27
10-4-78
256 NT 15

MASTER

MASTER

UCRL-50400
Volume 17, Part B, Rev. 1

**An Integrated System for Production of Neutronics and
Photonics Computational Constants
Volume 17, Part B, Rev. 1**

**PROGRAM SIGMA1 (VERSION 78-1): DOPPLER BROADEN
EVALUATED CROSS SECTIONS IN THE EVALUATED
NUCLEAR DATA FILE/VERSION B
(ENDF/B) FORMAT**

D. E. Cullen

July 4, 1978

Work performed under the auspices of the U.S. Department of
Energy by the UCLLL under contract number W 7405-ENG-48

**LAWRENCE
LIVERMORE
LABORATORY**
University of California, Livermore

LAWRENCE LIVERMORE LABORATORY

University of California Livermore, California 94550

UCRL-50400 Volume 17, Part B, Rev. 1

PROGRAM SIGMA1 (VERSION 78-1): DOPPLER BROADEN EVALUATED CROSS SECTIONS IN THE EVALUATED NUCLEAR DATA FILE/VERSION B (ENDF/B) FORMAT

D. E. Cullen

MS. date: July 4, 1978

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Notwithstanding, neither the United States Government nor the United States Department of Energy, nor any of its employees, nor any of its contractors, agents, or subcontractors, nor any of them, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, or method disclosed, or represents that its use would not infringe upon privately owned copyrights.

Foreword

The total cross section probability (TCP) system is designed to process evaluated neutron cross section data into a continuous energy or multigroup form. In the following figure, we have described the function of each of the computer codes in the TCP system by contrasting the form of the data before and after code processing.

Contents

Abstract	1
1978 Edition	1
Method	1
Doppler Broadening	1
Bootstrapping	4
Representations of Broadened Cross Sections	5
Truncating the Integration Range	7
Limitations and Assumptions	9
Requirements	10
Input Cards	11
Example Output	11
Error Messages	19
Operation at LLL	19
Conversion to Other Installations	20
Program Listing	21
Acknowledgments	45
1978 Edition	45
References	46

PROGRAM SIGMA1 (VERSION 77-1): DOPPLER BROADEN EVALUATED CROSS SECTIONS IN THE EVALUATED NUCLEAR DATA FILE/VERSION B (ENDF/B) FORMAT

Abstract

We have designed a code, SIGMA1, to Doppler broaden evaluated cross sections in the ENDF/B format. The code can only be applied to data that vary as a linear function of energy and cross section between tabulated points. This report describes the methods used in the code and serves as a user's guide to the code.

1978 Edition

This edition of the program has been designed for operation at Lawrence Livermore Laboratory on a CDC-7600 computer, but it can easily be converted for use at other installations. This edition includes improvements and corrections suggested by numerous users of earlier versions of the code. The code has been changed to ease the use of double precision on shorter word length computers (e.g. IBM-360) and to allow more efficient use of the scratch file. In addition, the underflow problem that occurred in earlier versions has been eliminated and coding added to properly broaden threshold reactions to controlled thermonuclear reactor (CTR) temperatures.

Method

DOPPLER BROADENING

Doppler broadening refers to a change in cross section resulting from thermal motion, rotation, and vibration of nuclei in a target material. The SIGMA1 method¹ may be used to Doppler broaden cross sections for any particle (e.g., neutron, proton, deuteron, etc.) incident at nonrelativistic energies upon a target in which the free-atom approximation is valid.

The SIGMA1 method is extensively described in Ref. 1. We have briefly described the method below, starting from the well known free-atom Doppler broadening equations in which energy [Eq. (1)] and speed [Eq. (2)] are the independent variables:

$$\sqrt{E}\sigma(E,T) = \frac{1}{2} \left(\frac{\alpha}{\pi E} \right)^{1/2} \int_0^\infty [\sqrt{E_r} \sigma(E_r, 0)] dE_r \{ \exp[-\alpha(\sqrt{E} - \sqrt{E_r})^2] - \exp[-\alpha(\sqrt{E} + \sqrt{E_r})^2] \} \quad (1)$$

$$V\sigma(V,T) = \frac{1}{V} \left(\frac{\beta}{\pi} \right)^{1/2} \int_0^\infty [V_r \sigma(V_r, 0)] V_r dV_r \{ \exp[-\beta(V - V_r)^2] - \exp[-\beta(V + V_r)^2] \} \quad (2)$$

where

$$\alpha = \frac{\lambda}{kT} : \beta = \frac{M}{2kT} : A = \frac{M}{m}$$

and

m = projectile mass (e.g., neutron, proton, alpha, etc.)

