cross section, and the units are converted to millibarns per steradian.

If required, the angular distribution is converted from the laboratory to the center of mass system.

3. File 5, Subsection 3 – Secondary Energy Distributions, Discrete Energy Loss

Using the Table 2 index for the required File 3 smooth cross-section data, the cross section for the desired energy range is found, using the File 3 method of retrieval.

The absolute value of the desired level excitation energy, $|Q|$, is checked against the ENDF/B parameter, θ ,* which is obtained from Table 2. The Table 2 index is modified as each value of the available θ 's is checked until the value of θ which is the closest to $|Q|$ is found. The match must be within 5%; if no match is found, a comment to that effect is displayed. The new Table 2 index is then used to examine the energy ranges that are available for the selected θ . The Table 2 index is modified to correspond to the available energy range in which the desired energy range begins. If discrete level inelastic data are available, the new Table 2 index is used to obtain the 900-word direct-access record number and appropriate word number from Table 2. The direct-access record is then read into core, using a 900-word array. Starting with the known word number, the energy - probability-for-excitation pairs in the desired energy range are transferred to the array which eventually will be displayed. If the desired information is continued in the next 900-word record, this record is read into core, and the transfer is continued. If the energy boundaries of the desired energy range are not included in the ENDF/B data, the probabilities at these boundaries are found by interpolation, using the ENDF/B interpolation scheme which is included in Table 2. Next, the probabilities are interpolated to the cross-section energy mesh of File 3, using the Table 2 interpolation scheme. The probabilities are then multiplied by the cross section and stored in the array which eventually will be displayed.

*ENDF/B specifications on θ are not clear; here, it is assumed that θ is the absolute value of the level excitation energy.

V. CONCLUSIONS

During this initial phase of the development of the SCORE system, several important results have been obtained. The most important conclusion is that automated neutron cross-section evaluation employing computer graphics techniques is not only feasible, but also economical. Experience has shown that computer graphics does provide a mechanism for improving man-computer communication. The ease and rapid response of this man-computer interaction leads to a more efficient use of technical manpower and computing facilities.

A data storage and retrieval system for experimental neutron cross-section data has been developed. Its primary feature is rapid retrieval of data satisfying a particular request. A rapid data retrieval system is essential to efficient operation of an interactive cross-section evaluation system. In order to overcome the slow response time resulting from a sequential search of many thousands of data points, we perform searches on successively more detailed indices; the result of one successful match in a table points to an entry in the next table. The final results are an address of a record on a disk from which data retrieval begins. Response time for a typical request has been shortened, in some cases, by as much as a factor of 100 over a purely sequential search.

Another indication of the utility of the interactive mode of data evaluation is the speed with which someone who is unfamiliar with the system can learn its operation. The user is presented with a graphical format to enter data. This format allows for a mixture of instruction data which the user supplies. Checks for data errors can be made, and necessary corrections applied, before large amounts of time can elapse or computing time be wasted. The sequence of operations is designed to allow maximum freedom of choice in executing a path through the program. The technique chosen to accomplish this end is the use of light-pen-sensitive switches.

A storage and retrieval system for evaluated neutron data has been included, in order to permit an evaluator to compare his results with those obtained previously by others. The mechanics of the operation of this storage and retrieval system is similar to that used for experimental data.

One of the most frequent jobs performed by an evaluator is choosing a smooth (evaluated) curve to represent a set of experimental data. We have been involved, not with developing new numerical methods for fitting data, but with adopting available methods to the interactive mode. In so doing, we have provided convenient methods for selecting nodal points for the smooth curves and entering that information through the cathode ray tube. Linear, spline, and least squares spline curves can be generated with the logic contained in SCORE.

Finally, we have provided the evaluator with a second analytical tool, namely, a mechanism for generating resonance parameters for resonance region cross sections. The method allows for iterative improvement of parameters for either a single-level or multilevel (Reich-Moore) formalism. By providing rapid response time, interactive graphics can allow an evaluator to analyze a new set of measurements in very short time.

This version of SCORE provides both the experience and the starting point for the further development of a tool which can be usefully employed by evaluators. There are large numbers of bookkeeping operations which could usefully be incorporated, as well as additional modules to perform more of the required analyses. The exact requirement would depend on the nature of the work of interest to various evaluation groups.

APPENDIX I

SUBROUTINE DESCRIPTIONS

MAIN: The MAIN subroutine of SCORE executes parameter initialization and provides the control logic for the various options available. This logic causes requested experimental data to be retrieved from storage and prepared for display. After the data display is created, the execution path is determined by a parameter returned to the main program following selection of an option with the light pen. A series of multiple GO TO statements causes transfer to a control section for the option chosen. Upon completion of any option, the basic data display is restored, so that a succeeding option may be selected.

BLK DATA: This is a nonexecutable subroutine which is used to initialize variables stored in COMMON when the program is first loaded into core.

DACON: All conversion of data from one machine format to another is accomplished with this subroutine, by use of multiple entries. The first entry converts floating point hexadecimal to Hollerith hexadecimal, or vice versa. The second entry (IDACON) converts fixed point to Hollerith, or Hollerith to fixed point. The third entry (ROUND) can be used to round a floating point number to a specified number of significant figures. These operations are accomplished, using READ and WRITE operations (IBM I/O routines) on an internal buffer. This buffer, and the necessary modifications to IBCOM, are generated with the subroutine INFILQ. When data is to be converted from Hollerith to fixed or floating point, the buffer is scanned for illegal characters which would cause an abnormal job termination on a READ statement. If such an illegal character is recognized, the READ operation is bypassed and an error index set.

CMBCD: When executed, this subroutine will transfer a string of characters, starting at a given position in an array, to another array starting a specified position.

CENTER: This routine is used to center the nonblank alphameric characters in an array. This operation is used to center display labels and titling information.

ERRCOR: There are several types of data errors or incompatibilities for which the user should be given a message and then allowed to proceed. This

subroutine will cause the appropriate error message to be displayed, and returns a flag identifying the option selected. The job can be restarted, terminated, or logically continued, which means that the program will execute the display required to permit corrected information to be entered.

CORLIM: The coordinate extrema for a set of experimental data are calculated in this subroutine. A secondary entry point, COR2, will modify the previously calculate extrema for any error bars placed on the data or for extrema for some overlaid smooth curve.

REFFIX: Data references are prepared for display by this subroutine. The ten or less references to be displayed are copied from an array containing all the reference information to a display array.

LCML: This subroutine calculates the transformation, and then converts a data point of an angular distribution from the center of mass to the laboratory system, or vice versa.

NORM: Arrays containing raw data points for curves or nodes to be displayed are converted to the required units and scaled, if logarithmic plotting is requested. Only points that are within the grid limits are transformed and stored in a second array. This second array provides the input data for the plotting arrays.

SCALE: This subroutine performs the scaling when a dimension requires logarithmic plotting.

DISPLA: All the graphical data displays are generated by this subroutine. The graphic commands are generated by three machine-language subroutines called from this subroutine.

UPDTIL: When a new frame, and hence new identifying display number, are generated, this subroutine is used to update the necessary titling information.

FIG1P: Initial case data are entered, using the display created from this subroutine. These data consist of two types. One type is for problem identification, and the other permits the selection of experimental data to be displayed. This subroutine also permits the printing of input data before returning control to the main program.

LABEL: The LABEL subroutine translates input abbreviations, such as 11 to SODIUM, by means of built-in dictionaries. This information is combined, in various ways, to generate titles and other identifying labels required in SCORE.

INPUT: This subroutine contains the retrieval logic for the experimental data. The input data includes nuclide reaction type and energy range. The subroutine returns arrays of data, experimental errors, and references. If no data exist which satisfy the request, then the appropriate error code is returned. A limit of 500 is set on the number of data points which may be retrieved.

POINT: A data point is retrieved in its compacted form, unpacked, and stored by this subroutine. The actual retrieval of the compacted form from the direct-access data set is done by a call to RECORD.

RECORD: This subroutine reads records from the direct-access data set. Since there are 56 data points to a blocked record, this routine must also de-block those records. Thus, it executes one direct-access read to retrieve 56 points.

DIRECT: All control information for a nuclide is retrieved from the direct-access data set and analyzed. If the nuclide is not stored in the direct-access data set, then this routine searches a table to find out where the correct data set is. The data are then retrieved and stored in the direct-access data set. DIRECT also searches the directory tables for the nuclide in the direct-access data set until the record number for the first record which contains an acceptable point is found. If the search fails to find an acceptable data point, the appropriate error flag is set.

SORT: Experimental data are transferred from the array in which they were stored, after being retrieved to the array to be plotted. If requested, a display will appear, allowing the user to select particular references and restrict the energy (or angular) range considered. In this case, data not satisfying these new restrictions are not transferred to the plotting arrays.

LIMITS: This subroutine uses a simple algorithm to obtain the maxima and minima of the grid coordinates, as well as the plotting mode (i.e., log or linear). An additional entry, DISPAR, is used when the user wishes to set his own grid parameters. A display appears which allows the user to select the plotting mode for each axis, such as the units, the maximum, the minimum, and the spacing between grid lines.

GRAPH: Subroutine GRAPH prepares the axis labels, depending on the reaction type and the units requested. Numeric labels for the grid marks are also prepared.

DNORM: This subroutine prepares all the experimental data points for displays. The data are transformed to the proper units, and scaled according to the plotting mode. All data for the overlay curves are prepared by means of calls to the NORM subroutine.

PRNT: Data describing any data display on the cathode ray tube may be listed for future reference. The frame identification number is printed, so that a correspondence between the listing and a particular display can be made. The data points, the references, and the display grid parameters are listed.

DELETE: A data point may be deleted from an array, using the DELETE subroutine and supplying the index of the point to be deleted. A second entry, RESTO, permits the most recently deleted data point to be restored to the data array. This is used when a data point has been erroneously deleted.

SEQOR: An array of integers is reordered by increasing numerical value by this subroutine.

DELP: Data deleted or corrected are listed by this subroutine.

CORRECT: This subroutine executes the data correction option. The coordinates of the selected data points are displayed, 15 pairs of coordinates at a time. A second entry provides a coordinate list option, using the same format as the correction option.

ESHIFT: When analyzing resonance region cross sections, it may be necessary to make flight path corrections to the reported energies. This subroutine permits all the data from a particular reference to correct according to

$$E_c = C_1 \left(\sqrt{\frac{1}{E}} + C_2 \right)^{-2}$$

PRINB: This subroutine prints the values of evaluated nuclear data which are currently being displayed.

CHISQR: A residual (X) is calculated for comparison of an overlay curve with the available experimental data from

$$X^2 = \frac{1}{N} \sum_{i=1}^N \left(\frac{\sigma_{\text{Calculated}} - \sigma_{\text{Experimental}}}{\Delta \sigma_{\text{Experimental}}} \right)_i^2$$

Whenever no experimental uncertainty ($\Delta\sigma$) is reported, then

$$\Delta\sigma \equiv \sigma_{\text{Experimental}}$$

SPLSUP: This subroutine prepares the arrays of experimental data which are to be used in the calculation of X^2 . An array of weights ($1/\Delta\sigma$) is calculated as these quantities are required of the least squares spline curve fitting procedure.

