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OUTLINE OF DIRECT METHODS USED IN COMPUTING THE CROSS SECTION SENSITIVITY OF NEUTRONIC PARAMETERS IN A FUSION REACTOR

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OAK RIDGE NATIONAL LABORATORY

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REACTOR DIVISION

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The numbers of the reports in this study, including this one are:
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OUTLINE OF DIRECT METHODS USED IN COMPUTING
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ABSTRACT

The methods by which cross section changes were effected in a sensitivity analysis of neutronic parameters in a D-T fusion reactor are recorded. Listings of auxiliary codes are presented.

I. INTRODUCTION

The purpose of this report is to describe the methods being employed in an investigation of the cross section sensitivity of neutronic parameters in a D-T fusion reactor. The methods to be described are designated "direct" methods since they are based on direct alterations of the nuclear data. In this context, "indirect" methods for cross section sensitivity analysis are those based on adjoint fluxes and perturbation theory. A perturbation theory method for cross section sensitivity analysis has recently been developed by members of the ORNL Mathematics and Neutron Physics Divisions¹ and is also being applied to fusion reactor neutronics. Each of the two methods, direct and indirect, exhibits characteristic advantages, and therefore it is desirable to possess developed capabilities in both methods.

*Operated by Union Carbide Corporation for the U. S. Atomic Energy Commission.

II. CALCULATIONAL PROCEDURES

The sensitivity analysis is being carried out with the discrete ordinates transport theory code XSDRN.² The reference for cross section data is the Evaluated Nuclear Data File, ENDF/B.³ The steps necessary to generate multigroup cross section data for use with XSDRN are as follows.

Cross sections in the ENDF/B files are accessed from the permanently mounted 2314 disk, NUCLIB. They are stored as the data sets named:

LMP.ENDFB2

LMP.ENDFB3

LMP.THERMAL.DATA

As the names indicate, the first is ENDF/B version 2 data; the second is ENDF/B version 3. The third contains ENDF/B format scattering law data (File 7 data) for graphite and other materials. These data are processed by the cross section processing code XLACS⁴ for subsequent use in XSDRN. The product of XLACS is called, in local jargon, a "new format XSDRN master tape" which must be altered by the CONVERT code to produce an "old format XSDRN master tape." (This program is described in the XLACS report.) The converted tape is then used in XSDRN. A product of the XSDRN code is the so-called "XSDRN working tape" which contains cross sections in "working tape" format. Cross section input to XSDRN may be either or both master tape and working tape data; use of the working tape for resonance nuclides is particularly advantageous when possible since the Nordheim treatment need not be repeated.

At the beginning of this study, the XLACS code was being debugged and improved. At a point where it was believed to be functioning accurately, a copy of XLACS was transferred to the 2311 disk THERM~~0~~ from the NUCLIB

disk using the UTILITY program IEHMOVE.⁵ The code, thus "frozen," could be used without fear of minor updates and changes producing spurious effects. (The XSDRN and CONVERT programs were likewise moved for the same reason.)

Typical running times and space requirements for the various codes are given in Table I.

III. MODIFICATIONS TO XLACS AND XSDRN

For the purposes of this study some of the subroutines of XLACS and XSDRN were reprogrammed to obtain desired information not normally provided. These modifications are introduced at run time by INCLUDE statements so that the original programs are actually unaltered. The modifications are the following:

XLACS - A data set named CRØS.L1ST.X1D on THERMØ over-rides the XLACS subroutines CRØS, L1ST, and X1D so that the XSDRN tape contains and displays under separate headings all the reaction types processed by XLACS, in particular ENDF/B MT's 22-28 and 51-91. The latter group are the inelastic scattering cross sections. MT=91 refers in the case of Li-7 to the (n,n') reaction.

XSDRN - A main program whose sole function is to set the size of the array D to 75,000 (or any other desired size) is compiled and included at each XSDRN run. A data set NØD.LST1D.RRATE.VS3 overrides the XSDRN subroutines LST1D and RRATE so as to output reaction rates for each nuclide by zone and energy group. These reaction rates will be designated "activities" in the following

TABLE I. RUNNING TIMES AND REGION REQUIREMENTS FOR VARIOUS CODES

CASE	CODE	360/75 RUNNING TIME**	REGION
1 Non-resonance nuclide	XLACS	4-5 minutes	378K
Niobium (123 groups)	XLACS	36 minutes	376K
Working tape	XSDRN	10-12 minutes	446K
Master tape with Nb	XSDRN	17 minutes	446K
—	CONVERT	5 seconds	212K

** Running times on the 360/91 are about 20-25% of the above.

discussion. The fractional activity for each energy group and the cumulative fractional activity up to and including that group are given. That is, if A_G is the activity over all zones for a given reaction type in an energy group G , then the fractional activity is

$$A_G / \left(\sum_{G'=1}^{GMAX} A_{G'} \right)$$

and the cumulative fractional activity through group G is

$$\sum_{G'=1}^G A_{G'} / \left(\sum_{G'=1}^{GMAX} A_{G'} \right)$$

where $GMAX$ is the maximum number of energy groups (100 or 123 in this work).

The subroutines in all cases were changed only in the sense of producing additional results. All original features were retained.