$\bar{V}$ = projectile velocity

$V = |\bar{V}|$ = projectile speed

$E = \frac{1}{2}mV^2$ = projectile energy

M = target nuclei mass

$\bar{V}_T$ = target velocity

$V_T = |\bar{V}_T|$ = target speed

$E_T = \frac{1}{2}MV_T^2$ = target energy

$A = M/m$ = atomic weight ratio (target mass/projectile mass)

$\bar{V}_r = \bar{V} - \bar{V}_T$ = relative velocity

$V_r = |\bar{V}_r|$ = relative speed

$E_r = \frac{1}{2}mV_r^2$ = relative energy of the neutron as "seen" by the target

$\sigma(V,0)$ = cold (0 K) cross section

$\sigma(V,T)$ = Doppler broadened cross section

By changing variables in Eq. (2) so that

$$y^2 = \alpha E = \beta V^2$$

$$x^2 = \alpha E_r = \beta V_r^2 \quad (3)$$

the Doppler broadening equation becomes

$$\sigma(y, T_2) = \frac{1}{y^2} \left(\frac{1}{\pi} \right)^{1/2} \int_0^{\infty} x^2 \sigma(x, T_1) \{ \exp[-(x-y)^2] - \exp[-(x+y)^2] \} dx. \quad (4)$$

The ensuing development can be simplified by defining

$$\sigma^*(y, T_2) = \frac{1}{y^2} \left(\frac{1}{\pi} \right)^{1/2} \int_0^{\infty} x^2 \sigma(x, T_1) \exp[-(x-y)^2] dy \quad (5)$$

and noting that the Doppler broadened cross section is

$$\sigma(y, T_2) = \sigma^*(y, T_2) - \sigma^*(-y, T_2). \quad (6)$$

Next, we will assume that the cross section to be Doppler broadened is given as a table of cross sections and their corresponding energies. Values between the tabulated points will be assumed to vary as a linear function of energy and cross section:

$$\sigma(E, T_1) = \left[\frac{E - E_k}{E_{k+1} - E_k} \right] \sigma_{k+1} + \left[\frac{E_{k+1} - E}{E_{k+1} - E_k} \right] \sigma_k = A_k + B_k E \quad : \quad E \in (E_k, E_{k+1}) \quad (7)$$

$$\sigma(x, T_1) = A_k + C_k x^2 \quad : \quad x \in (x_k, x_{k+1}). \quad (8)$$

Since tabulated cross sections span only a finite energy range (e.g., 10^{-5} eV to 20 MeV), we will also assume that the cross section will be continued as constant outside the range of the table. If we make these two assumptions (data within the energy range of the table are linear; data outside the energy range of the table are constant), then Eq. (5) becomes

$$\sigma^*(y, T_2) = \frac{1}{y^2} \left(\frac{1}{\pi} \right)^{1/2} \sum_k \int_{x_k}^{x_{k+1}} x^2 (A_k + C_k x^2) \exp[-(x-y)^2] dx. \quad (9)$$

By changing variables to $Z = x - y$ and collecting terms in powers of Z , we get

$$\begin{aligned} \sigma^*(y, T_2) = \frac{1}{y^2} \left(\frac{1}{\pi} \right)^{1/2} \sum_k \int_{x_k}^{x_{k+1}-y} [C_k Z^4 + 4C_k y Z^3 + (A_k + 6C_k y^2) Z^2 + (2A_k y + 4C_k y^3) Z \\ + (A_k y^2 + C_k y^4)] \exp(-Z^2) dZ. \end{aligned} \quad (10)$$

Equation (10) can be defined exactly in terms of the functions

$$H^n(a,b) = F^n(a) - F^n(b) \quad (11)$$

$$F^n(a) = \frac{2}{\sqrt{\pi}} \int_0^a z^n \exp(-z^2) dz \quad (12)$$

where

$$n = 0, 1, 2, 3, 4.$$

These functions can easily be shown to satisfy the recursion relationship

$$F^n(a) = \frac{(n-1)}{2} F^{n-2}(a) - \left(\frac{1}{\pi}\right)^{1/2} a^{n-1} \exp(-a^2) + \left(\frac{1}{\pi}\right)^{1/2} \delta_{n,1}. \quad (13)$$

By explicitly evaluating Eq. (12) for $n = 0$ and 1, as well as by applying the recursion relationship, we can derive the required functions

$$\begin{aligned} F^0(a) &= \text{ERF}(a) \\ F^1(a) &= \left(\frac{1}{\pi}\right)^{1/2} [1 - \exp(-a^2)] \\ F^2(a) &= \frac{1}{2} \text{ERF}(a) - \frac{a}{\sqrt{\pi}} \exp(-a^2) \\ F^3(a) &= \left(\frac{1}{\pi}\right)^{1/2} [1 - (1 + a^2) \exp(-a^2)] \\ F^4(a) &= \frac{3}{4} \text{ERF}(a) - \left(\frac{1}{\pi}\right)^{1/2} \left(\frac{3a}{2} + a^3\right) \exp(-a^2). \end{aligned} \quad (14)$$

With the definition of these functions, the algorithm describing the Doppler broadened cross section at any arbitrary energy is complete.