BSETUP: The contents of the right center box of the data display for the RES CALC and DATA FIT options are prepared by this subroutine. If the data points are displayed with characters, then the corresponding references appear in the box. If the data are displayed as points and an overlay curve is plotted, then the residual for that curve is printed in the box. Finally, if a second overlay curve appears in the display, the residual for that curve is also displayed.

INTERP: Subroutine INTERP will perform linear or spline curve interpolation, depending on the type of curve displayed. The entry, LOGOLN, will convert any array of numbers to an array of the logarithms of those numbers, in preparation for interpolation. It will also reconvert the numbers after interpolation.

SPLINE: SPLINE will calculate a set of second derivatives for a set of input nodes, according to the constraining conditions for a cubic spline curve.

DAFIT: The DAFIT subroutine controls the logical flow of the curve-fitting option in SCORE.

RESFIT: This subroutine controls the logical flow of the resonance theory option in SCORE.

CHIP: Information relating to a smooth evaluated curve fit to the current set of experimental data is printed by this subroutine. This information includes parameters for the evaluated curve and residuals for each experimental data point.

ENGSP: This subroutine performs a least squares cubic spline fit to a set of experimental data. The x-coordinates of the nodes are kept fixed, and the

y-coordinates are adjusted to yield a minimum residual. This subroutine was supplied to us by the data evaluation group at Aldermaston.

SONO: Coordinates returned by the light-pen tracking routine are properly normalized and inserted into the nodal coordinate arrays. The entry, DELNO, deletes a selected node from the arrays.

LEGEND: This subroutine computes Legendre coefficients for a set of points representing an angular distribution, by assuming linearity between points.

SERIES: SERIES will evaluate Legendre series, given the set of coefficients and a set of angle cosines.

LISTN: This subroutine allows the evaluator to list and/or modify the nodes for an evaluated curve, using techniques and displays similar to the CORRECT option.

MULP: Information related to a resonance theory calculation is printed by this subroutine. The output consists of a list of the input parameters, a list of resonance parameters, a list of the calculated energy-dependent cross sections, and finally a list of the experimental data points and their residuals.

RESD: Subroutine RESD is a multiple-entry subroutine. REASET reads the resonance parameters from disk storage. STORES stores the current resonance parameters on the disk. EXPCHG permits the modification of the experimental environment parameters (e.g., flight path).

RESMOD: This subroutine controls the modification of resonance parameters by the user during operation of SCORE. An entry point, ADDRES, is provided for use when the user wishes to add new resonances.

RESORT: The resonance parameters must be stored in order of increasing resonance energy. If any resonance energies are modified, then this subroutine is used to reorder the resonance parameter array. The entry, INSERT, is used when a single new resonance is to be added to the parameter array.

COMBCO: This subroutine controls the calculation of the resonance cross section for any one of four reaction types: total, elastic, capture, or fission. The zero degree line shape is both Doppler and resolution broadened numerically, in order to compare with experimental data. This subroutine was

supplied by M. Moore (Idaho Nuclear) and N. Marshall (Phillips Petroleum). However, we have made considerable revisions to meet the requirements of SCORE.

LINESP: The zero degree resonance line shape is calculated by this subroutine. The two-channel multilevel portions of LINESP were supplied by Moore and Marshall. We have added a single-level Breit-Wigner calculation including scattering interference.

LAIN: This is a Lagrange interpolation subroutine used by COMBCO.

INFILQ: INFILQ allocates temporary buffer storage, so that a read or write statement may be executed in core. A call to this routine always precedes a

READ (I, N) list

or a

WRITE (I, N) list

where I is 98 or 99. This is a North American Rockwell routine.

ENDFB: This is the control routine for the acquisition of ENDF/B data.

RITDSK: This routine controls the transfer of a material file on a SCOFF tape to a disk as a direct-access data set. A check is made for proper tape mounting.

TAPERS: This routine brings in the material correspondence and tape requirements tables from Record 40 in the direct-access data set. The logic for card input is also available.

MOUNT: This routine is entered if the wrong SCOFF tape is mounted. It provides mounting instructions to the operator.

TABLE: This routine examines the last record of a material file to obtain the control information. This information is used to bring into core the three tables which catalogue the data and the file contents directory.

TRAN1: This routine transfers a member of the file contents directory from a 900-word floating-point storage area to a fixed-point array. Continuation of the member into the next direct-access record is allowed.

TRAN2: This routine transfers a member of the file contents directory from a 900-word floating-point storage area to a floating-point array. Continuation of the member into the next direct-access record is allowed.

REACT: This routine converts the SCORE reaction number into an ENDF/B file and reaction number, and packs the result into one word.

TAB1: This routine operates upon the file contents directory. It searches Table 1, using the ENDF/B file and reaction numbers (packed into one word) to obtain the Table 1 and Table 2 indices for the desired ENDF/B file and reaction numbers.

FL3: This routine controls the methods used in obtaining ENDF/B File 3 data (smooth cross sections). Table 2 is checked for the appropriate energy range. The required data are brought into core by direct-access reads and interpolated to the end points of the energy range, using the ENDF/B interpolation scheme given in Table 2.

SELECT: This routine controls the transfer of data from a 900-word array, obtained by a direct-access read, to the X, Y arrays that eventually will be displayed. Continuation of the data into the next direct-access record is allowed.

TRPL8: This routine interpolates between (X1, Y1) and (X2, Y2) to obtain Y at X, using the ENDF/B interpolation scheme given in Table 2.

FL4: This routine controls the methods used in obtaining ENDF/B File 4 data (secondary angular distributions). The appropriate File 3 cross section is found by entering subroutine FL3. Table 2 is checked for the desired energy. Either Legendre coefficients or the tabulated angular distribution are brought into core by direct-access reads. The data may be at the desired energy, or at energies bracketing that energy. Interpolation to the desired energy is done, using the ENDF/B interpolation scheme given in Table 2. If Legendre coefficients are involved, they are used to generate a tabulated distribution. The units of the distribution are converted to millibarns per steradian. Conversion to the center of mass system is done if required.

MUTERP: This routine interpolates a (X1, Y1) pair of arrays, defined at NP1 points, to a larger X grid, defined at NP points, using the ENDF/B interpolation scheme given in Table 2. The interpolated result is placed in the Y1 array, which is then defined at NP points.

XERIES: This routine generates angular distributions from Legendre polynomial coefficients. The results are multiplied by the File 3 cross section divided by 2π .

FL5: This routine controls the methods used in obtaining ENDF/B File 5, Subsection 3, data (inelastic level cross sections). The appropriate File 3 cross sections are found by entering subroutine FL3. Table 2 is checked for the desired energy range. The level excitation probabilities for the desired Q value are brought into core by direct-access reads. The probabilities are interpolated to the boundaries of the desired energy range. The probabilities are then interpolated to the File 3 cross-section energy grid. The probabilities are multiplied by the File 3 cross section.

RETREV: This routine either reads a 900-word record from a SCOFF tape and writes it on a direct-access disk (data set Reference Number 16), or effects a direct-access read of 900-word record number ($|NR|$) from the disk.

WTOR: This routine prints a line on the operator's console and returns the operator's one-character reply.

HELP: This routine prints one line of text on the 2250 and returns one of three options detected by the user's light pen.

FIG 1: FIG 1 produces the initial data input (Figure 3) display on the 2250 and returns the parameters typed by the user on an END signal.

FIG 2: This routine displays summary information.

FIG 2A: FIG 2A overlays the basic display created by FIG 2. Text, representing the selected references and energy limits, is returned on an END signal. In addition, the program sets a flag and returns control, if the reference list is detected by the light pen.

FIG 2B: FIG 2B overlays the display produced by FIG 2. This subprogram displays light-pen switches for the axis types and units. In addition to returning the selected setting of all the switches, text representing axis limits, etc. is returned at the END signal.

FIG 3A: This program creates the basic data display. Return is effected when any light-pen switches are detected; sensitive areas are the option list and the reference list.

FIG 3B: This routine creates the data display. The points, hats, and letters shown on the screen are light-pen sensitive per an argument. Any light-pen detect of sensitive areas, or the END or CANCEL signal, results in an immediate return to the caller with appropriate parameter values.

FIG 4: The picture on the 2250 will either be a list of data points for perusal or a list of data points which may be corrected by use of the keyboard and light pen. The first option will return control on the END or CANCEL signal. The CORRECT option returns parameters which indicate whether an END or CANCEL was selected. In addition, a light-pen detect of a displayed number causes the index of that number to be returned immediately.

GIO: Interfaces with the Basic Graphics support of Operating System/360. It opens and closes the 2250, assigns buffer space, and dispatches attentions. It is required for any action at the 2250, and must reside in the root segment. Users of SCORE who run under pre-Release 11 of OS/360 must replace this subprogram with one available from the authors.

GTVDD: When the 2250 is opened for operation under OS/360, the name on the DD card specifying the 2250 must be known. This subroutine gets the ddname from the first DD card which allocates a 2250.

GT2250: Specifies the size of the 2250 buffer to be used by SCORE. The data set, FT05F001, is read under format control (I5). The value obtained (or 8192, if there is no card) is used to indicate the number of bytes wanted in the buffer. If this amount is not available, 4096 is used; and, if allocation is still unsuccessful, execution is terminated.

DISPLAY: A number of entry points, used by FORTRAN programs to control the 2250, compose this subprogram.

REPRNT: Multiple lines may be printed on the 2250 screen, as on a line printer. The direction is reversed, however, with new lines appearing at the top and old ones disappearing from the bottom.

WAITR: This subprogram effects multiple partition operation during execution of SCORE by releasing the scheduler and unit record equipment when using the MFT option of OS/360.

PICT: Records are read from FT10F001 and printed sequentially on the 2250, using REPRNT.

RJCTIM: Releases the CPU and waits for an interval of time specified in tens of milliseconds.

TIMER: Waits for an interval specified in seconds by using RJCTIM.

TRACK: Superimposes on the current 2250 picture a pattern for indicating x, y coordinates with the light pen.

RJCF2I: A subprogram to convert and scale floating-point 2250 dimensions to half-word integer raster units, and vice versa.

A set of Job Control Language cards for the execution of SCORE are given in Table 3. These cards may be used with minor modifications at most installations wishing to use SCORE.