IV. DESIGNATION OF CROSS SECTION TYPES IN XSDRN AND THEIR RELATION TO ENDF REACTION CLASSIFICATION

Appendix B of BNL 50274³ lists the reaction types designated by the integers MT used in the ENDF files. For historical reasons, the numbering system and definitions used in XLACS and XSDRN are different. (It may be the case that future versions of these codes will be changed to conform to the ENDF system. Here we refer only to those versions of these codes which were used during this study.) Table II shows the

TABLE II. CORRESPONDENCE BETWEEN XSDRN REACTION NUMBERS AND ENDF MT'S

<u>XSDRN NO.</u>	<u>ENDF MT</u>	<u>PROCESS</u>
1	---	Absorption
2	18	Fission
5	1	Total
6	2	Elastic scatter
7	102	n-gamma
8	107	n- α
9	---	Sum of all processes with more than one neutron in exit channel (n,2n), (n,3n), etc.
10	4	Total inelastic, the sum of all processes with one neutron in exit channel.
11	103	n-p
12	104	n-d
13	105	n-t
16	108	n,2 α
21	---	Infinite dilute capture
22	---	Infinite dilute fission
24	17	n,3n
25	22	(n,n') α
26	23	(n,n')3 α
27	24	(n,2n) α
28	25	(n,3n) α
32-71	51-90	(n,n') reactions to the (MT-50)th excited state
72	91	(n,n') to the continuum

correspondence between the numbering systems in XSDRN and ENDF/B. The XSDRN numbers are those to be used in preparing XSDRN inputs for extra cross section positions and activities. XSDRN numbers 21 and 22 refer to the resonance portion of the respective cross section calculated on an infinite dilution basis. XSDRN numbers 24-72 were added to the code by the subroutine modifications.

V. LAYOUT OF "OLD FORMAT TAPES" AND "WORKING TAPES" FOR XSDRN

In order to make cross section changes on either the "Old Format Tapes" or the "Working Tapes" for XSDRN, it is necessary to know how information is stored. (The word "tapes" refers actually to data sets stored on disks.)

A. Old Format XSDRN Tapes

Record 1: 103 items

Item 1, tape identification number

Item 2, number of nuclides on the tape, NNUC

Item 3, number of groups, NGP

Items 4-103 are 5 title card images copied from XLACS input.

Records 2 to NNUC+1: Table of Contents, 33 items for each nuclide.

Record NNUC+2: L1, L2, L3, L4. Lengths of escape probability tables for slabs and cylinders and of a tabulation of the function $J(\xi, k)^{6,7}$ which are in the next record.

Record (NNUC+3): Table, L4 items.

Record (NNUC+4): Energy-lethargy tabulation, high-to-low, energy in e.v., $2*(NG+1)$ items.

For each nuclide, the following records are given:

- R_a 33 Items: ID(1-18), title
 ID(19), nuclide identification number
 ID(20), number of resolved resonances
 ID(21), number of unresolved energies
 ID(22), number of 1-D cross sections
 ID(23), length of P_0 elastic scattering matrix list
 ID(24), length of P_1, P_2, P_3 lists
 ID(25), length of inelastic matrix list
 ID(26), length of $n, 2n$ matrix list
 ID(27), number of fission yields
 ID(28), number of records for this nuclide besides this one
 ID(29-33) zeros in this study
- R_b Resonance data, $6*ID(20)+ID(21)+9$ items if $ID(20) + ID(21) \neq 0$
- R_c One-D cross sections, $ID(22)*(NGP+1)$ items
- R_d P_0 elastic matrix, ID(23) items
- R_e, R_f, R_g ID(24) items each, the P_1, P_2 , and P_3 matrices respectively
- R_h ID(25) items, the inelastic matrix
- R_i ID(26) items, the $n, 2n$ matrix

B. Working Tape Layout

Record 1: 93 items

- Item 1, tape identification
- Item 2, number of nuclides, NNUC
- Item 3, number of groups, NGP
- Items 4-93, five title card images

Records 2 (NNUC+1), 19 items each

Items 1-18, descriptive of a nuclide whose identification number is
the 19th item

The information for each nuclide is provided in the succeeding records:

R₂: 33 items

Items 1-18, descriptive

Item 19, nuclide identification number

Item 20, number of resolved resonances

Item 21, 0 in this study

Item 22, number of one-dimensional cross sections

Item 23, length of one-dimensional arrays + NGP "magic words"*** +
length of P₀ scattering array

Item 24, length of P₁, P₂, P₃ arrays

Item 25, length of inelastic array

Item 26, length of n,2n array

Item 28, number of records for the nuclide beside this one

All other items were zero in this study.

VI. ALTERING CROSS SECTIONS

Cross sections can be altered at any stage of the calculation if a listing of the records is available. A computer code ROSETTA,⁸ which takes advantage of the extended error handling facility to enable the reading of records of unknown length, was written to permit record listing in readable form. In this way, cross sections may be read in from working

*** See page 84 of Reference 4 for a discussion of "magic words."

or old format XSDRN tapes and changed in any way desired. For instance, to avoid repetition of the Nordheim integral treatment for the niobium resonances by XSDRN, the data was broken up so that two fictitious niobiums could be used. One had all scattering cross sections suppressed while the other had all absorption cross sections suppressed. Changes in the scattering cross sections could then be made without disturbing the absorption cross sections.