BOOTSTRAPPING

The Doppler broadening equations can be slightly generalized by recognizing that not only can they be used to broaden cross sections from 0 K to a temperature T K, but can also be used to broaden cross sections from any temperature T_1 K to any higher temperature T_2 K (Ref. 2). For example, it is possible to start from experimentally measured data at room temperature (293 K) and Doppler broaden it to 600 K, which in turn can be broadened to 1000 K, etc. For each of these steps to be independent, the Doppler broadening equations must be in the laboratory system (as opposed to the center-of-mass system) and the above definition of E_r must be used. The generalized equations are:

$$v\sigma(v, T_2) = \frac{1}{v} \left(\frac{E}{E_r}\right)^{1/2} \int_0^\infty [V_r \sigma(V_r, T_1)] V_r dv_r \{ \exp[-\beta(v - V_r)^2] - \exp[-\beta(v + V_r)^2] \};$$

$$\beta = \frac{M}{2k(T_2 - T_1)} \quad , \quad (15)$$

$$\sqrt{E}\sigma(E, T_2) = \frac{1}{2} \left(\frac{E}{E_r}\right)^{1/2} \int_0^\infty [\sqrt{E_r} \sigma(E_r, T_1)] dE_r \times \{ \exp[-\alpha(\sqrt{E} - \sqrt{E_r})^2] - \exp[-\alpha(\sqrt{E} + \sqrt{E_r})^2] \};$$

$$\alpha = \frac{A}{k(T_2 - T_1)} \quad , \quad (16)$$

where the V_r and E_r associated with the T_1 K cross sections $\sigma(V_r, T_1)$ and $\sigma(E_r, T_1)$ are merely the laboratory speed and energy of the neutron, respectively.

REPRESENTATIONS OF BROADENED CROSS SECTIONS

If the programs that produce multigroup and continuous Monte Carlo data from evaluated cross-section libraries (the library data being subject to linear-linear interpolation) are to be applicable to Doppler broadened cross sections, the latter cross sections must also be subject to linear-linear interpolation. Although the Doppler broadening algorithm described above allows the cross section to be calculated at any given energy, it does not guarantee that the broadened cross section is subject to linear-linear interpolation between any two given energies. Use of an iterative scheme, such as interval halving, can be prohibitively expensive. Use of the same energy grid that was used to represent the unbroadened cross section can lead to pitfalls. For example, the 0-K hydrogen-elastic cross section is roughly 20 barns from 10^{-5} eV to 1 keV. Linear variation in energy and cross section can be used to define the 0-K cross section from 10^{-5} eV to 1 keV and to calculate Doppler-broadened cross sections at 10^{-5} eV and 1 keV. The broadened cross section is certainly not subject to linear-linear interpolation between these two energies. Large errors will result if a multigroup processing code assumes that it is. Figure 1 illustrates this error by comparing linear-linear variation to a $1/v$ cross section variation between 0.01 and 100 eV. The figure speaks for itself as far as the errors that would occur.

Although Doppler broadening is a smoothing process, it is the reaction rate, not the cross section, that is becoming smoother. Therefore, if the energy grid that represents the unbroadened reaction rate is sufficiently dense, the smoother Doppler broadened reaction rate can be adequately represented on

the same energy grid. At higher energies ($av \gg 1$), this smoothing process applies equally well to the cross section. However, at lower energies, although the reaction rate is becoming smoother, the same may not be true of the cross section because the two differ by a factor of $1/V$ [i.e., $\sigma(V,T) = R(V,T)/V$]. To ensure that this low-energy $1/V$ tail does not prevent the cross section from being in a form subject to linear-linear interpolation, all we have to do is choose an energy grid for the broadened data that is the same as the energy grid for the unbroadened data, except that the latter is supplemented by an additional set of energy points. These additional points should be added in such a way that between any two energy points of the final energy grid, the difference between linear-linear and $1/V$ variations in the cross section is always less than some allowable error ϵ .

Consider two possible representations of the same cross section: a $1/V$ variation and a linear-linear variation in energy. By insisting that the two representations agree exactly at the two ends of an interval V (V_1, V_2) and that $V_2 = SV_1$, we get

$$\sigma_1(V) = \frac{1}{V} \quad (1/V \text{ variation})$$

$$\sigma_2(V) = \frac{1}{V} - \frac{(V^2 - V_1^2)}{V_1^3 S(S+1)} \quad \left(\begin{array}{l} \text{linear-linear in} \\ \text{cross section-energy} \end{array} \right)$$

$$V \in (V_1, SV_1). \quad (17)$$

Fig. 1. Linearized $1/V$ cross section.

The fractional difference between these two representations is

$$\delta(V) = \frac{\sigma_1(V) - \sigma_2(V)}{\sigma_1(V)} = 1 - \frac{V^3 - V_1^2}{V_1^3 S(S+1)} - \frac{V}{V_1}$$

and the variation in the fractional difference is

$$\frac{d\delta}{dV}(V) = \frac{3V^2 - V_1^2}{V_1^3 S(S+1)} - \frac{1}{V_1} \quad (18)$$

Therefore, the point of maximum difference and the value of the difference at that point are

$$V_{\max} = V_1 \left[\frac{1}{3} (1 + S + S^2) \right]^{1/2}$$

$$\delta(V_{\max}) = 1 - \left(\frac{2}{3} \right) \left(\frac{1}{3} \right)^{1/2} \frac{(1 + S + S^2)^{3/2}}{S(S+1)} \quad (19)$$

Note $\delta(V_{\max})$ is independent of V , and only depends on s , the spacing between tabulated points. This means that a $1/V$ variation can be represented by a linear-linear variation in energy to within any allowable error ϵ , simply by ensuring that the energies for successive tabulated values are within $S^2\epsilon$ of one another (independent of E).