TABLE 3
JOB CONTROL LANGUAGE CARDS

LISTING OF DATASET SCORE.KUNDECK

//JGULLB	DD	DSNAME=SCORE.SUPER,DISP=OLD,UNIT=SYSDA,VOLUME=SER=SCORE	RUN00010
//SCORE	EXEC	PGM=SCORE	RUN00020
//SCOPE	DD	UNIT=2250	RUN00030
//TAPE01	DD	UNIT=2400,VOLUME=(PRIVATE,RETAIN,SER=SAP),DISP=(OLD,PASS),LABEL=(1,NL),DSNAME=SCISRS	XRUN00040
//		UNIT=2400,VOLUME=(PRIVATE,RETAIN,SER=SCOFF),DISP=(OLD,PASS),LABEL=(1,NL),DSNAME=ENDFB	RUN00050
//TAPE02	DD	UNIT=SYSDA,VOLUME=(RETAIN,SER=SCORE),DISP=(OLD,PASS)	XRUN00060
//		VOLUME=REF=*.DISK01,DISP=OLD,	RUN00070
//DISK01	DD	DSNAME=ISTABL4,DCB=(RECFM=V,LRECL=3620,BLKSIZE=3624)	XRUN00080
//FT08F001	DD	VOLUME=REF=*.DISK01,DISP=OLD,DCB=(RECFM=VB,BLKSIZE=3604,LRECL=80)	RUN00090
//FT10F001	DD	DCB=(RECFM=VB,BLKSIZE=3604,LRECL=80)	RUN00100
//		VOLUME=REF=*.DISK01,DISP=OLD,	RUN00110
//FT16F001	DD	DSNAME=ENDFB,DCB=(RECFM=F,BLKSIZE=3600,LRECL=3600)	RUN00120
//		VOLUME=REF=*.DISK01,DISP=OLD,	XRUN00130
//FT17F001	DD	DSNAME=AIDIRECT,DCB=(RECFM=F,BLKSIZE=3584,LRECL=3584)	RUN00140
//		VOLUME=REF=*.DISK01,DISP=OLD,	XRUN00150
//FT19F001	DD	DSNAME=RESDATA,DCB=(RECFM=FB,LRECL=80,BLKSIZE=800)	RUN00160
//		VOLUME=REF=*.DISK01,DISP=OLD,	XRUN00170
//FT20F001	DD	DSNAME=SAP.LABEL,DCB=(RECFM=V,LRECL=68,BLKSIZE=72)	XRUN00180
//		VOLUME=REF=*.TAPE01,LABEL=(2,NL),DISP=OLD,	RUN00190
//FT21F001	DD	DSNAME=NA023,DCB=(RECFM=VB,BLKSIZE=3812,LRECL=68)	XRUN00200
//		VOLUME=REF=*.TAPE01,LABEL=(3,NL),DISP=OLD,	RUN00210
//FT22F001	DD	DSNAME=FL000,DCB=*.FT21F001	XRUN00220
//		VOLUME=REF=*.TAPE01,LABEL=(4,NL),DISP=OLD,	XRUN00230
//FT23F001	DD	DSNAME=FE054,DCB=*.FT21F001	RUN00240
//		VOLUME=REF=*.TAPE01,LABEL=(5,NL),DISP=OLD,	XRUN00250
//FT24F001	DD	DSNAME=L1000,DCB=*.FT21F001	RUN00260
//		VOLUME=REF=*.TAPE01,LABEL=(6,NL),DISP=OLD,	XRUN00270
//FT25F001	DD	DSNAME=L1007,DCB=*.FT21F001	RUN00280
//		VOLUME=REF=*.TAPE01,LABEL=(7,NL),DISP=OLD,	XRUN00290
//FT26F001	DD	DSNAME=PU241,DCB=*.FT21F001	RUN00300
//		VOLUME=REF=*.TAPE02,LABEL=(1,NL),DISP=OLD,	XRUN00310
//FT27F001	DD	DSNAME=SCUFF.LABEL,DCB=(RECFM=V,LRECL=3604,BLKSIZE=3608)	XRUN00320
//		VOLUME=REF=*.TAPE02,LABEL=(2,NL),DISP=OLD,	XRUN00330
//FT28F001	DD	DSNAME=L1007B,DCB=*.FT27F001	XRUN00340
//		VOLUME=REF=*.TAPE02,LABEL=(3,NL),DISP=OLD,	RUN00350
//FT29F001	DD	DSNAME=NA023B,DCB=*.FT27F001	XRUN00360
//		VOLUME=REF=*.TAPE02,LABEL=(4,NL),DISP=OLD,	XRUN00370
//FT30F001	DD	DSNAME=FE000B,DCB=*.FT27F001	XRUN00380
//		VOLUME=REF=*.TAPE02,LABEL=(5,NL),DISP=OLD,	RUN00390
//FT31F001	DD	DSNAME=PU241B,DCB=*.FT27F001	XRUN00400
//		SYSDA	RUN00410
//FT06F001	DD		RUN00420
//FT05F001	DD		RUN00430
//*			RUN00440
			RUN00450

- 1) The VOLUME=SER=SCORE appearing on the JOBLIB and the DISK01 card will have to be changed to reflect the name of the disk volume on which SCORE resides.
- 2) TAPE01 is a dummy card for the SAP tapes (S), and TAPE02 is a dummy card for the SCOFF tapes (S). These tapes are nonlabeled, in order that multiple tapes may be used with one set of DD cards.
- 3) DISK01 is a dummy, referring to the direct-access unit (2311 or 2314). FT17F001 and FT16F001, the direct-access data sets, and FT19F001 must be on this volume. Other data sets are optionally on this unit or another tape unit.
- 4) The data set names (DSNAME) on FT20F001-FT32F001 are meaningless, since the tapes are unlabeled. They only reflect what is currently on our tapes. The tape label file generated by SAP is FT20F001, and that generated by SCOFF is FT27F001. SCORE assures that the right data are in the SAP and SCOFF data files by checking the tape label files, rather than using DSNAME on standard label tapes.
- 5) One input data card is optional. This card is used to specify the desired space in the 2250 buffer. The default condition is 8K (no card). If any other size is desired, then an I5 format is used. For example, if 4K were desired, Columns 1-5 would be 04096.
- 6) The printer, FT06F001, may be dummied out to speed execution time.

APPENDIX III DATA SET DESCRIPTIONS

All the data sets required for execution of SCORE, or containing program source cards, will be described in this appendix. The description will contain the contents of the data set and its organization parameters, using standard IBM-360 notation. The parameters given are:

1) Data Set Organization (DSORG)

Sequential (PS)

Partitioned (PO)

2) Record Format (RECFM)

Fixed (F)

Fixed, Blocked (FB)

Variable (V)

Variable, Blocked (VB)

Unformatted (U)

3) Logical Record Length (LRECL)

4) Blocksize (BLKSIZE)

A. DATA SETS REQUIRED FOR EXECUTION

AIDIRECT DSORG = PS, RECFM = F, BLKSIZE = 3584

This data set is the direct-access data set used to store the experimental data from SCISRS for a given isotope or element which has been selected by the user. The data set requires approximately 500 tracks on a 1316 disk pack, and must be kept on a disk.

ENDFB DSORG = PS, RECFM = F, BLKSIZE = 3600

This is the direct-access data set for the evaluated neutron data. It requires approximately 40 tracks of disk storage, and must be kept on a disk.

ISTABL4 DSORG = PS, RECFM = V, LRECL = 3620, BLKSIZE = 3624

The table of contents of the available experimental data sets is stored in this data set. The set is created and maintained by the SAP program, and is described in more detail in Appendix V. The set requires 2 disk tracks.

SAP.LABEL DSORG = PS, RECFM = V, LRECL = 68, BLKSIZE = 72

This is a tape identifier label, created by SAP. This data set is checked to make sure that the correct tape is mounted, so that the requested isotope file can be transferred to the direct-access data set.

NA023 DSORG = PS, RECFM = VB, LRECL = 68, BLKSIZE = 3812

This data set contains the SCISRS experimental data for sodium-23 in the format required by SCORE. The file is created by SAP, and is generally stored on tape because of the large size of experimental data sets.

FE000, FE054, LI000, LI007, PU241

Same as NA023, but containing experimental data for natural iron, iron-54, natural lithium, lithium-7, and plutonium-241.

SCOFF.LABEL DSORG = PS, RECFM = V, LRECL = 3604, BLKSIZE = 3608

This is a tape identifier label created by SCOFF. Its use is the same as SAP.LABEL for the evaluated data files.

NA023B DSORG = PS, RECFM = V, LRECL = 3604, BLKSIZE = 3608

The evaluated neutron cross sections for sodium from ENDF/B are stored in the data set. The file is created by SCOFF, and may be stored either on tape or disk.

FE000B, LI007B, PU241B

Same as NA023B, but containing the evaluated data (ENDF/B) for iron, lithium-7, and plutonium-241, respectively.

RESDATA DSORG = PS, RECFM = FB, LRECL = 80, BLKSIZE = 800

The resonance parameters for the resonance calculation option are stored in this data set. The data consist of 80-column card images for the Reich-Moore parameters for 21 plutonium-241 resonances. The parameters in order are: energy (ev), reduced neutron width (ev)^{1/2}, capture width (ev), first fission channel width (ev), second fission channel width (ev), and statistical weight factor (G).

SCORE.SUPER DSORG = PO, RECFM = U, BLKSIZE = 3072

This partitioned data set contains four executable load modules. The members are SCORE, SAP, SCOFF, and SUPERZAP.

SCORE 2.LOADMODS DSORG = PO, RECFM = U, BLKSIZE = 3072

Same as SCORE.SUPER.

SCORE.RUNDECK DSORG = PS, RECFM = FB, LRECL = 80, BLKSIZE = 3200

This data set contains the Job Control Language Cards for execution of SCORE. Some modifications may be needed for a given installation.

SCORE.OVERLAY DSORG = PS, RECFM = FB, LRECL = 80, BLKSIZE = 3200

The cards required to generate the overlay structure for SCORE are contained in this data set.

FINAL.PICTURE DSORG = PS, RECFM = VB, LRECL = 80, BLKSIZE = 3604

The data for the termination display is contained in this data set.

B. DATA SETS CONTAINING FORTRAN OR ASSEMBLY LANGUAGE SOURCE CARDS

All the source card data sets are card images with DSORG = PS, RECFM = FB, LRECL = 80, BLKSIZE = 3520. All assembly language source cards are in one data set, as are the SCORE subroutines containing direct-access statements. The remainder are primarily separated according to the overlay segment.

SCORE.SOURCE.S1	This data set contains source cards for all FORTRAN subroutine in the root segment of the overlay structure.
SCORE.SOURCE.S10S11	Fortran source cards for overlay Segments 10 and 11.
SCORE.SOURCE.S2S3	Fortran source cards for overlay Segments 2 and 3.
SCORE.SOURCE.S4	Fortran source cards for overlay Segment 4.
SCORE.SOURCE.S5S6S9	Fortran source cards for overlay Segments 5, 6, and 9.

SCORE.SOURCE.S7S8	Fortran source cards for overlay Segments 7 and 8.
SCORE.SOURCE.DIRECT	Contains all subroutines with direct-access statements. Must be compiled in FORTRAN G if Version 13 (OS/360) or less is used. Compatible with FORTRAN H for Version 14 or greater.
SCORE.SOURCE.ENDFB	Contains all subroutines for the retrieval of ENDF/B data for SCORE.
SCORE.GRAPH.ASEMB	Source for all assembly language routines.
SCORE.GRAPH.FORT	Source for all SCORE graphics routines written in Fortran.
SAP.SOURCE	Card image data set for the source cards for SAP.
SCOFF.SOURCE	Source cards for SCOFF in card image form.