At the ENDF/B level, the EDITOR⁹ code proves highly useful. The ENDF/B data for any nuclide is easily converted to card image form as a data set on a disk, or as physical cards. The ROSETTA code, appropriately modified, can be used to change the numbers, or the ENDF processing code CRECT¹⁰ may be used. (Because of its flexibility, a ROSETTA modification was used.) Once the card images are changed, EDITOR can be used again to convert the data back to binary form. Careful attention to the requirements of ENDF/B formats must be exercised; all necessary information is available in Reference 3.

It may be the case that interpolation is necessary, as was the case in dealing with fluorine cross sections in the ENDF/B-2 files. A subroutine, TERP, exhibited in the appendix is useful in matching cross section lists. For instance, the inelastic cross section may be given at fewer points than the total cross section. TERP enables a change in the inelastic cross section to be properly reflected as a corresponding change in the total cross section by interpolating the inelastic cross section at the intermediate points.

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10. Description of the ENDF/B Processing Codes CHECKER, CRECT, DAMMET, PLDTFB, and Retrieval Subroutines, Revised April 1969, BNL 13582.

APPENDIX A

IEHMOVE - An IBM Utility Program Used Here to Copy
Data Sets from One Disk to Another

```
//MLTRD001 JOB (13803,,,50),'Y-12 9104-2 TOBIAS',MSGLEVEL=(1,1),
// CLASS=D, TYPRUN=HOLD
// EXEC PGM=IEHMOVE
//SYSPRINT DD SYSOUT=A
//SYSUT1 DD UNIT=SYSDA,SPACE=(CYL,(10))
//DD1 DD UNIT=2311,VOLUME=SER=THERMO,DISP=OLD
//DD2 DD UNIT=2314,VOLUME=SER=ZX1111,DISP=OLD
//SYSIN DD *
    COPY DSN=MLT.DWC12871.F.N.NPRIME.HI,
    TO=2311=THERMO,FROM=2314=ZX1111
    COPY DSN=MLT.DWC12871.F.N.NPRIME.LO,
    TO=2311=THERMO,FROM=2314=ZX1111
    COPY DSN=MLT.DWC12871.F.XA.ALDER,
    TO=2311=THERMO,FROM=2314=ZX1111
    COPY DSN=MLT.DWC12871.N2N.BE.HI,
    TO=2311=THERMO,FROM=2314=ZX1111
    COPY DSN=MLT.DWC12871.N2N.BE.LO,
    TO=2311=THERMO,FROM=2314=ZX1111
    COPY DSN=MLT.DWC12871.N2N.BE.STD,
    TO=2311=THERMO,FROM=2314=ZX1111
```

/*

//

APPENDIX B

XLACS DECK SETUP - Deck Set up to Create an XSDRN
Old Format "Tape" XLACS.BEFF.OLD

The utility IEHPRGGM has been used to scratch the data set before-hand to avoid restart difficulties. An in-line procedure is used for XLACS which is followed by a CONVERT step.

```

75
//MLTZD015 JOB (13803,,,50),'Y-12 9104-2 TOBIAS',MSGLEVEL=(1,1),
// CLASS=D,TPRUN=HOLD
//ERASE EXEC PGM=IEHPRGGM
//SYSPRINT DD SYSOUT=A
//DDZ DD UNIT=2311,VOLUME=SER=THERMO,DISP=SHR
//SYSIN DD *
  SCRATCH VOL=2311=THERMO,
    DSN=XLACS.BEFF.NEW
  SCRATCH VOL=2311=THERMO,
    DSN=XLACS.FROW.NEW
  SCRATCH VOL=2311=THERMO,
    DSN=XLACS.BEFF.OLD
  SCRATCH VOL=2311=THERMO,
    DSN=WURK.G100.BEFF
/*
//XLACS PROC V=3,FT21=NULLFILE,FT22=NULLFILE
//LINK EXEC PGM=IEWL,PARM=(MAP,LIST,XREF,OVLY),REGION=150K
//SYSPRINT DD SYSOUT=A
//SYSUT1 DD UNIT=SYSDA,SPACE=(CYL,(6,1))
//SYSLIB DD DSN=SYS1.FORTLIB,DISP=SHR
//LIB DD DSN=LALIB,DISP=SHR
//SYSLMOD DD DSN=8&FJ03LIB(XLACS),UNIT=SYSDA,DISP=(NEW,PASS),
// SPACE=(CYL,(8,1,1),RLSE)
//SYSLIN DD DDNAME=SYSIN
// DD DSN=NMG.XLACS.OVERLAY,UNIT=2311,VOL=SER=THERMO,DISP=SHR
//XLACS -DD DSN=NMG.XLACS.PGM,UNIT=2311,VOL=SER=THERMO,DISP=SHR
//GO EXEC PGM=XLACS,COND=(5,LT,LINK),REGION=375K
//STEPLIB DD DSN=8&FJ03LIB,DISP=(OLD,DELETE)
//FT06F001 DD SYSOUT=A,DCB=(RECFM=FA,BLKSIZE=133)
//FT08F001 DD UNIT=SYSDA,SPACE=(3520,(100,40)),
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=3520)
//FT09F001 DD UNIT=SYSDA,SPACE=(3520,(100,40)),DCB=*.FT08F001
//FT10F001 DD UNIT=SYSDA,SPACE=(3520,(100,40)),DCB=*.FT08F001
//FT11F001 DD DSN=LMP.ENDFR&V,UNIT=2314,VOL=SER=NUCLIB,DISP=SHR
//FT12F001 DD UNIT=SYSDA,SPACE=(3520,(100,40)),DCB=*.FT08F001
//FT14F001 DD UNIT=SYSDA,SPACE=(3520,(100,40)),DCB=*.FT08F001
//FT15F001 DD UNIT=SYSDA,SPACE=(3520,(100,40)),DCB=*.FT08F001
//FT16F001 DD UNIT=SYSDA,SPACE=(3520,(100,40)),DCB=*.FT08F001
//FT17F001 DD UNIT=SYSDA,SPACE=(3520,(100,40)),DCB=*.FT08F001
//FT18F001 DD UNIT=SYSDA,SPACE=(3520,(100,40)),DCB=*.FT08F001
//FT20F001 DD UNIT=SYSDA,SPACE=(3520,(100,40)),DCB=*.FT08F001
//FT21F001 DD DSN=8&FT21,UNIT=TAPE9,VOL=SER=21,DISP=OLD,LABEL=(,NL),
// DCB=*.FT08F001
//FT22F001 DD DSN=8&FT22,UNIT=TAPE9,VOL=SER=22,DISP=OLD,LABEL=(,NL),
// DCB=*.FT08F001
//FT23F001 DD UNIT=SYSDA,SPACE=(3520,(100,40)),DCB=*.FT08F001