Table 1 illustrates the typical factor (ϵ) required for a number of allowable tolerances (δ), when ϵ is in the range 0.1 to 2.0. The table also shows the number of points that would be required to space points $S^2\epsilon$ apart between 10^{-5} eV and 20 MeV. For example, an allowable tolerance of 0.5% would require 124 points or roughly 10 per energy decade.

Therefore, to ensure that the Doppler broadened cross sections are subject to linear-linear interpolation, we must start from the same energy points as the 0-K data and supplement this grid in any interval where the points are more widely spaced than $S^2\epsilon$ (where S^2 depends on the allowable error ϵ).

TRUNCATING THE INTEGRATION RANGE

Although the algorithm as previously described can exactly evaluate the Doppler broadened cross section, it can be a costly procedure since the calculational time can vary as the square of the number of points used to represent a given reaction. To reduce the cost, we can use the strongly convergent

Gaussian character of the Doppler broadening kernel to truncate the Doppler broadening integral. Because of the exponential term $\exp[-(x - y)^2]$ [see Eq. (5)], the major contribution to the integral $x \in (0, \infty)$ is from an interval centered about y ; the interval is defined by $x \in (y - N, y + N)$. Therefore, it is only necessary to integrate over this interval. The truncation procedure should recognize that although $\exp[-(x - y)^2]$ is rapidly decreasing, the term $x^2 \sigma(x, T)$ may be rapidly increasing, particularly $\sigma(x, T)$ in the resonance region. Therefore, the truncation procedure should be:

$$\int_0^\infty x^2 \sigma(x, T) \exp[-(x - y)^2] dx = \int_{y-N}^{y+N} x^2 \sigma(x, T) \exp[-(x - y)^2] dx + R(y), \quad (20)$$

Table 1. Linear-Linear approximation of a $1/V$ cross section.

Tolerance	Factor	Points ^a
0.001	1.0530	276
0.002	1.0757	195
0.003	1.0935	160
0.004	1.1087	139
0.005	1.1223	124
0.006	1.1347	114
0.007	1.1463	105
0.008	1.1571	99
0.009	1.1674	93
0.010	1.1772	88
0.011	1.1865	84
0.012	1.1956	81
0.013	1.2043	78
0.014	1.2128	75
0.015	1.2210	72
0.016	1.2290	70
0.017	1.2367	68
0.018	1.2444	66
0.019	1.2518	65
0.020	1.2591	63

^a Points span 10^{-5} eV to 20 MeV.

$$R(y) = \int_0^{y-N} x^2 \sigma(x, T) \exp[-(x-y)^2] dx + \int_{y+N}^{\infty} x^2 \sigma(x, T) \exp[-(x-y)^2] dx \quad (21)$$

$$R(y) = 2 \cdot \sigma \cdot \int_N^{\infty} (Z+y)^2 \exp(-Z^2) dZ \quad (22)$$

If we assume that the cross section will vary no more than four orders of magnitude (10^4) and that the error will be no more than 0.1%, then we can safely truncate the integral when $N = 4$. Thus, the truncated integral should only be extended over those intervals in which at least one end is within four units of y . In particular, the second term $\sigma^*(-y, T_2)$ [Eq. (6)] need not be calculated unless $y \leq 4$.

Limitations and Assumptions

The program nonselectively Doppler broadens all sections of file 3 data on the original ENDF/B format tape (i.e., all sections between the tape label card and the tape end card),³ except for the parameters $\bar{\mu}$, $\bar{\epsilon}$, and γ (MT = 251-253). This program does not require the evaluations to be in MAT³ order; e.g., they may be in ZA order.

The program only uses the ENDF/B BCD format (as opposed to binary) and copies all sections except file 3 as hollerith. As such, the program may be used on data in the ENDF/B - I, II, III, IV or V format, since all sections of file 3 data are identical in all ENDF/B versions.

The program reads and Doppler broadens the data a page at a time, so there is no limit to the number of points in any section (i.e., each section may be described by any number of points - up to 500 000 points).

The program is written entirely in FORTRAN-IV and can be easily modified to run on any medium-sized computer.

We recommend the LINEAR program as the best way to linearize data in the ENDF/B format.⁴ If the data do not vary as a linear function of energy and cross section between tabulated points, the program will check the interpolation law and abort.

During Doppler broadening, three pages of data are core resident: the page being broadened, the page below it in energy, and the page above it in energy. If at any time the integral extends beyond the limits of these pages, the cross section is extended as a constant and an "EXTENSION" warning message is printed out, advising the user of the maximum temperature step allowable to avoid "EXTENSION." In this case we recommend rerunning the program by boot-

strapping the cross section up to the final temperature, in temperature steps smaller than or equal to that recommended in the "EXTENSION" message.

The program will automatically select the energy grid consistent with the input allowable error to avoid problems resulting from the onset of the low energy 1/V cross section. If an allowable error of less than 0.1% is specified, it will be used for output thinning, but maximum energy point spacing will be limited to 0.1%.

If the original ENDF/B data are given at a temperature that is higher than the final temperature, the section will not be Doppler broadened and the original temperature will be left in the section. If the original ENDF/B data are given at a temperature between 0 K and the final temperature, the program will broaden the data by the temperature difference (see Bootstrapping).