APPENDIX IV SPLINE CURVES

A. DEFINITION

Copying T. N. E. Greville,⁽⁹⁾ consider the problem of interpolating between N given data points (x_i, f_i) ($i = 1, 2, \dots, N$) by means of a function $Y(x)$ which has continuous derivatives of orders $1, 2, \dots, k$ (where $1 \leq k \leq N$) and, moreover, is the "smoothest" such function in the sense that

$$I = \int_a^b \left[Y^{(k)}(x) \right]^2 dx$$

is made as small as possible, where

$$a \leq x_1 \leq x_2 \quad \dots \quad x_N \leq b \quad . \quad \dots (1)$$

For $k = N$, the Lagrangian interpolation polynomial (which is of degree $k-1$) is the unique solution. For $k < N$, there is again a unique solution, which is a piecewise function given in any interval $[x_i, x_{i+1}]$ by a polynomial of degree at most $2k-1$, in general, by a different polynomial in each such interval. Moreover, the polynomial arcs that make up the graph of the function Y "join smoothly," in the sense that the two polynomials that represent Y to the left and to the right of each x_i have the same ordinate and the same values of the derivatives of order $1, 2, \dots, 2k-2$ for $x = x_i$. The function Y has the further property that, in each of the intervals $(-\infty, x_1)$ and (x_N, ∞) , it reduces to a polynomial of degree $k-1$ (rather than $2k-1$).

The function Y just described belongs to a class of functions known as spline functions.

B. CUBIC SPLINE

Copying B. Wendroff,⁽¹⁰⁾ to construct an interpolating spline to $f(x)$, we note that, if $Y(x)$ is a spline, then Y has a second derivative at each interpolation point x_i ; so let

$$Y''(x_i) = S_i \quad , \quad i = 1, 2, \dots, N$$

Now, since $Y(x)$ is cubic on $[x_i, x_{i+1}]$, on that interval Y'' is linear, or

$$Y''(x) = S_i \left(\frac{x_{i+1} - x}{x_{i+1} - x_i} \right) + S_{i+1} \left(\frac{x - x_i}{x_{i+1} - x_i} \right), \quad x_i \leq x \leq x_{i+1} \quad \dots(2)$$

If we integrate Y'' twice and determine the two constants of integration, so that

$$Y(x_i) = f(x_i) = f_i, \quad i = 1, \dots, N, \quad \dots(3)$$

we find that

$$Y(x) = \frac{S_i(x_{i+1} - x)^3}{6h_i} + \frac{S_{i+1}(x - x_i)^3}{6h_i} + \left(\frac{f_{i+1}}{h_i} - \frac{S_{i+1}h_i}{6} \right) (x - x_i) + \left(\frac{f_i}{h_i} - \frac{S_i h_i}{6} \right) (x_{i+1} - x), \quad \dots(4)$$

where:

$$h_i = x_{i+1} - x_i, \quad \dots(5)$$

and

$$x_i \leq x \leq x_{i+1}.$$

Of course, the second derivatives (S_i) are unknown; however, in order for $Y(x)$ to be a spline, $Y'(x)$ must be continuous. Since

$$Y'(x_i) = -\frac{S_i}{2} h_i + \frac{f_{i+1}}{h_i} - \frac{S_{i+1}}{6} h_i + \frac{S_i h_i}{6} - \frac{f_i}{h_i} \quad \dots(6)$$

and

$$Y'(x_i) = \frac{S_i}{2} h_{i-1} + \frac{f_i}{h_{i-1}} - \frac{S_i h_{i-1}}{6} + \frac{S_{i-1} h_{i-1}}{6} - \frac{f_{i-1}}{h_{i-1}}, \quad \dots(7)$$

equating these expressions for $Y'(x_i)$, we have

$$h_{i-1} S_{i-1} + 2(h_{i-1} + h_i) S_i + h_i S_{i+1} = 6 \left(\frac{f_{i+1} - f_i}{h_i} - \frac{f_i - f_{i-1}}{h_{i-1}} \right), \quad \dots(8)$$

for $i = 2, \dots, N - 1$. This is a linear system with $N - 2$ equations in N unknowns, S_1, \dots, S_N ; therefore, two additional conditions are needed. We will take these to be

$$S_1 = S_N = 0 \quad \dots(9)$$

[Other choices are presented in Ahlberg, Nilson, and Walsh⁽¹⁰⁾].

Equation 8 is then just a special case of the general tridiagonal matrix equation:

$$A_k \mu_{k-1} + B_k \mu_k + C_k \mu_{k+1} = D_k \quad ; \quad k = 2, \dots, N - 1 \quad ; \quad \mu_1 = \alpha \quad ; \quad \mu_N = \beta \quad \dots(10)$$

The simple algorithm for solving this system is, let

$$\mu_{k-1} = p_k \mu_k + q_k \quad \dots(11)$$

Substituting into Equation 11, we have

$$A_k(p_k \mu_k + q_k) + B_k \mu_k + C_k \mu_{k+1} = D_k \quad \dots(12)$$

or

$$\mu_k = -\frac{C_k}{A_k p_k + B_k} \mu_{k+1} + \frac{D_k - A_k q_k}{A_k p_k + B_k} \quad \dots(13)$$

This has the same form as Equation 11; therefore,

$$p_{k+1} = -\frac{C_k}{A_k p_k + B_k} \quad \text{and} \quad q_{k+1} = \frac{D_k - A_k q_k}{A_k p_k + B_k} \quad \dots(14)$$

Now take $p_2 = 0$, $q_2 = \alpha$, so that $\mu_1 = \alpha$, then Equation 14 recursively defines all p_k and q_k , provided none of the denominators vanish. Starting Equation 11 with $k = N$ and $\mu_N = \beta$, we can then compute $\mu_{N-1}, \mu_{N-2}, \dots, \mu_2$. It can be shown, in our case, that none of the denominators vanish.

Thus, we have a cubic spline determined from (x_i, f_i) by the preceding method.

C. USE OF SPLINE IN SCORE

Using the tracking pattern in SCORE to enter the spline nodes (x_i, Y_i) , $i = 1, \dots, N$ in the space (log-log, lin-log, lin-lin, log-lin) displayed on the screen, SPLINE is then called to produce the spline curve in this space. This curve is then displayed on the screen, and can then be refined as desired to approximate the experimental data also displayed on the screen by simply adjusting the spline nodes (moving, adding, or removing).

D. LEAST SQUARES CUBIC SPLINE SUBROUTINE

This subroutine uses a sophisticated technique for spline curve fitting experimental data.⁽⁷⁾ Given M experimental points, (XD_i, YD_i, WD_i) , $i = 1, \dots, M$, where

$$WD_i = \frac{1}{|Y - YD_i|} ,$$

and N values, XN_j , $j = 1, \dots, N$, the subroutine calculates the spline curve which minimized the least squares residual

$$R = \sum_{i=1}^M WD_i (Y - YD_i)^2 ,$$

and returns the values YN_j at XN_j , and GN_j which are the first derivatives at XN_j . These can be used to compute Y at any desired points.

E. USE OF LEAST SQUARES SPLINE SUBROUTINE IN SCORE

Using the tracking pattern in SCORE to enter the x values (nodes), x_j , $j = 1, \dots, N$, in the space as previously, ENGSPL is then called to produce the least squares spline to the given experimental data in this space. The curve may then be refined by adjusting the nodes, and by deleting or correcting experimental points. Use of this method for data evaluation has been described by Horsley et al.⁽⁵⁾

F. INTEGRATING AND DIFFERENTIATING SPLINES

Some very simple formulas can be derived:

$$x_i \leq x \leq x_{i+1} , \quad h_i = x_{i+1} - x_i \quad ;$$

$$Y'(x) = -\frac{1}{2} \frac{S_i}{h_i} (x_{i+1} - x)^2 + \frac{1}{2} \frac{S_{i+1}}{h_i} (x - x_i)^2 + \left(\frac{f_{i+1}}{h_i} - \frac{S_i h_i}{6} \right) - \left(\frac{f_i}{h_i} - \frac{S_i h_i}{6} \right) ;$$

$$Y''(x) = \frac{S_i}{h_i} (x_{i+1} - x) + \frac{S_{i+1}}{h_i} (x - x_i) ;$$

$$Y'''(x) = \frac{S_{i+1} - S_i}{h_i} ;$$

$$\int_{x_i}^{x_{i+1}} Y(x) dx = \left(\frac{f_i + f_{i+1}}{2} \right) h_i - \left(\frac{S_i + S_{i+1}}{24} \right) h_i^3$$

APPENDIX V

SCISRS ADAPTION PROGRAM (SAP)

A. INTRODUCTION

The SAP library tape containing SCISRS data that is used by SCORE is basically a record-by-record transformation by program SAP from an EBCD SCISRS data tape to a hexadecimal tape. For each isotope, the 16-word records are blocked with 56 records per block, and are written on the SAP tape as one file. As the data are processed, two tables are created which describe the reaction types and energy ranges in the file. This information is to be used to allow direct-access reads of specific energy ranges for a reaction type when the isotope file resides on a disk. These two tables are included in the final records written on the tape; the last four words in the final record consist of control information which may be used later to obtain the two tables from the direct-access data set.

During the isotope processing, a tape identifier and isotope table data set is generated and/or updated; when new isotopes are added to the tape, the required additions are made at the end of the table. This table may be punched, printed, or written as data set Reference Number 11. SAP may be run without processing any isotopes, in order to effect the output of these tables as well as the output of the reaction types and energy ranges tables.

In order to use SAP on a standard SCISRS data tape, the tape must first be converted from BCD to EBCD (see Section F of this appendix).

Program SAP is designed to perform the following options:

- 1) Convert SCISRS EBCD data to SCORE input format (an isotope file on a SAP tape)
- 2) Create the identifier file on a new SAP tape
- 3) Create the direct-access data set used by SCORE
- 4) Construct, update, list, and punch the table of tape identifiers and isotopes
- 5) Print the reaction and energy tables for any data file on a SAP tape

- 6) Print the identifier file of a SAP tape
- 7) Create the final picture data set for SCORE.

B. TAPE IDENTIFIER AND ISOTOPE TABLE

The tape identifier and isotope table is contained in data set Reference Number 11. The first word of the data set contains the number of isotope entries in the table. The second word contains the number of SAP tape identifiers in the table. The next five words are repeated for each isotope; they are:

- 1) The atomic number times 1000, plus the mass number (the mass number may be zero, if the material is a naturally occurring mixture of isotopes)
- 2) The SAP tape and file numbers packed into one word (explained below)
- 3) The first word of the literal date
- 4) The second word of the literal date
- 5) A dummy word.

The next two words are repeated for each SAP tape identifier; they are:

- 1) The first word of the SAP literal tape identifier
- 2) The second word of the SAP literal tape identifier.

The SAP tape (NT) and file (NF) numbers for the latest entry for an isotope, along with the SAP tape (NT_p) and file (NF_p) numbers for the previous, out-of-date entry for an isotope, are contained in one word (NTT):

$$NTT = (NT * 100 + NF) * 10000 + NT_p * 100 + NF_p$$

By storing the previous tape and file number, a traceback record of updates and a record of what is stored on every tape are available. Since new additions to the table are made at its end, the table must be searched backward to obtain the latest entry for an isotope. The tape number (NT) is the index (I) of the SAP literal tape identifier contained in a doubly dimensioned array, TAPE (J, I) where J = 1, 2. The file number (NF) is the sequential file number minus one for the isotope file on the tape.