```

```

//FT25F001 DD DSN=LMP.THERMAL.DATA,UNIT=2314,VOL=SER=NUCLIB,DISP=SHR 00000320
//FT30F001 DD UNIT=SYSDA,SPACE=(3520,(400,40)),DCB=*.FT08F001 00000330
//GO.FT31F001 DD UNIT=SYSDA,SPACE=(3604,(500,1)) 00000340
//FT51F001 DD SYSOUT=A,DCB=*.FT06F001 00000350
// PEND
//XLACS EXEC XLACS,REGION.GO=425K
//LINK.F DD DSN=CRUS.LIST.X10,UNIT=2311,DISP=SHR,VOL=SER=THERMO
//LINK.SYSIN DD *
  INCLUDE F
//GO.FT11F001 DD DSN=LMP.ENDFB2,UNIT=2314,VOL=SER=NUCLIB,DISP=SHR
//GO.FT20F001 DD UNIT=2311,VOL=SER=THERMO,DISP=(NEW,KEEP),
// DSN=XLACS.FROM.NEW,
// SPACE=(3520,(20,10),RLSE),
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=3520)
//GO.FT21F001 DD DSN=XLACS.BEFL.NEW,UNIT=2311,VOL=SER=THERMO,DISP=SHR
//GO.FT22F001 DD DSN=XLACS.BEFF.NEW,UNIT=2311,VOL=SER=THERMO,
// SPACE=(3520,(20,10),RLSE),DISP=(NEW,KEEP),
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=3520)
//GO.FT05F001 DD *

```

XLACS INPUT DATA FOLLOWS (SEE REF. 4)

CREATION OF XLACS.FROM.NEW, JANUARY 10, 1973

70\$\$\$ 2323 23 1 3 3 0 23 1 11 T

73** 300. T

11\$\$\$ 1620 1 3 0 0 1 T

15\$\$\$ 2323 1154 23

16\$\$\$ 0 1 8R0 T

/*

//CONVERT EXEC LINKNGO,

// REGION.GO=270K

//LINK.SYSLIB DD DSN=SYS1.FORTLIB,DISP=SHR

//LINK.SYSLIN DD DSN=CONVERT,UNIT=2311,DISP=SHR,VOL=SER=THERMO

// DD DDNAME=SYSIN

//LINK.SYSLIN DD *

//GO.FT01F001 DD UNIT=SYSDA,SPACE=(3520,(400,40)),

// DCB=(RECFM=VS,BLKSIZE=3600)

//FT06F001 DD SYSOUT=A,DCB=(RECFM=FBA,LRECL=133,BLKSIZE=3458),

// SPACE=(3458,(200),RLSE)

//GO.FT08F001 DD UNIT=2311,VOL=SER=THERMO,DISP=SHR,

// DSN=XLACS.RFFF.NFW

//GO.FT09F001 DD UNIT=2311,VOL=SER=THERMO,DISP=(NEW,KEEP),

// DSN=XLACS.BEFF.OLD,

// SPACE=(3520,(20,10),RLSE),

// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=3520)

//FT10F001 DD UNIT=SYSDA,SPACE=(CYL,(1,1))