In the unresolved resonance region, starting from energy-averaged cross sections the SIGMA1 algorithm will conserve the averages and return the same values. This program does not use unresolved parameters directly.

Requirements

The I/O units are defined as follows:

<u>Filename</u> *	<u>Unit</u>	<u>Description</u>
INPUT	5	Input card
OUTPUT	6	Output report
ENDFIN	21	Evaluated data to be Doppler broadened in the ENDF/B format
ENDFOUT	22	Doppler broadened evaluated data in the ENDF/B format
SCRATCH	23	Scratch file

All read and write statements use variable I/O unit numbers. To convert to any other set of unit numbers, it is necessary to redefine the unit numbers as described in the program listing.

The program, when run on the Livermore CDC-7600, requires 21 000 words of small core memory and 6 000 words of large core memory (I/O buffers). It takes 0.7 min to Doppler broaden ENDF-78⁵ tape 6 from 0 to 300 K and to thin the output to 0.1% accuracy [it takes 7.92 min to Doppler broaden the entire

* The filenames apply to the program run at Livermore. Disk files that have these names will be used by the program.

ENDL-76⁵ library (88 complete evaluations) from 0 to 300 K and thin the output to 0.1% accuracy].

Input Cards

The program requires a single input card to define the allowable fractional error and temperature to which cross sections should be broadened.

Card	Columns	Format	Description
1	1 - 11	E11.4	Fractional output thinning criteria
	12 - 22	E11.4	Output Kelvin temperature

To Doppler broaden to 300 K and thin the output to 0.1% the following input card is required:

1.0000E-03 3.0000E+02

A 0.0 thinning criteria means that there will not be any output thinning but there will be maximum output spacing in order to keep the result within 0.1% of 1/V.

Example Output

Table 2 presents the output that results from Doppler broadening ENL-76 tape 6 to 300 K and thinning the output to 0.1%. Figures 2 through 5 illustrate the wide range of applications of the SIGMA code. Note that it can be applied to Doppler broadening at

- Reactor core-like temperatures (300 - 10000 K) (Fig. 2)
- Controlled thermonuclear reactor core and stellar temperatures (1 eV-10 keV)* (Fig. 3)
- Initially constant cross sections from 0.01 eV to 10 MeV (Fig. 4)
- Initially 1/V cross section from 0.01 eV to 10 MeV (Fig. 5)

* For those who are unfamiliar with the convention of expressing temperature in eV, note the unit of KT is energy and can be used to describe temperature (e.g., 1 eV $\sim$ 12 000 K; 10 keV $\sim$ 1.2×10^8 K).

Table 2. Example output listing.

1 DOPPLER BROADEN ENDF/B CROSS SECTIONS (SIGMA1 78-1)									
THINNING CRITERIA-- 1.00000- 3									
TEMPERATURE----- 3.00000+ 2 KELVIN									
TAPE LABEL									
LAWRENCE LIVERMORE EVALUATED LIBRARY (ENDL) 6/01/78									
ZA	MAT	MT	KELVIN		Q-VALUE		POINTS		POINTS
			IN		EV		IN		OUT
90231	7863	1	0.	+ 0	0.	+ 0	246		320
90231	7863	2	0.	+ 0	0.	+ 0	43		72
90231	7863	4	0.	+ 0	0.	+ 0	22		22
90231	7863	16	0.	+ 0	-5.12000+	6	19		19
90231	7863	17	0.	+ 0	-1.19100+	7	11		11
90231	7863	18	0.	+ 0	1.80000+	8	152		195
90231	7863	37	0.	+ 0	-1.71500+	7	5		4
90231	7863	91	0.	+ 0	0.	+ 0	22		22
90231	7863	102	0.	+ 0	6.43000+	6	138		183
90231	7863	251	0.	+ 0	0.	+ 0	20		20
90231	7863	252	0.	+ 0	0.	+ 0	20		19
90231	7863	253	0.	+ 0	0.	+ 0	20		19
MAT TOTALS							718		806
90232	7864	1	0.	+ 0	0.	+ 0	6261		5323
90232	7864	2	0.	+ 0	0.	+ 0	2983		2898
90232	7864	4	0.	+ 0	0.	+ 0	62		51
90232	7864	16	0.	+ 0	-6.34000+	6	17		16
90232	7864	17	0.	+ 0	-1.15600+	7	8		8
90232	7864	18	0.	+ 0	1.70000+	8	34		34
90232	7864	37	0.	+ 0	-1.63500+	7	2		2
90232	7864	91	0.	+ 0	0.	+ 0	62		51
90232	7864	102	0.	+ 0	4.79000+	6	5535		5451
90232	7864	251	0.	+ 0	0.	+ 0	14		13
90232	7864	252	0.	+ 0	0.	+ 0	14		14
90232	7864	253	0.	+ 0	0.	+ 0	14		13
MAT TOTALS							15006		13874
90233	7865	1	0.	+ 0	0.	+ 0	296		219
90233	7865	2	0.	+ 0	0.	+ 0	43		72
90233	7865	4	0.	+ 0	0.	+ 0	21		21
90233	7865	16	0.	+ 0	-4.78000+	6	19		19
90233	7865	17	0.	+ 0	-1.12200+	7	14		14
90233	7865	18	0.	+ 0	1.80000+	8	130		174
90233	7865	37	0.	+ 0	-1.63400+	7	5		4
90233	7865	91	0.	+ 0	0.	+ 0	21		21
90233	7865	102	0.	+ 0	6.18000+	6	121		157
90233	7865	251	0.	+ 0	0.	+ 0	16		15
90233	7865	252	0.	+ 0	0.	+ 0	16		15
90233	7865	253	0.	+ 0	0.	+ 0	16		16
MAT TOTALS							718		747
92233	7866	1	0.	+ 0	0.	+ 0	2884		2353
92233	7866	2	0.	+ 0	0.	+ 0	343		352
92233	7866	4	0.	+ 0	0.	+ 0	32		30
92233	7866	16	0.	+ 0	-5.90000+	6	12		11