C. SAP TAPE LAYOUT

When the SAP program creates a new SAP hexadecimal tape, the first file of that tape has a single 16-word record containing the tape identifier. The first two words are the tape identifier, and the last 14 words may be any arbitrary information. This identifier is checked by subsequent SAP runs or by SCORE to determine whether the desired tape is mounted.

All subsequent files on the tape consist of records containing 16 words; there are 56 records to the block.

The first record is a 16-word literal title, which may be any arbitrary information. The second record contains five words of information:

- 1) ZNUM, the isotope atomic number. The input format is A2.
- 2) ANUM, the isotope mass number. The input format is A3.
- 3) AMASS, the isotope atomic weight. The input format is E.
- 4) DATE (1), the first word of the date of entry. The input format is A4.
- 5) DATE (2), the second word of the date of entry. The input format is A4. Eleven dummy words fill out the record.

The succeeding records are a record-by-record transformation of the corresponding information from the EBCD SCISRS tape. Each record contains the 16 words enumerated in Table 3. Each entry in Table 4 is detailed in the SCISRS document.⁽⁴⁾

The next group of records contains a table of the reaction types (σ -type in the SCISRS document) for which data are available. Each entry in this table has an associated index number. This index gives the location of the initial point in the energy table which is associated with this reaction type. The table is stored as pairs of reaction type and index, eight pairs per record, for as many records as are needed.

The next group of records contains the table of energy points and their associated record numbers. The energy for the initial data point, and every 250th point thereafter of each reaction type, and the record number in the direct-access data set for that point are stored in the table. This table is stored as pairs of energy and record number, eight pairs per record, for as many records as are needed.

TABLE 4
 FORMAT OF SAP EXPERIMENTAL DATA RECORD

Entry	Symbol	Input Format
1) Energy	EN	(E)
2) Energy Error/Resolution	*	(E)
3) Secondary Energy or Other Numerical Quantity	EN2	(E)
4) Cos θ	U	(E)
5) Cos θ Error or Resolution	*	(E)
6) Value of Cross Section	SIG1	(E)
7) Error in Value	ERS	(E)
8) Identification of Secondary Energy or Other Numerical Quantity	STYPE2	(A1)
Error Type	ETYPE	(A1)
Lab System Indicator	CML	(A1)
Information Source	SOURCE	(A1)
9-12) Reference	REFER (4)	(4A4)
13) Energy Error Units	*	(A1)
Energy Error Type	*	(A1)
Cos θ Error Resolution Units	*	(A1)
Cos θ Error or Resolution Indicator	*	(A1)
14) Status	*	(1X, A1, A2)
Method	*	
15) Standard	*	(A1, A3)
Institution	*	
16) Date of Entry	*	(A3, A1)
Comment Entries	*	

*This item is stored by SAP but is not used in SCORE

The last record of the file has four words of information and 12 dummy words to fill out the record. This record contains four constants which control the reading of the direct-access data set (Table 5).

TABLE 5
DIRECT-ACCESS CONTROL INFORMATION

Item	Symbol	Input Format
1) The starting record number of the table of reaction types	ISAVE	(I)
2) The number of pairs in the table of reaction types	KU	(I)
3) The number of pairs in the table of energy points	KE	(I)
4) The total number of records in the file	NRS	(I)

The file is organized in this manner, so that SAP can do a one-pass record-by-record transformation from the EBCD SCISRS tape to the SCORE tape. At the same time, SAP builds the tables and control information which are placed after the last record of SCISRS information, followed by an end-of-file mark.

D. RESTRICTIONS

In converting the SCISRS data, SAP deletes comment cards, data whose reaction type is SEL where the secondary energy identification is L, and data whose secondary energy is nonblank where the secondary energy identification is blank. SAP converts "last figures" error to percent error.

1. Dimensioning Considerations

<u>Item</u>	<u>Maximum Value</u>
Number of pairs in the table of reaction types	175
Number of pairs in the table of energy points	500*
Number of entries in the isotope table	400
Number of entries in the tape identifier table	20

*This is sufficient to allow for the approximately 28,000 data points which SCORE can store in the direct-access data set.

2. Input-Output Assignments

<u>Symbol</u>	<u>Data Set Reference Number</u>	<u>Explanation</u>
IN	5	Input stream
IO	6	Printout
N7	7	Punchout
NTAPE	8	SCISRS EBCD tape
NEW	9	SCORE output tape
NOLD	10	SCORE tape for printing of reaction and energy tables
NTAB	11	Tape identifier and isotope table data set
NPCT	12	Final picture data set
N17	17	Direct-access data set

E. INPUT PREPARATION

1. Control Card (2A4, 1X, I3, 5I12)

<u>Symbol</u>	<u>Explanation</u>
DATE	The date, 2 EBCD words (e.g., 12/31/67)
NF	The number of files to be processed on the SCISRS EBCD tape 0 If a SCISRS tape is not to be processed
IFILE 1	0 Do not create the identifier file 1 Create the identifier file on a new SCORE tape
IDACS	0 Do not create the direct-access data set 1 Create the direct-access data set
IUPD	-1 Construct the table of tape identifiers and the isotope table, based on the processing of the SCISRS EBCD tape (NF not equal to 0); or, if NF equals 0, do not print and punch these tables 0 Use the table of tape identifiers and the isotope table from the disk

Symbol

Explanation

1 Read the table of tape identifiers and the isotope table as input

For IUPD = 0 or 1:

If NF does not equal 0, these tables will be updated, written into the data set, printed, and punched.

If NF equals 0, these tables will be written into the data set, printed, and punched.

NPRINT The number of files to be processed on the SCORE tape for printing of tables or tape identifier

0 If a SCORE tape is not to be processed for printing

IPICT 0 Do not create the final picture data set

1 Create the final picture data set

2. Identifier File Card (16A4)

Omit if IFILE1=0.

TAPEX The tape identifier, 2 EBCD words (e.g., SCORE001)

HEAD 14 EBCD words of arbitrary information

3. Final Picture Data (19A4)

Omit if IPICT=0.

The final picture data deck is 170 EBCD cards which are distributed with SAP.

4. Tape Identifier and Isotope Tables

Omit if IUPD≠1.

a. Control Card (2I12)

NIS Number of entries in the isotope table to be read in (0<NIS≤400)

NTS Number of tape identifiers in table to be read in (0<NTS≤20)

b. Tape Identifier Table (2A4, 4X, 2A4, 4X, etc.)

TAPE(J, I) NTS tape identifiers (2 EBCD words each) are read in, six per card (J=1, 2 and I=1, NTS), where I is the tape number NT

c. Isotope Table (2I12, 2A4, 4X, I12)

ISOTOP(I) Isotope number $Z*1000+A$

ISNUM(I) Tape and file number of the current data set, and tape and file number of the data set which this supercedes (see Section B of this appendix)

$$=(NT*100+NF)*10000+NT_p * 100+NF_p$$

DATEIS(J, I) Date, 2 EBCD words, (J=1, 2)

NRECS(I) The total number of records in this file

NIS cards are read in (I=1, NIS)

5. Selected Isotopes (for conversion from SCISRS to SCORE format)

Omit if NF=0.

a. Title Card (16A4)

TITLE 16 EBCD words of arbitrary information

b. Isotope Card (A2, A3, 7X, E12.8, 2I12)

ZNUM Two-character EBCD Z number (e.g., 03 or 26)

ANUM Three-character EBCD A number (e.g., 007 or 000)

AMASS Atomic weight (based on $C^{12} = 12.0$)

NT Tape number (NT) (see Section III-D)

NF File number (NF) excluding the identifier file (see Section C of this appendix)

Repeat Cards a and b for each selected isotope. The selected isotope cards must be arranged in the order the isotopes appear in the SCISRS EBCD file, or the order of the DD cards, if in separate files. ZNUM and ANUM must agree identically with the corresponding values on the SCISRS EBCD tape.

F. OPERATING INSTRUCTIONS

1. SCISRS BCD to SCISRS EBCD

The following job control language (JCL) cards are designed to convert a standard BCD SCISRS data tape (isotope, reaction, energy, etc., sorted) to a blocked EBCDSCISRS tape, using the OS/360 utility program IEBGENER.

TAPE-TAPE PROCEDURE

```
//GO EXEC PGM=IEBGENER
//SYSPRINT DD SYSOUT=A
//SYSUT1 DD UNIT=2400-2, DISP=OLD, LABEL=(K1†, NL), X
// DSNAME=BCDDATA, VOLUME=SER=YYYYYY, X
// DCB=(DEN=1, TRTCH=ET, RECFM=F, BLKSIZE=84, LRECL=84)
//SYSUT2 DD UNIT=2400, DISP=(NEW, KEEP), LABEL=(K2§, NL), X
// DSNAME=EBCDDATA, VOLUME=SER=ZZZZZZ, X
// DCB=(RECFM=FB, LRECL=80, BLKSIZE=4480)
//SYSIN DD *
GENERATE MAXFLDS=1
RECORD FIELD=(80, 1, HE, 1)
/*
```

† K1 is the desired file on the SCISRS BCD.

§ K2 is the next available file on the SCISRS EBCD tape.

2. SAP Procedure

The following job control language (JCL) cards are designed to execute SAP from a job library. The load module for SAP, the direct-access data set, the tape and file tables, and the data for PICT are all on the same disk pack. The SCORE tapes must be nonlabeled.

SAP PROCEDURE

```
//JOB LIB DD UNIT=2311, VOLUME=SER=SCPACK, DSNAME=SCLMOD, DISP=OLD
//GO EXEC PGM=SAP
//FT05F001 DD DDNAME=SYSIN
//FT06F001 DD SYSOUT=A, DCB=(, RECFM=UA)
//FT07F001 DD UNIT=(SYSCP, , DEFER), DISP=(MOD, PASS), DCB=(STACK=2)
//FT08F001 DD UNIT=2400, DISP=OLD, LABEL=(M1†, NL), X
//          DSNAME=EBCDDATA, VOLUME=SER=ZZZZZZ, X
//          DCB=(RECFM=FB, LRECL=80, BLKSIZE=4480)
//FT08F002 DD DISP=OLD, LABEL=(M2†, NL), X
//          DSNAME=MOREDATA, VOLUME=REF=*. FT08F001 X
//          DCB=(RECFM=FB, LRECL=80, BLKSIZE=4480)
    Etc.
//FT09F001 DD UNIT=2400, DISP=(NEW, KEEP), LABEL=(N1§, NL), X
//          DSNAME=FILE1, VOLUME=SER=WWWWW, X
//          DCB=(RECFM=V, LRECL=68, BLKSIZE=72)
//FT09F002 DD DISP=(NEW, KEEP), LABEL=(N2§, NL), X
//          DSNAME=FILE2, VOLUME=REF=*. FT09F001, X
//          DCB=(RECFM=VB, LRECL=68, BLKSIZE=3812)
    Etc.
//FT10F001 DD UNIT=2400, DISP=OLD, LABEL=(L1††, NL), X
//          DSNAME=FILE1, VOLUME=SER=XXXXXX, X
//          DCB=(RECFM=V, LRECL=68, BLKSIZE=72)
//FT10F002 DD DISP=OLD, LABEL=(L2††, NL), X
//          DSNAME=FILE2, VOLUME=REF=*. FT10F001, X
//          DCB=(RECFM=VB, LRECL=68, BLKSIZE=3812)
    Etc.
//FT11F001 DD UNIT=2311, VOLUME=SER=SCPACK, DISP=OLD, X
//          DSNAME=TFTABLE, DCB=(RECFM=V, LRECL=3620, BLKSIZE=3624), X
//          SPACE=(TRK, (2, 1))
//FT12F001 DD UNIT=2311, VOLUME=SER=SCPACK, DISP=(NEW, KEEP), X
//          DSNAME=PICTDATA, DCB=(RECFM=V, LRECL=3620, BLKSIZE=3624), X
//          SPACE=(TRK, (5, 1))
//FT17F001 DD UNIT=2311, VOLUME=SER=SCPACK, DISP=(NEW, KEEP), X
//          DSNAME=SCDIRECT, SPACE=(3584, (500, 1)), X
//          DCB=(RECFM=F, BLKSIZE=3584)
//SYSIN DD *
```

[DATA]

/*

†M1,M2 are the desired files on the SCISRS EBCD tape.