//GO.FT20F001 DD DSN=NMG.XSDRN.X123,UNIT=2314,VOL=SER=NUCLIB,DISP=SHR

//GO.FT05F001 DD *

3			
23	23		0
2323	2323		0
1154	1154		0

/*

APPENDIX C

An XSDRN Job Setup

```

//XSDRN PROC FT02=NULLFILE,SIZE=450K,DSP3=NEW,DSP4=DELETE 00000010
//LINK EXEC PGM=IEWL,PARM=(MAP,LIST,OVLY),REGION=150K 00000020
//SYSPRINT DD SYSOUT=A 00000030
//SYSUT1 DD UNIT=SYSDA,SPACE=(CYL,(6,1)) 00000040
//SYSLIB DD DSN=SYS1.FORTLIB,DISP=SHR 00000050
//LIB DD DSN=LALIB,DISP=SHR 00000060
//SYSLMOD DD DSN=88FJOB LIB(XSDRN),UNIT=SYSDA,DISP=(NEW,PASS), 00000070
// SPACE=(CYL,(8,1,1),RLSE) 00000080
//SYSLIN DD DDNAME=SYSIN 00000090
// DD DSN=ONLINEA.MLT13803.XSDRN1(M&SIZE),UNIT=2314,VOL=SER=ZZZZZ, 00000100
// DISP=SHR 00000101
// DD DSN=ONLINEA.MLT13803.XSDRN2,UNIT=2314,VOL=SER=ZZZZZ,DISP=SHR 00000110
//XSDRN DD DSN=ONLINEA.MLT13803.PGM,UNIT=2314,VOL=SER=ZZZZZ,DISP=SHR 00000120
//GO EXEC PGM=XSDRN,COND=(5,LT,LINK),REGION=8SIZE 00000130
//STEPLIB DD DSN=88FJOB LIB,DISP=(OLD,DELETE) 00000140
//FT01F001 DD DSN=NMG.XSDRN.X123,UNIT=2314,VOL=SER=NUCLIB,DISP=SHR 00000150
//FT02F001 DD DSN=8FT02,UNIT=TAPE9,LABEL=(,ML),DISP=OLD,VOL=SER=2, 00000160
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=3520) 00000170
//FT03F001 DD DSN=8FT03,UNIT=SYSDA,SPACE=(3520,(400,40)), 00000180
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=3520),DISP=(8DSP3,DELETE) 00000190
//FT04F001 DD DSN=8FT04,UNIT=SYSDA,SPACE=(3520,(400,40)),DISP=(,8DSP4), 00000200
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=3520) 00000210
//FT06F001 DD SYSOUT=A,DCB=(RECFM=FA,BLKSIZE=133) 00000220
//FT07F001 DD SYSOUT=B,DCB=(RECFM=F,BLKSIZE=80) 00000230
//FT08F001 DD UNIT=SYSDA,SPACE=(3604,500) 00000240
//FT09F001 DD UNIT=SYSDA,SPACE=(3604,500) 00000250
//FT12F001 DD UNIT=SYSDA,SPACE=(3520,(400,40)),DCB=*.FT04F001 00000260
//FT18F001 DD UNIT=SYSDA,SPACE=(3520,(400,40)),DCB=*.FT04F001 00000270
//FT19F001 DD UNIT=(SYSDA,SEP=FT18F001),SPACE=(3520,(400,40)), 00000280
// DCB=*.FT04F001 00000290
//FT20F001 DD UNIT=(SYSDA,SEP=(FT18F001,FT19F001)),DISP=(,PASS), 00000300
// SPACE=(3520,(400,40),RLSE),DCB=*.FT04F001,DSN=8LIBOUT 00000310
//FT51F001 DD SYSOUT=A,DCB=*.FT06F001 00000320
// PEND
//FORT EXEC FORTHC
//FORT.SYSIN DD *
COMMON/DATA/D(75000)
CALL XSDRN(75000)
RETURN
END
/*
//XSDRN EXEC XSDRN,REGION.G0=475K
//LINK.F DD DSNNAME=ONLINEA.MLT13803.VS3,UNIT=2314,DISP=SHR, X
// VOL=SER=ZZZZZ
//LINK.G DD DSN=88UT30,DISP=(OLD,DELETE)
//LINK.SYSIN DD *

```

```
INCLUDE F
INCLUDE G
//GO.FT01F001 DD UNIT=2314,VOL=SER=ZX1111,DISP=SHR,
// DSN=MLT.DWC12871.NIOBIUM.WO.ABS.N2NL25.PCT
//GO.FT02F001 DD DSN=80RKN IO,UNIT=SYSDA,DISP=(SHR,PASS),VOL=,LABEL=
//FT05F001 DD *
```

XSDRN INPUT DATA FOLLOWS (SEE REF. 2)