Table 2. (Continued).

92233	7866	17	0.	+ 0	-1.31800+ 7	6	5
92233	7866	18	0.	+ 0	1.80000+ 8	1613	1608
92233	7866	91	0.	+ 0	0.	32	30
92233	7866	102	0.	+ 0	6.84000+ 6	1954	1949
92233	7866	251	0.	+ 0	0.	21	21
92233	7866	252	0.	+ 0	0.	21	21
92233	7866	253	0.	+ 0	0.	21	20
				MAT TOTALS			
				6939 6400			
92234	7867	1	0.	+ 0	0.	188	190
92234	7867	2	0.	+ 0	0.	37	57
92234	7867	4	0.	+ 0	0.	19	17
92234	7867	16	0.	+ 0	-6.84000+ 6	13	13
92234	7867	17	0.	+ 0	-1.25900+ 7	7	7
92234	7867	18	0.	+ 0	1.80000+ 8	40	40
92234	7867	91	0.	+ 0	0.	19	17
92234	7867	102	0.	+ 0	5.31000+ 6	128	166
92234	7867	251	0.	+ 0	0.	29	28
92234	7867	252	0.	+ 0	0.	29	29
92234	7867	253	0.	+ 0	0.	29	27
				MAT TOTALS			
				538 591			
92235	7868	1	0.	+ 0	0.	2294	2292
92235	7868	2	0.	+ 0	0.	235	264
92235	7868	4	0.	+ 0	0.	25	25
92235	7868	16	0.	+ 0	-5.23000+ 6	16	16
92235	7868	17	0.	+ 0	-1.20000+ 7	7	7
92235	7868	18	0.	+ 0	1.80000+ 8	1511	1585
92235	7868	37	0.	+ 0	-1.78900+ 7	3	3
92235	7868	91	0.	+ 0	0.	25	25
92235	7868	102	0.	+ 0	6.55000+ 6	767	837
92235	7868	251	0.	+ 0	0.	29	27
92235	7868	252	0.	+ 0	0.	29	29
92235	7868	253	0.	+ 0	0.	29	27
				MAT TOTALS			
				4970 5137			
92236	7869	1	0.	+ 0	0.	179	176
92236	7869	2	0.	+ 0	0.	35	58
92236	7869	4	0.	+ 0	0.	21	19
92236	7869	16	0.	+ 0	-6.56000+ 6	14	14
92236	7869	17	0.	+ 0	-1.18500+ 7	8	8
92236	7869	18	0.	+ 0	1.80000+ 8	40	71
92236	7869	91	0.	+ 0	0.	21	19
92236	7869	102	0.	+ 0	5.12000+ 6	127	183
92236	7869	251	0.	+ 0	0.	29	28
92236	7869	252	0.	+ 0	0.	29	29
92236	7869	253	0.	+ 0	0.	29	28
				MAT TOTALS			
				532 633			
92237	7870	1	0.	+ 0	0.	299	206
92237	7870	2	0.	+ 0	0.	45	68
92237	7870	4	0.	+ 0	0.	31	30
92237	7870	16	0.	+ 0	-5.12000+ 6	11	11
92237	7870	17	0.	+ 0	-1.16700+ 7	7	7
92237	7870	18	0.	+ 0	1.80000+ 8	104	132
92237	7870	91	0.	+ 0	0.	31	30

Table 2. (Continued).