§N1,N2 are the output files on the SCORE tape.

††L1,L2 are the desired files for printing.

G. SAMPLE INPUT SHEETS

FORTRAN FIXED 10 DIGIT DECIMAL DATA

DECK NO. _____ PROGRAMMER _____ DATE _____ PAGE 1 of 4 JOB NO. _____

	NUMBER	IDENTIFICATION	DESCRIPTION	DO NOT KEY PUNCH
1	2 / 3 1 / 6 7	2	DATE, NF	
13		1	IFILE1	
25		1	IDACS	
37		1	IUPD	
49		3 73 .80	NPRINT	
61		1 1 0	IPICT	(2A4, 1X, I3, 5I12)
1	S C O R E 0 0 2 S E C		TAPEX, HEAD	
13	O N D S C O R E T A			
25	P E 1 2 / 3 1 / 6 7			Omit if IFILE1=0.
37	B E R L A N D , D U N F			
49	O R D , C R E A S Y	73 .80		
61		2 0		(16A4)
1			Final Picture Data	
13			(170 cards)	
25				
37				Omit if IPICT=0.
49		73 .80		
61		3 0		(19A4)
1		3	NIS	
13		1	NTS	
25				Omit if IUPD#1.
37				
49		73 .80		
61		4 0		(21I2)

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FORTRAN FIXED 10 DIGIT DECIMAL DATA

DECK NO. _____ PROGRAMMER _____ DATE _____ PAGE 2 of 4 JOB NO. _____

	NUMBER	IDENTIFICATION	DESCRIPTION	DO NOT KEY PUNCH
1	S C O R E 0 0 1		TAPE	
13				
25				Omit if IUPD#1.
37				
49		73 .80		
61		5 0		(2A4, 4X, 2A4, 4X, etc.)
1	1 1 0 2 3		ISOTOP	
13	1 0 1 0 0 0 0		ISNUM	
25	1 1 / 1 9 / 6 7		DATEIS	Omit if IUPD#1.
37	2 2 3 0		NRECS	
49		73 .80		
61		6 0		(21I2, 2A4, 4X, I12)
1	2 6 0 0 0		ISOTOP	
13	1 0 2 0 0 0 0		ISNUM	
25	1 1 / 1 9 / 6 7		DATEIS	
37	7 4 8 5		NRECS	
49		73 .80		
61		7 0		
1	2 6 0 5 4		ISOTOP	
13	1 0 3 0 0 0 0		ISNUM	
25	1 1 / 2 0 / 6 7		DATEIS	
37	2 3 8		NRECS	
49		73 .80		
61		8 0		

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FORTRAN FIXED 10 DIGIT DECIMAL DATA

DECK NO. _____ PROGRAMMER _____ DATE _____ PAGE 3 of 4 JOB NO. _____

	NUMBER	IDENTIFICATION	DESCRIPTION DO NOT KEY PUNCH
1	PLUTONIUM 2	73 80	TITLE
13	4 1 FROM BNL		
25	1 2 / 1.5 / 6.7		Omit if NF=0
37			
49			
61			9 0 (16A4)
1	9 4 2 4 1	73 80	ZNUM, ANUM
13	2 4 1 . 0 5 6 6		AMASS
25	2		NT
37	1		NF
49			
61			1 0 0 (A2, A3, 7X, E12.8, 2I12)
1	NATURAL LIT	73 80	TITLE
13	H I U M F R O M B N		
25	L 1 2 / 2.0 / 6.7		
37			
49			
61			1 1 0
1	0 3 0 0 0	73 80	ZNUM, ANUM
13	6 . 9 3 6 1 2		AMASS
25	1		NT
37	4		NF
49			
61			1 2 0

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FORTRAN FIXED 10 DIGIT DECIMAL DATA

DECK NO. _____ PROGRAMMER _____ DATE _____ PAGE 4 of 4 JOB NO. _____

	NUMBER	IDENTIFICATION	DESCRIPTION DO NOT KEY PUNCH
1	LITHIUM 7, F	73 80	TITLE
13	R O M . B . N . L . 1 2 / 2		
25	0 / 6.7		
37			
49			
61			1 3 0
1	0 3 0 0 7	73 80	ZNUM, ANUM
13	7 . 0 1 6		AMASS
25	1		NT
37	5		NF
49			
61			1 4 0
1		73 80	
13			
25			
37			
49			
61			
1		73 80	
13			
25			
37			
49			
61			

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APPENDIX VI SCOFF PROGRAM

A. INTRODUCTION

The SCOFF program converts ENDF/B EBCDIC data for a material into continuous 900-word hexadecimal records, and writes these records onto a tape as one file. As the data are processed, a file contents directory, consisting of three tables, is created. This information is to be used to allow direct-access reads of specific records, when the material file resides on a disk. The file contents directory is included in the final records written on the tape; the last five words in the final record consist of control information which may be used later to obtain the file contents directory from the direct-access data set.

As many materials as desired may be processed by program SCOFF; however, for a given run, the order of the materials requested must be the same as on the ENDF/B Mode 3 tape. Subsequent runs may be made in which the requested materials will be added to the tape at the end of the last file.

Not all of the ENDF/B data for a material may be processed by program SCOFF. Data which are not processed are:

- 1) File 1: Although the literal data are processed, the dictionary is ignored. Radioactive decay data and fission product yield data are skipped.
- 2) File 2: Resolved resonance parameters for resonance formula other than single-level Breit-Wigner, with or without multilevel scattering (LRF = 1 or 2), cannot be processed. Unresolved resonance parameters for resonance formula other than LRF = 1 cannot be processed. Attempts to process such data will cause the program to fail.
- 3) File 3: Temperature-dependent records are skipped.
- 4) File 4: The transformation matrix, if present, is skipped. Temperature-dependent records are not allowed; their presence will cause the program to fail.

- 5) File 5: All records other than the tabulated probability for each partial distribution are skipped. Temperature-dependent records are not allowed; their presence will cause the program to fail.
- 6) File 6: Not processed.
- 7) File 7: Not processed.

When a new SCOFF tape is created, the first file written is a tape identifier file. During the material processing, a material correspondence table and a tape requirement table are generated and/or updated; when new materials are added to the tape, the required additions are made at the end of the tables. These tables may be punched, printed, or written as Record 40 on the direct-access data set used by SCORE. SCOFF may be run without processing any materials, in order to effect the output of these tables.

B. MATERIAL CORRESPONDENCE AND TAPE REQUIREMENTS TABLES

The material correspondence and tape requirements tables are contained in one 900-floating-point-word record (Record Number 40). The first word of the record contains the number of materials that exist on SCOFF tapes; the second word contains the number of SCOFF tapes. The next six words are repeated for each material; they are:

- 1) The atomic number times 1000 plus the mass number (the mass number may be zero, if the material is naturally occurring)
- 2) The ENDF/B material identification (MAT)
- 3) The total number of 900-word records in the SCOFF file for this material
- 4) The SCOFF tape and file numbers packed into one word (explained below)
- 5) The first word of the literal date
- 6) The second word of the literal date.

The next two words are repeated for each SCOFF tape; they are:

- 1) The first word of the SCOFF tape literal identification
- 2) The second word of the SCOFF tape literal identification.

The SCOFF tape (NT) and file (NF) numbers for the latest entry for a material, along with the SCOFF tape (NT_p) and file (NF_p) numbers for the previous, out-of-date entry for a material, are contained in one word (NTT):

$$NTT = (NT * 100 + NF) * 10,000 + NT_p * 100 + NF_p$$

By storing the previous tape and file number, a traceback record of updates, and a record of what is stored on every tape, are available. Since new additions to the tables are made at their end, the table must be searched backward to obtain the latest entry for a material. The tape number (NT) is the index (I) of the SCOFF tape literal identification when transferred to a doubly dimensional array, TAPID (I,J), where J = 1, 2. The file number (NF) is the sequential file number minus one for the material file on the tape.

C. SCOFF TAPE LAYOUT

When the SCOFF program creates a new SCOFF hexadecimal tape, the first file that is written contains the tape identifier. This file contains a 16-word record. The first two words are the tape identifier, and the last 14 words are zeros. This identifier is checked by subsequent SCOFF runs or by SCORE, to determine whether the desired tape is mounted.

All subsequent files on a SCOFF tape consist of records containing 900 hexadecimal words; there is one record per block.

In the first record, the first 16 words contain a title, which may be any arbitrary information read from input cards by program SCOFF. The next five words contain the atomic number, the mass number, the atomic mass, and the first and second words of the date of the run; this information is also read from cards. Words 22 through 36 are 0.0.

Information from Files 1 through 5 of the ENDF/B Mode 3 tape is then processed and written on the SCOFF tape in a continuous fashion. Within each record, there is no indication of where data of one type ends and data of another type begins. When one record is filled up and written on the tape, the data are continued in the next record.

The arrangement of data for each ENDF/B file is given in the following paragraphs. The abbreviation FCD for file contents directory will be used.

The term NDIF is the number of pairs of X, Y values in a tabulation defined for a specific X interval; its value may be determined by subtracting the beginning word number for the desired tabulation (or X interval) found in Table 2 of the FCD from that for the next tabulation (or X interval) and dividing by 2.

1. File 1

Parameters, indicating whether the material is fissile and whether it contains resonance parameters, are given in Table 1 of the FCD. A parameter, indicating literal data or a tabulation of the average number of neutrons per fission, is given in Table 2 of the FCD.

File 1 \ data start in the 37th word of the first record; literal data will always be first. Each word of the literal information, 18 words per card, is stored in the first record, and may be continued into the second and third records. The number of cards may be found in Table 2 of the FCD.

Next, the average number of neutrons per fission (ν), if present, is placed on the tape. If the data are given in terms of polynomial coefficients, a tabulation is generated; the energy grid (E) starts at 0.001 ev and increases, by a factor of 10, until 1.0×10^5 ev is reached; then, the energy values increase, by addition of 1.0×10^5 ev to the previous energy value, until 1.5×10^7 evis reached. The interpolation code for the generated tabulation is log-log; one energy range is specified. If the data are given as a tabulation, it is used directly; the number of interpolation regions determines the number of energy ranges. The data for each energy range is written in the record as

$$(E(I), \nu(I), I = 1, NDIF) \ .$$

The lower energy of the energy range and the ENDF/B interpolation code are stored in Table 2 of the FCD.