APPENDIX D

ENDF Cross Section Changing

A job which changes ENDF/B cross sections utilizing the subroutine TERP.

```

75
//MLT 6A005 JOB (13803,,,,9999,,,,60),'Y-12 9104-2 TOBIAS',
// MSGLEVEL=(1,1),CLASS=A
//ERASE EXEC PGM=IEHPRGM
//SYSPRINT DD SYSOUT=A
//DDZ DD UNIT=2314,VOLUME=SER=ZX1111,DISP=SHR
//SYSIN DD *
  SCRATCH VOL=2314=ZX1111,
                                DSNAME=MLT.DWC12871.F.N.NPRIME.LO
  SCRATCH VOL=2314=ZX1111,
                                DSNAME=MLT.DWC12871.F.N.NPRIME.HI
/*
//EDIT EXEC LINKGO,PARM.LINK='NOMAP,NOLIST',
// PARM.GO='TIME=2,SI=5,SO=6',
// REGION.GO=256K
//LINK.FT33F001 DD VOL=REF=AZZZZZ,DISP=SHR,
// DSNAME=AA.G4.P36087.C12807.WHITE.EDITOR
//LINK.SYSIN DD *
  INCLUDE FT33F001
//GO.FT17F001 DD DSNAME=LMP.ENDF82,
// DISP=SHR,UNIT=2314,VOL=SER=NUCLIB
//GO.FT16F001 DD UNIT=SYSDA,DCB=(RECFM=VBS,LRECL=X,BLKSIZE=3520),
// SPACE=(3520,(50,20),RLSE),DSN=&FRQW,DISP=(NEW,PASS)
//GO.FT50F001 DD *
  17      3      16      2
  23

  16      1      6      5
  23      -3      1      4      91

/*
//ALTER EXEC FORTHCLG,REGION.GO=256K
//FORT.SYSIN DD *
  DIMENSION X(20)
  DIMENSION X1(200),E1(200),N1(70)
  DIMENSION X4(200),F4(200),N4(70)
  DIMENSION X91(200),E91(200),N91(70),X91H(200),X91L(200),X4H(200)
  DIMENSION X4L(200),X1H(200),X1L(200)
1388  CONTINUE
      LREAD=16
      JLO=1
      JHI=62
      CALL SKIP(JLO,JHI,X,LREAD)
1357  CONTINUE

```

```

      JLO=63
      JHI=110
      CALL READ(JLO, JHI, E1, X1, L1, M3, M1, N1, LREAD)
1358      CONTINUE
      JLO=111
      JHI=166
      CALL SKIP(JLO, JHI, X, LREAD)
1359      CONTINUE
      JLO=167
      JHI=194
      CALL READ(JLO, JHI, E4, X4, L1, M3, M4, N4, LREAD)
1360      CONTINUE
      JLO=195
      JHI=281
      CALL SKIP(JLO, JHI, X, LREAD)
1361      CONTINUE
      JLO=282
      JHI=292
      CALL READ(JLO, JHI, E91, X91, L1, M3, M91, N91, LREAD)
1362      CONTINUE
      K33=33
      K44=144
      K84=84
      NM=2
      CALL TERP(E1, X1, E4, X4, K44, K84, NM)
1363      CONTINUE
      CALL TERP(E4, X4, E91, X91, K84, K33, NM)
1365      CONTINUE
      DO 50 JQ=1, 200
      X4H(JQ)=X4(JQ)
      X1H(JQ)=X1(JQ)
      X4L(JQ)=X4(JQ)
      X1L(JQ)=X1(JQ)
      50      CONTINUE
1366      CONTINUE
      DO 100 JR=1, 33
      X91H(JR)=1.25*X91(JR)
      X91L(JR)=0.75*X91(JR)
      100      CONTINUE
      7      CONTINUE
      NM=-2
      CALL TERP(E4, X4L, E91, X91L, K84, K33, NM)
1367      CONTINUE
      CALL TERP(E4, X4H, E91, X91H, K84, K33, NM)
1368      CONTINUE
      CALL TERP(E1, X1L, E4, X4L, K44, K84, NM)
1369      CONTINUE
      CALL TERP(E1, X1H, E4, X4H, K44, K84, NM)

```

```

1370  CONTINUE
      REWIND 16
      JLO=1
      JHI=62
      LREAD=16
      LWRITE=3
      LWRT2=4
      CALL RDRP(JLO, JHI, X, LREAD, LWRITE, LWRT2)
1371  CONTINUE
      JLO=63
      JHI=110
      CALL SKIP(JLO, JHI, X, LREAD)
      CALL WRITE(JLO, JHI, E1, X1H, L1, M3, M1, N1, LWRITE)
1372  CONTINUE
      LWRITE=4
      CALL WRITE(JLO, JHI, E1, X1L, L1, M3, M1, N1, LWRITE)
1373  CONTINUE
      LWRITE=3
      JLO=111
      JHI=166
      CALL RDRP(JLO, JHI, X, LREAD, LWRITE, LWRT2)
1374  CONTINUE
      JLO=167
      JHI=194
      CALL SKIP(JLO, JHI, X, LREAD)
      CALL WRITE(JLO, JHI, E4, X4H, L1, M3, M4, N4, LWRITE)
1376  CONTINUE
      LWRITE=4
      CALL WRITE(JLO, JHI, E4, X4L, L1, M3, M4, N4, LWRITE)
1377  CONTINUE
      JLO=195
      JHI=281
      LWRITE=3
      CALL RDRP(JLO, JHI, X, LREAD, LWRITE, LWRT2)
1378  CONTINUE
      JLO=282
      JHI=292
      CALL SKIP(JLO, JHI, X, LREAD)
      CALL WRITE(JLO, JHI, E91, X91H, L1, M3, M91, N91, LWRITE)
1379  CONTINUE
      LWRITE=4
      CALL WRITE(JLO, JHI, E91, X91L, L1, M3, M91, N91, LWRITE)
1380  CONTINUE
      JLO=293
      JHI=459
      LWRITE=3
      CALL RDRP(JLO, JHI, X, LREAD, LWRITE, LWRT2)
1381  CONTINUE
      END FILE 3
      END FILE 4
      RETURN
      END