92237	7870	102	0.	+ 0	6.14000+	6	173	214
92237	7870	251	0.	+ 0	0.	+ 0	21	20
92237	7870	252	0.	+ 0	0.	+ 0	21	21
92237	7870	253	0.	+ 0	0.	+ 0	21	21
MAT TOTALS							764	760
92238	7871	1	0.	+ 0	0.	+ 0	1744	1565
92238	7871	2	0.	+ 0	0.	+ 0	453	464
92238	7871	4	0.	+ 0	-4.50000+	4	72	61
92238	7871	16	0.	+ 0	-6.04000+	6	15	15
92238	7871	17	0.	+ 0	-1.14500+	7	9	9
92238	7871	18	0.	+ 0	1.80000+	8	4	40
92238	7871	37	0.	+ 0	-1.78200+	7	3	3
92238	7871	51	0.	+ 0	-4.50000+	4	21	21
92238	7871	52	0.	+ 0	-1.48000+	5	13	13
92238	7871	53	0.	+ 0	-3.08000+	5	8	8
92238	7871	54	0.	+ 0	-6.80000+	5	17	17
92238	7871	55	0.	+ 0	-7.32000+	5	16	16
92238	7871	56	0.	+ 0	-8.27000+	5	13	13
92238	7871	57	0.	+ 0	-9.30000+	5	14	14
92238	7871	58	0.	+ 0	-9.67000+	5	12	12
92238	7871	59	0.	+ 0	-1.00000+	6	12	12
92238	7871	60	0.	+ 0	-1.04100+	6	12	12
92238	7871	61	0.	+ 0	-1.06000+	6	12	12
92238	7871	62	0.	+ 0	-1.12000+	6	12	12
92238	7871	63	0.	+ 0	-1.16000+	6	10	10
92238	7871	64	0.	+ 0	-1.22000+	6	11	11
92238	7871	65	0.	+ 0	-1.27000+	6	10	10
92238	7871	66	0.	+ 0	-1.30000+	6	9	9
92238	7871	67	0.	+ 0	-1.36000+	6	9	9
92238	7871	68	0.	+ 0	-1.41900+	6	8	8
92238	7871	69	0.	+ 0	-1.43700+	6	9	9
92238	7871	70	0.	+ 0	-1.47000+	6	11	11
92238	7871	71	0.	+ 0	-1.62500+	6	13	13
92238	7871	72	0.	+ 0	-1.87500+	6	11	11
92238	7871	91	0.	+ 0	0.	+ 0	22	22
92238	7871	102	0.	+ 0	4.80000+	6	1473	1519
92238	7871	251	0.	+ 0	0.	+ 0	28	27
92238	7871	252	0.	+ 0	0.	+ 0	28	26
92238	7871	253	0.	+ 0	0.	+ 0	28	25
MAT TOTALS							4179	4039
TAPE TOTALS							34364	32987

Fig. 3. Doppler broadening of the cross section in Fig. 2. to stellar or CTR core temperatures ($KT = 0$ to 10 keV; $T = 0$ to $\sim 1.2 \times 10^8$ K).

Fig. 4. Doppler broadening of an initially constant cross section from temperatures of 1 eV to 1 MeV. The results agree with theoretical predictions over the entire energy range.

Fig. 5. Doppler broadening of an initially $1/V$ cross section. Although the cross section should be temperature independent, it does not deviate until well above 100 keV — and then only at extremely low energies.

Error Messages

In the following error messages the underlined items are variables.

EXTENSION

CROSS SECTION EXTENSION CAN BE AVOIDED BY THINNING DATA OR DOPPLER BROADENING IN STEPS OF LESS THAN 2.7419+6 KELVIN

The Doppler integrals have extended beyond the three pages of core resident data. This normally occurs only for large temperature changes. Doppler broaden to the final temperature in steps (in the above example each step is not to exceed about 2.7×10^6 K).

INTERPOLATION LAW IS NOT LINEAR-LINEAR

EXECUTION TERMINATED

The data in the ENDF/B format must be subject to linear-linear interpolation for valid Doppler broadening by SIGMA1. Convert the data to linear-linear form using program LINEAR.⁴

SCRATCH MAXIMUM PAGE COUNT EXCEEDED

EXECUTION TERMINATED

The scratch disk file is designed to allow each section to include up to 500 000 points. In the unlikely event that this limit is exceeded, this error message is printed out.

Operation at LLL

At Livermore a compiled, loaded, ready-to-execute version of the program is available from the photostore as file

.19:025:PROGRAMS:SIGMA1

The program is small enough (21 000 words of SCM, 6 000 words of LCM) to run at standby during the daytime as file

SIGMA1 / 1 S

The program will automatically use disk files as illustrated in Fig. 6.

Fig. 6. Linear operations.

Conversion to Other Installations

This edition of the code is designed for operation at Lawrence Livermore Laboratory on a Cdc-7600 computer. It uses special I/O routines to avoid the inefficiency of FORTRAN binary reads and writes. All points in the code that use these special routines are preceded and followed by comment cards of the form,

C**** LTSS*****

to indicate the Livermore time sharing system. For conversion to standard FORTRAN binary I/O, the required statements are included in the program as comment cards and can easily be activated. Alternatively, by recognizing all of these points one can easily implement his own direct disk access routines, which are equivalent to those used at Livermore. If FORTRAN binary I/O is used, subroutines

IONAME

FILE IO

WAIT

are not required.