2. File 2*

The number of isotopes for which resonance parameters are given for this material is given in Table 1 of the FCD. The isotope (Z, A) identification, a resolved or an unresolved resonance parameter flag, the ENDF/B resonance formula index, and a fission widths flag are given in Table 2 of the FCD. The isotope

*Data processed here must be in the original ENDF/B format; pending changes in the formats are not included here.

abundance, the lower and upper boundaries of the energy range, and the number of l states are given in Table 3 of the FCD.

For resolved resonance parameters, the data are placed in the record in the following order (Formula No. 1 or 2):

SPI, AP, LIS, $(C(l), AM(l), L(l), NRS(l), (ER(i, l), AJ(i, l),$
 $GT(i, l), GN(i, l), GG(i, l), GF(i, l), i = 1, NRS(l)), l = 1, NLST)$

where

SPI = nuclide spin

AP = A_+ spin-dependent scattering length, in units of 10^{-12} cm

LIS $\left\{ \begin{array}{l} = 0 \text{ add smooth File 3 cross section to calculation} \\ = 1 \text{ use smooth File 3 cross section only} \end{array} \right.$

$C(l)$ = constant used in the calculation of the penetration factor

$AM(l)$ = A_- spin-dependent scattering length, in units of 10^{-12} cm

$L(l)$ = value of L , angular momentum

$NRS(l)$ = number of resonances

$ER(i, l)$ = resonance energy (ev)

$AJ(i, l)$ = value of J , spin state

$GT(i, l)$ = total width, Γ (ev)

$GN(i, l)$ = neutron width, Γ_n (ev)

$GG(i, l)$ = radiation width, Γ_γ (ev)

$GF(i, l)$ = fission width, Γ_f (ev)

NLST = number of L states given in Table 3 of the FCD.

For unresolved resonance parameters with fission widths given, the data are placed in the record in the following order (Formula No. 1):

SPI, A, LIS, NE, $(ES(i), i = 1, NE), (C(l), L(l), NJS(l), (MUF(i, l),$
 $D(i, l), AJ(i, l), AMU(i, l), GNO(i, l), GG(i, l), 0.0, (GF(k, i, l),$
 $k = 1, NE), i = 1, NJS(l)), l = 1, NLST)$

where

A = scattering length, in units of 10^{-12} cm

NE = number of energy points at which fission widths are tabulated

$ES(i)$ = energy (ev) of the i^{th} point used to tabulate fission widths

$NJS(\ell)$ = number of spin (J) states

$MUF(i, \ell)$ = number of degrees of freedom used in the fission width distribution

$D(i, \ell)$ = mean level spacing

$AMU(i, \ell)$ = number of degrees of freedom used in the neutron width distribution

$GNO(i, \ell)$ = the average reduced neutron width

$GG(i, \ell)$ = the average radiation width

$GF(k, i, \ell)$ = the average fission width at energy $ES(k)$

For unresolved resonance parameters with fission widths not given, the data are placed in the record in the following order (Formula No. 1):

$SPI, A, LIS, (C(\ell), L(\ell), NJS(\ell), (D(i, \ell), AJ(i, \ell), AMU(i, \ell),$
 $GNO(i, \ell), GG(i, \ell), i = 1, NJS(\ell)), \ell = 1, NLST)$

3. File 3

The Q for the reaction and the final state index are given in Table 1 of the FCD. The lower energy boundary of the energy range and the ENDF/B interpolation code are given in Table 2 of the FCD.

Smooth cross sections for a specific energy range are placed in the record in the following order:

$(E(I), SIG(I), I = 1, NDIF)$

where

$E(I)$ = energy (ev)

$SIG(I)$ = cross section.

4. File 4

Flags, indicating laboratory or center-of-mass system and Legendre coefficients or tabulations, are given in Table 1 of the FCD. For Legendre coefficients, the lower energy of the energy range and the ENDF/B energy interpolation code are given in Table 2 of the FCD. For tabulations, the lower μ of the μ range, the ENDF/B μ interpolation code, the ENDF/B energy interpolation code, and the energy for the tabulation are given in Table 2 of the FCD.

For Legendre coefficients, the data are placed in the record in the following order for a specific energy range:

$$(E(I), L(I), (F(\ell, I), \ell = 1, L(I)), I = 1, NDIF)$$

where

$E(I)$ = energy (ev)

$L(I)$ = number of coefficients

$F(\ell, I)$ = coefficients.

For tabulations, the data are placed in the record in the following order for a specific μ range:

$$(CMU(I), DSIG(I), I = 1, NDIF)$$

where

$CMU(I)$ = cosine of the angle, μ

$DSIG(I)$ = value of the distribution.

5. File 5

The number of ENDF/B subsections in File 5 for a given reaction type is found in Table 1 of the FCD. The lower energy boundary of the energy range, the interpolation code, the subsection formula index (LF), and the value of θ for the formula are given in Table 2 of the FCD.

The data for the probability for each partial distribution are placed in the record in the following order for a specific energy range:

$$(E(I), P(I), I = 1, NDIF)$$

where

$E(I)$ = energy (ev)

$P(I)$ = probability for the partial distribution.

6. File Contents Directory, Table 1

The FCD, Table 1, consists of four arrays. The INDX2 array contains the Table 2 index, pointing to the location in Table 2 where the appropriate data may be found. The MTX array contains the ENDF/B file number (MF) and the ENDF/B reaction number (MT), packed into one word:

$$MTX = MF * 1000 + MT$$

The QTAB1 and ITAB2 arrays contain parameters appropriate to the corresponding ENDF/B file. In Table 6, the last three figures of the MTX number would take on all values of MT that occur for the material for Files 3 through 5.

TABLE 6
FILE CONTENTS DIRECTORY, TABLE 1

INDX2	MTX	QTAB1	ITAB2	ENDF/B File No.
↓ Table 2 Index ↓	1451	0 = no resonances 1 = resonances	0 = nonfissile 1 = fissile	1
	2151	number of isotopes	nothing	2
	3001	reaction Q	final state index	3
	4002	1 = laboratory system 2 = center of mass	1 = Legendre coefficients 2 = tabulation	4
	5004	number of subsections	nothing	5

7. File Contents Directory, Table 2

The FCD, Table 2, consists of four arrays. The NBLOK array contains the 900-word direct-access record number (N1) and the word number (N2), within the record:

$$NBLOK = 1000 * N1 + N2$$

The RANGE array contains the lower boundary of the X range for a X, Y tabulation; however, in the case of resonance data, it contains the Z, A identification of the isotope. The INTERP array contains two parameters, N₃ and N₄, whose character depends upon the ENDF/B file involved:

$$\text{INTERP} = 1000 * \text{N3} + \text{N4}$$

The ENER array also contains ENDF/B file-dependent parameters. In Table 7, the type of entry in Table 2 of the FCD is illustrated for each ENDF/B file. There are entries for each energy or μ range of every reaction type in ENDF/B Files 3 through 5.

TABLE 7
FILE CONTENTS DIRECTORY, TABLE 2

NBLOK	RANGE	INTERP*		ENER	Description
		N3	N4		
1000 * record number + word number ↓	nothing	nothing	0	number of cards	literal data
	lower energy	interpolation code	1 or 2	nothing	$\bar{\nu}$ tabulation
	Z, A isotope identification	1 = resolved 2 = unresolved	formula number	1 = fission widths 0 = no fission widths	resonance parameters
	lower energy	interpolation code	nothing	nothing	smooth cross sections
	lower energy	energy interpolation code	nothing	nothing	Legendre coefficients
	lower μ	μ interpolation code	energy interpolation code	energy of distribution	tabulated distributions
	lower energy	interpolation code	subsection code	formula constant, θ	partial energy distributions

*INTERP = 1000 * N3 + N4

8. File Contents Directory, Table 3

The FCD, Table 3, consists of four arrays which are used only for ENDF/B File 2, resonance, data. The ABUND array contains the abundance of the isotope. The ELO array contains the lower energy of the energy range over which

the resonance parameters apply; the EHI array contains the upper energy of that range. The NLST array contains the number of l states. There are entries for each energy range of every isotope.

D. RESTRICTIONS

In addition to the types of ENDF/B data which may be processed and the order in which materials must be handled, given in the introduction of this appendix, several dimensioning considerations must be considered:

- 1) Each array in the FCD Table 1 is dimensioned 100.
- 2) Each array in the FCD Table 2 is dimensioned 900.
- 3) Each array in the FCD Table 3 is dimensioned 50.
- 4) The maximum number of materials that may be included in one material correspondence table is 100.
- 5) The maximum number of tapes containing SCOFF data for materials in one tape requirements table is 10.
- 6) SCOFF data for a material must be contained within 39 records of 900 words each.

Further restrictions are:

- 1) Temperature-dependent ENDF/B records will cause the program to fail; except in ENDF/B File 3, the records are skipped.
- 2) Materials to be processed in a given run must be on the ENDF/B tape; if a material is not on the ENDF/B tape, the entire tape will be searched and the program will be terminated. Materials that have been processed previous to this will be all right, and will be recorded in the material correspondence and tape requirements tables.

E. INPUT PREPARATION

1. Card No.1 Format (2I12, 4X, 2A4, 2I12)

NEW = 1, for new SCOFF tape preparation

= 0, for addition of new materials to end of an old SCOFF
tape

= -1, for print of material correspondence and tape requirements tables.

NSKIP = 0, if NEW = 1 or -1

= number of SCOFF material files to be skipped before additions of new materials are made.

NSCORE = literal SCOFF tape identification (8 bytes), two EBCDIC words.

NENDF = ENDF/B tape identification, LABEL on ENDF/B LABEL card.

NOMAT = number of materials to be processed.

2. Card No. 2 Format (2I12)

NUT1 = 1, read old material correspondence and tape requirements tables from direct-access data set, Record 40, on disk.

= 0, read old tables from cards.

= -1, no old table (NEW = 1).

NUT2 = 1, write new material correspondence and tape requirements tables on direct-access data set, Record 40, on disk.

= 0, punch new table on cards.

= -1, do both 1 and 0.

The third and fourth cards are repeated for each material to be processed (NOMAT sets of cards); however, if NEW = -1, this set of cards is omitted. The card sets for each material must be ordered by increasing MAT1 number. The set of cards for the first material to be processed must be followed by the material correspondence and tape requirements tables, if NUT1 = 0.

3. Card No. 3 Format (I12, 3E12.4, 2A4)

MAT1 = ENDF/B material identification number

ZNUM = material atomic number

ANUM = material mass number (0.0, if mixture of isotopes)

AMASS = material atomic weight

DATE = date for this run (8 bytes), two EBCDIC words.

4. Card No. 4 Format (16A4)

TITLE = 64-character literal title.

The remaining cards contain the material correspondence and tape requirements tables, and are used only if NUT1 = 0; they are inserted after the set of cards for the first material.

5. Card No. 5 Format (3I12)

NUM = number of materials in the material correspondence table.

NOT = number of SCOFF tapes on which the NUM materials reside.