```

```

SUBROUTINE WRITE(JLO,JHI,E1,X1,L1,M3,M1,N1,L4)
  DIMENSION X1(200),E1(200),M1(200)
  J3=0
  J=-2
  DO 260 JJ=JLO,JHI
    J3=J3+1
    J=J+3
    J1=J+1
    J2=J+2
    WRITE(L4,30)(E1(K),X1(K),K=J,J2),L1,M3,M1,N1(J3)
260  CONTINUE
30   FORMAT(3(1PE11.5,1PE11.4),I4,I2,I3,I5)
  RETURN
  END

```

```

SUBROUTINE READ(JLO,JHI,V,W,L,M,N,N4,L1)
DIMENSION V(200),W(200),N4(200)
J3=0
J=-2
DO 210 I=JLO,JHI
J3=J3+1
J=J+3
J1=J+1
J2=J+2
READ(L1,30)(V(K),W(K),K=J,J2),L,M,N,N4(J3).
210 CONTINUE
30  FORMAT(3(1PE11.5,1PE11.4),I4,I2,I3,I5)
RETURN
END

```



```
SUBROUTINE RDRP(JLO,JHI,X,LREAD,LWRITE,LWRIT2)
  DIMENSION X(20)
  DO 250 I=JLO,JHI
    READ(LREAD,20)X
    WRITE(LWRITE,20)X
    WRITE(LWRIT2,20)X
250 CONTINUE
  20 FORMAT(20A4)
    RETURN
  END
```

/*

```

SUBROUTINE TERP(E1,X1,E2,X2,MAX1,MAX,INT)
DIMENSION X1(200),E1(200)
DIMENSION X2(200),E2(200)
XSINT=1.
IF(INT.GT.0)GO TO 24
1382 CONTINUE
XSINT=-1.
1383 CONTINUE
24 CONTINUE
JJ=1
DO 14 J=1,MAX1
IPRIN=0
IF(E1(J).NE.E2(JJ))GO TO 3
X0=X1(J)
X01=X2(JJ)
GO TO 8
3 IF(E1(J).NE.E2(JJ+1))GO TO 5
JK=JJ+1
X0=X1(J)
X01=X2(JK)*XSINT
X1(J)=X1(J)-X01
WRITE(51,44)X1(J),E1(J),X01,X0,X2(JK)
1384 CONTINUE
IF(JK.EQ.MAX)GO TO 6
JJ=JK
GO TO 4
5 IF(E1(J).LT.E2(JJ))GO TO 4
JK=JJ+1
X0=X1(J)
1385 CONTINUE
INX=IABS(INT)
IF(INX.EQ.5)GO TO 7
D1=X2(JK)-X2(JJ)
D2=E2(JK)-E2(JJ)
D3=E1(J)-E2(JJ)
X01=X2(JJ)+(D3/D2)*D1
1386 CONTINUE
GO TO 8
7 D1=ALOG(X2(JK)/X2(JJ))
D2=ALOG(E2(JK)/E2(JJ))
D3=ALOG(E1(J)/E2(JJ))
X2JJ=ABS(X2(JJ))
X=ALOG(X2JJ)+(D3/D2)*D1
1387 CONTINUE
X0=X1(J)
X01=EXP(X)
8 X01=X01*XSINT
X1(J)=X1(J)-X01
WRITE(51,44)X1(J),E1(J),X01,X0,X2(JJ)
4 CONTINUE
14 CONTINUE
6 CONTINUE
44 FORMAT(1H,1P5E13.5)
RETURN
END

```

```
SUBROUTINE SKIP(LOW,LIE,X,LREAD)  
  DIMENSION X(20)  
  DO 200 I=LOW,LIE  
    READ(LREAD,20)  
200  CONTINUE  
  20  FORMAT(20A4)  
  RETURN  
END
```

```

//GO.FT16F001 DD UNIT=SYSDA,DSN=&FRQW,DISP=( SHR, PASS)
//GO.FT03F001 DD UNIT=SYSDA,DCB=(RECFM=VBS,LRECL=X,BLKSIZE=3520),
// SPACE=(3520,(50,20),RLSE),DSN=&FALTH,DISP=( NEW, PASS)
//GO.FT04F001 DD UNIT=SYSDA,DCB=(RECFM=VBS,LRECL=X,BLKSIZE=3520),
// SPACE=(3520,(50,20),RLSE),DSN=&FALTL,DISP=( NEW, PASS)
/*
//EDIT2 EXEC LINKGO,PARM.LINK='NOMAP,NOLIST',
// PARM.GO='TIME=2,SI=5,SO=6',
// REGION.GO=256K
//LINK.FT33F001 DD VOL=REF=AZZZZ,DISP= SHR,
// DSN=AA.G4.P36087.C12807.WHITE.EDITOR
//LINK.SYSIN DD *
INCLUDE FT33F001
//GO.FT02F001 DD UNIT=2314,DCB=(RECFM=VBS,LRECL=X,BLKSIZE=3520),
// SPACE=(3520,(5,1),RLSE),DSN=MLT.DWC12871.F.N.NPRIME.HI,
// VOL=SER=ZX1111,DISP=(NEW,KEEP)
//GO.FT03F001 DD UNIT=2314,DCB=(RECFM=VBS,LRECL=X,BLKSIZE=3520),
// SPACE=(3520,(5,1),RLSE),DSN=MLT.DWC12871.F.N.NPRIME.LO,
// VOL=SER=ZX1111,DISP=(NEW,KEEP)
//GO.FT17F001 DD UNIT=SYSDA,DSN=&FALTH,DISP=( SHR, PASS)
//GO.FT18F001 DD UNIT=SYSDA,DSN=&FALTL,DISP=( SHR, PASS)
//GO.FT50F001 DD *
18 1 3 4
23

3 3 6 5
23 -3 1 4 91

17 1 2 4
23

2 3 6 5
23 -3 1 4 91

/*
//LISTER EXEC LISTER
//FT50F001 DD *
L35,ZX1111,MLT+
/*
//