NPRINT = 1, print the material correspondence and tape requirements tables.

The next card is repeated NUM times, once for each material.

6. Card No. 6 Format (4I12, 4X, 2A4)

IZAT = Z, A number for the material, 1000 times the atomic number plus the mass number.

MATT = ENDF/B material identification number.

NTOREC = the total number of 900-word records in which this material resides.

NTT = the SCOFF tape and file numbers, NT and NF, along with the previous values, NT_p and NF_p , for this material.

$$NTT = (NT * 100 + NF) * 10000 + NT_p * 100 + NF_p$$

DATEET = literal date (8 bytes) when this material was processed; two EBCDIC words.

The next card is repeated until all NOT tapes are specified.

7. Card No. 7 Format (6(4X, 2A4))

TAPID = literal SCOFF tape identification (8 bytes), two EBCDIC words; there may be six identifications per card.

F. SAMPLE INPUT SHEETS

FORTRAN FIXED 10 DIGIT DECIMAL DATA

DECK NO. _____ PROGRAMMER _____ DATE _____ PAGE 1 of _____ JOB NO. _____

NUMBER	IDENTIFICATION	DESCRIPTION DO NOT KEY PUNCH
1	0	NEW Add to old SCOFF tape
13	3	NSKIP Skipp 3 material files on old SCOFF tape
25	S C O F F 0 0 1	NSCORE SCOFF literal tape identification
37	1 1 4	NENDF ENDF/B tape identification (LABEL)
49	2	NOMAT Add 2 materials to SCOFF tape
61		Format (2I12, 4X, 2A4, 2I12)
1	0	NUT1 Read } Cards for material correspondence
13	0	NUT2 Punch } and tape requirements tables
25		
37		
49		
61		Format (2I12)
1	1 0 0 6	MAT1 ENDF/B Lithium-7 identification
13	3 0	ZNUM Lithium-7 atomic number
25	7 0	ANUM Lithium-7 mass number
37	7 0 1	AMASS Lithium-7 atomic weight
49	0 2 / 1 4 / 6 8	DATE Date of run
61		Format (I12, 3E12.4, 2A4)
1	L I T H I U M - 7 E	TITLE Literal information (arbitrary)
13	N D F / B T A P E 1	
25	1 4	
37		
49		
61		Format (16A4)

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FORTRAN FIXED 10 DIGIT DECIMAL DATA

DECK NO. _____ PROGRAMMER _____ DATE _____ PAGE 2 of _____ JOB NO. _____

NUMBER	IDENTIFICATION	DESCRIPTION DO NOT KEY PUNCH
1	3	NUM 3 materials on old SCOFF tape
13	1	NOT 1 SCOFF tape
25	1	NPRINT Print material correspondence and
37		tape requirements tables
49		
61		Omit if NUT1 ≠ 0 Format (3I12)
1	2 6 0 0 0	IZAT Iron Z, A number
13	1 0 2 0	MATT Iron ENDF/B identification
25	2 2	NTOREC 22 records of 900 words in iron material file
37	1 0 1 0 0 0 0	NTT SCOFF tape and file number for iron
49	0 2 / 1 3 / 6 8	DATET Date of run
61		Omit if NUT1 ≠ 0 Format (4I12, 4X, 2A4)
1	9 4 2 3 9	IZAT Pu-239 Z, A number
13	1 0 5 1	MATT Pu-239 ENDF/B identification
25	8	NTOREC 8 records of 900 words in Pu-239 material file
37	1 0 2 0 0 0 0	NTT SCOFF tape and file number for Pu-239
49	0 2 / 1 3 / 6 8	DATET Date of run
61		Omit if NUT1 ≠ 0 Format (4I12, 4X, 2A4)
1	9 4 2 4 1	IZAT Pu-241 Z, A number
13	1 0 5 4	MATT Pu-241 ENDF/B identification
25	1 4	NTOREC 14 records of 900 words in Pu-241 material file
37	1 0 3 0 0 0 0	NTT SCOFF tape and file number for Pu-241
49	0 2 / 1 3 / 6 8	DATET Date of run
61		Omit if NUT1 ≠ 0 Format (4I12, 4X, 2A4)

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FORTRAN FIXED 10 DIGIT DECIMAL DATA

	DECK NO.	PROGRAMMER	DATE	PAGE 3 of	JOB NO.
	NUMBER	IDENTIFICATION	DESCRIPTION	DO NOT KEY PUNCH	
1	S C O F F 0 0 1		TAPID	Literal tape identification for first	
13				SCOFF tape	
25					
37					
49		73		80	
61			Omit if NUT1 ≠ 0	Format (6 (4X, 2A4))	
1	1 0 5 9		MAT1	ENDF/B Na-23 identification	
13	1 1 . 0		ZNUM	Na-23 atomic number	
25	2 3 . 0		ANUM	Na-23 mass number	
37	2 2 . 9 9		AMASS	Na-23 atomic weight	
49	0 2 / 1 4 / 6 8	73	DATE	Date of run	
61				Format (112, 3E12.4, 2A4)	
1	S O D I U M - 2 3 E		TITLE	Literal information (arbitrary)	
13	N D F / B T A P E 1				
25	1 4				
37					
49		73		80	
61				Format (16A4)	
1					
13					
25					
37					
49		73		80	
61					

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G. OPERATING INSTRUCTIONS

1. Input-Output Assignments

<u>Date-Set Reference No.</u>	<u>Explanation</u>
5	Input stream
6	Printout
7	Punchout (14, if compiled at AI)
8	SCOFF tape, old or new
9	ENDF/B EBCDIC tape
16	Direct-access data set

Data set 16 is used only if NUT1 = 1 and/or NUT2 = 1 or -1 on the input cards.

Data set 7 is used only if NUT2 = 0 or -1 on the input cards.

2. SCOFF Procedure

The following job control language (JCL) cards are designed to execute SCOFF from a job library. The load module for SCOFF and the direct-access

SCOFF PROCEDURE

```

//          MSG LEVEL = 1
//JOB LIB DD DSNAME = SCORE2.LOADMODS, DISP = OLD, UNIT = 2311, VOLUME = SER = GPAK10
//G      EXEC PGM = SCOFF
//FT05F001 DD DDNAME = SYSIN
//FT06F001 DD SYSOUT = A
//FT07F001 DD UNIT = (SYSCP, , DEFER), DISP = (MOD, PASS), DCB = (STACK = 2)
//FT08F001 DD DISP = OLD, DSNAME = SCOFF01, VOLUME = SER = XXXXXX, LABEL = (1, NL),      X
//          DCB = (RECFM = V, LRECL = 3604, BLKSIZE = 3608), UNIT = TAPE9              8
//FT08F002 DD DISP = OLD, DSNAME = LI007B, LABEL = (2, NL),                          X
//          VOLUME = (, RETAIN, REF = *. FT08F001),                                  X
//          DCB = (RECFM = V, LRECL = 3604, BLKSIZE = 3608)                          11
//FT08F003 DD DISP = OLD, DSNAME = NA023B, LABEL = (3, NL),                          X
//          VOLUME = (, RETAIN, REF = *. FT08F002),                                  X
//          DCB = (RECFM = V, LRECL = 3604, BLKSIZE = 3608)                          14
//FT08F004 DD DISP = OLD, DSNAME = FE000B, LABEL = (4, NL),                          X
//          VOLUME = (, RETAIN, REF = *. FT08F003),                                  X
//          DCB = (RECFM = V, LRECL = 3604, BLKSIZE = 3608)                          17
//FT08F005 DD DISP = OLD, DSNAME = PU241B, LABEL = (5, NL),                          X
//          VOLUME = (, RETAIN, REF = *. FT08F004),                                  X
//          DCB = (RECFM = V, LRECL = 3604, BLKSIZE = 3608)                          20
//FT08F006 DD DISP = (NEW, KEEP), DSNAME = YYYYYY, LABEL = (6, NL),                  X
//          VOLUME = (, RETAIN, REF = *. FT08F005),                                  X
//          DCB = (RECFM = V, LRECL = 3604, BLKSIZE = 3608)                          23
    Etc.
//FT09F001 DD DISP = OLD, VOLUME = SER = UUUUUU, DSNAME = VVVVVVVV,                  X
//          UNIT = (2400, , DEFER), DCB = (RECFM = F, LRECL = 80, BLKSIZE = 80)        30
//SYSIN      DD *
    [Data]
/*

```

```

where   XXXXXX = SCOFF tape number
        YYYYYY = DSNAME for new material to be processed
        UUUUUU = ENDF/B tape number
        VVVVVVVV = DSNAME for ENDF/B tape

```

data set are on the same disk pack. A SCOFF tape containing five files, including the identification file, has been prepared; the SCOFF files are:

- 1) Identification file
- 2) ENDF/B data for lithium-7
- 3) ENDF/B data for sodium-23
- 4) ENDF/B data for natural iron
- 5) ENDF/B data for plutonium-241

APPENDIX VII SYSTEM CHANGE

Starting with Release 15/16 of the IBM 360 Operating System, the use of the "CANCEL" key is reserved by special system purposes. Since SCORE makes extensive use of the "CANCEL" key, we are including enough information so that any system support person can patch your system and allow unrestricted use of the "CANCEL" key.

The program SUPERZAP is included in the SCORE.SUPER load module. This program is a standard IBM program, and should be used to produce the patch.

The required patch is as follows:

The member of SYS1.SVCLIB named IGG0190E has the instruction 4780 at location 016A relative to the CSECT name IGG0190E. This instruction must be 4700 to prevent the system from possibly intercepting CANCEL key attentions from the 2250.

REFERENCES

1. H. Alter and C. L. Dunford, "Compilation, Evaluation, and Production of Nuclear Data for Reactor Calculations" NAA-SR-11980 Vol. 1 (1966)
2. H. C. Honeck, "Specifications for an Evaluated Nuclear Data File for Reactor Applications, ENDF/B," BNL 50066 (T-467) (July 1967)
3. "System/360 Component Description-2250 Display Unit Model 1," IBM Systems Reference Library, A27-2701
4. J. M. Friedman and M. Platt, "SCISRS, Sigma Center Information Storage and Retrieval System," BNL883(T-357) (July 1964)
5. A. Horsley, J. B. Parker, K. Parker, and J. A. Price, "Curve Fitting and Statistical Techniques for Use in the Mechanized Evaluation of Neutron Cross Sections," Nucl. Instr. Methods 62 (1968) p 29
6. M. Goldberg et al., "SCISRS Newsletter, Part A," BNL 50061A (L-391) (June 1967)
7. M. J. D. Powell, "Curve Fitting by Cubic Splines," AERE Report TP 307
8. "Operating System/360 FORTRAN (H) Programmer's Guide," IBM Systems Reference Library, C28-6602-3
9. T.N.E. Greville, "Spline Functions, Interpolation, and Numerical Quadrature," Mathematical Methods for Digital Computers, Vol II (John Wiley & Sons, Inc., New York, N. Y., 1967)
10. B. Wendroff, Theoretical Numerical Analysis (Academic Press, 1966) p 27
11. J. H. Ahlberg, E. N. Nelson, and J. L. Walsh, Theory of Splines and Their Applications (Academic Press, 1967)