```

APPENDIX E

A Version of ROSETTA

75

//MLTBD001 JOB (13803,,,,,9999,,,,,60),'Y-12 9104-2 TOBIAS',

// CLASS=D, TYPRUN=HOLD

//ROSET EXEC FORTHCLG, PARM.FORT='XREF', REGION.GQ=256K

//FORT.SYS IN DD *

C***** PROGRAM ROSETTA*****

DIMENSION X(10000)

CALL ERRSET(213,255,-1,0,0)

NS=10000

M=51

NT=NS+1

P=12345

READ(50,507)LD

507 FORMAT(I5)

WRITE(51,508)LD

508 FORMAT('THE NUMBER OF DATA SETS TO BE READ IS',I5//)

DO 506 L=1,LD

LL=L

1 CONTINUE

REWIND L

J=0

READ(50,501)IRS,IRF,IEN

501 FORMAT(3I5)

IRSP1=IRS+1

WRITE(51,509)IRSP1,IRF,LL

509 FORMAT('RECORDS',I6,' TO',I6,' FROM LOGICAL',I3,' FOLLOW'//)

IF(IRS.EQ.0)GO TO 505

DO 503 I=1,IRS

J=J+1

503 READ(L,END=200)

505 CONTINUE

IJ=IRS+1

IF(L.NE.1) GO TO 8000

DO 1504 K=IJ,IRF

DO 1357 N=1,NS

1357 X(N)=12345

KK=K

198 READ(L,END=201)X

J=J+1

IF(K.NE.24) GO TO 7000

M1=33

N1=3

N2=32

N3=30

DO 1500 NG=1,100

M1=M1+1

F=1.1

IF(NG.GT.21.AND.NG.LE.59)F=1.05

IF(NG.GT.59)F=1.03

```

      Q=X(N1)*(1.-F)
      Q=-Q
      X(N1)=X(N1)-Q
      X(N2)=X(N2)-Q
      X(N3)=X(N3)-Q
      N1=N1+M1
      N2=N2+M1
      N3=N3+M1
1500 CONTINUE
7000 DO 22 JJ=1,NS
      JK=NT-JJ
      IF(X(JK).NE.P)GO TO 33
22 CONTINUE
33 WRITE(2)(X(JN),JN=1,JK)
1504 CONTINUE
      IF(L.EQ.1) GO TO 2504
8000 CONTINUE
      DO 504 K=IJ,IRF
      DO357 N=1,NS
357 X(N)=12345
      KK=K
98 READ(L,END=201)X
      J=J+1
      DO2 JJ=1,NS
      JK=NT-JJ
      IF(X(JK).NE.P)GO TO 3
2 CONTINUE
3 WRITE(51,5555)J,JK
6002 WRITE(51,6005)(JN,X(JN),JN=1,JK)
3334 WRITE(51,75)(X(JN),JN=1,33)
      IF(JK.EQ.NS)WRITE (51,5556)
3336 WRITE (51,8888)J
8888 FORMAT(1H0,'END OF RECORD',I6//)
504 CONTINUE
2504 CONTINUE
      IF(IEN.LT.0)GO TO 506
1775 GO TO 1
200 WRITE(51,8)IRS,LL
      GO TO 506
201 WRITE(51,10)LL,KK
506 CONTINUE
5 FORMAT(1H ,6(' (',I5,')',1PE13.5))
8 FORMAT(1H0,30X,'ENDFILE ENCOUNTERED WHILE TRYING TO SKIP',I6,' REC
XORDS ON LOGICAL',I3//)
10 FORMAT(1H0,30X,'ENDFILE ENCOUNTERED TRYING TO READ LOGICAL',I4,',
XRECORD',I6)
75 FORMAT(1H ,18A4/1H ,15I8)
5555 FORMAT(1H , 'RECORD',I6,5X,I6,' ITEMS')

```

```
5556 FORMAT(1H0,'*****WARNING***** ABOVE RECORD MAY REALLY BE LONGER*')
6005 FORMAT(1H,6('(',I6,')',1PE13.5))
```

```
STOP 99
```

```
END
```

```
/*
```

```
//LINK.SYSLIB DD DSN=SYS1.FORTLIB,DISP=SHR
```

```
//GO.FT01F001 DD UNIT=2311,VOL=SER=THERMO,DSN=WORK.G100,DISP=SHR
```

```
//GO.FT02F001 DD UNIT=2311,VOL=SER=THERMO,DSN=WORK.G100.L6NA.LO,
```

```
// SPACE=(3520,(57,10),RLSE),DISP=(NEW,KEEP),
```

```
// DCB=(RECFM=VBS,LRECL=X,RLKSIZE=3520)
```

```
//GO.FT50F001 DD *
```

```
2
```

```
0 100 -1
```

```
0 100 -1
```

```
/*
```