Program Listing

```

PROGRAM SIGMA1 (INPUT,OUTPUT,TAPES=INPUT,TAPE6=OUTPUT,
1 TAPE21,TAPE22)
C**** LTSS *****
C FORTRAN BINARY I/O REQUIRES AN ADDITIONAL UNIT (TAPE23)
C 1 TAPE21,TAPE22,TAPE23)
C**** LTSS *****
C
C PROGRAM SIGMA1
C VERSION 73-1 (MARCH 1973)
C VERSION 76-1 (FEBRUARY 1976)
C VERSION 76-2 (OCTOBER 1976)
C VERSION 77-1 (JANUARY 1977) (REPORT UCRL-50400, VOL. 17, PART B)
C VERSION 78-1 (JULY 1976)
C
C WRITTEN BY DERMOTT E. CULLEN
C L-71
C UNIVERSITY OF CALIFORNIA
C LAWRENCE LIVERMORE LABORATORY
C P.O. BOX 808
C LIVERMORE, CALIFORNIA
C TELEPHONE 415-447-1100 X-3134
C
C THIS PROGRAM IS DESIGNED TO READ SECTIONS OF FILE 3 ENDF/B
C DATA THAT HAVE ALREADY BEEN CONVERTED TO LINEAR-LINEAR
C INTERPOLATION IN ENERGY AND CROSS SECTION. THE DATA IS THEN
C DOPPLER BROADENED, THINNED AND OUTPUT IN THE ENDF/B FORMAT.
C
C THIS PROGRAM ONLY USES THE ENDF/B BCD FORMAT AND COPIES ALL
C SECTIONS EXCEPT FILE 3 AS HOLLERITH. AS SUCH IT MAY BE USED ON
C DATA IN THE ENDF/B-1, II, III, IV OR V FORMAT (SINCE A SECTION
C OF FILE 3 DATA IS IDENTICAL IN ALL ENDF/B VERSIONS).
C
C THE PROGRAM OPERATES NON-SELECTIVELY ON AN ENTIRE ENDF/B TAPE
C (ALL CARD IMAGES BETWEEN THE TAPE LABEL AND THE TAPE END CARD).
C ALL SECTIONS OF FILE 3, EXCEPT MU-BAR, XI OR GAMMA (MT=251-253)
C ARE BROADENED. ALL SECTIONS ARE THINNED (INCLUDING MT=251-253).
C
C THE PROGRAM BROADENS A PAGE OF DATA AT A TIME (1 PAGE=1002 POINTS)
C USING 3 PAGES OF DATA AT THE ORIGINAL TEMPERATURE (THE PAGE
C BEING BROADENED, THE PAGE BELOW IT IN ENERGY AND THE PAGE
C ABOVE IT IN ENERGY). OPERATING IN THIS MANNER THERE IS NO LIMIT
C TO THE NUMBER OF POINTS IN A SECTION.
C
C THE ENERGY GRID FOR THE DOPPLER BROADENED CROSS SECTIONS IS
C SELECTED TO INSURE THAT THE BROADENED DATA IS LINEAR-LINEAR
C INTERPOLATABLE. AS SUCH THE ENERGY GRID FOR THE BROADENED
C DATA MAY NOT BE THE SAME AS THE ENERGY GRID FOR THE ORIGINAL
C UNBROADENED DATA.
C
C IF THE ORIGINAL DATA IS NOT AT ZERO KELVIN THE PROGRAM
C WILL BROADEN THE DATA BY THE EFFECTIVE TEMPERATURE DIFFERENCE TO
C THE FINAL TEMPERATURE. IF THE DATA IS ALREADY AT A TEMPERATURE
C THAT IS HIGHER THAN THE FINAL TEMPERATURE DOPPLER BROADENING
C IS NATURALLY NOT PERFORMED AND THE TEMPERATURE IN THE SECTION
C IS LEFT AT ITS ORIGINAL VALUE.
C
C THE PRESENT VERSION ONLY DOPPLER BROADENS TO ONE FINAL TEMPERATURE
C (IF THERE IS SUFFICIENT INTEREST EXPRESSED BY USERS FUTURE
C VERSION MAY BROADEN TO MULTIPLE TEMPERATURES. PLEASE
C CONTACT THE AUTHOR IF YOU ARE INTERESTED IN A MULTIPLE

```

```

SIG00010
SIG00020
SIG00030
SIG00040
SIG00050
SIG00060
SIG00070
SIG00080
SIG00090
SIG00100
SIG00110
SIG00120
SIG00130
SIG00140
SIG00150
SIG00160
SIG00170
SIG00180
SIG00190
SIG00200
SIG00210
SIG00220
SIG00230
SIG00240
SIG00250
SIG00260
SIG00270
SIG00280
SIG00290
SIG00300
SIG00310
SIG00320
SIG00330
SIG00340
SIG00350
SIG00360
SIG00370
SIG00380
SIG00390
SIG00400
SIG00410
SIG00420
SIG00430
SIG00440
SIG00450
SIG00460
SIG00470
SIG00480
SIG00490
SIG00500
SIG00510
SIG00520
SIG00530
SIG00540
SIG00550
SIG00560
SIG00570
SIG00580
SIG00590
SIG00600

```

C	TEMPERATURE OPTION).	SIG00610
C		SIG00620
C	INPUT FILES	SIG00630
C	-----	SIG00640
C	UNIT DESCRIPTION	SIG00650
C	-----	SIG00660
C	5 INPUT CARDS	SIG00670
C	21 SOURCE FILE (DATA AT ORIGINAL TEMPERATURE)	SIG00680
C	23 SCRATCH FILE FOR BROADEN DATA	SIG00690
C		SIG00700
C	OUTPUT FILES	SIG00710
C	-----	SIG00720
C	UNIT DESCRIPTION	SIG00730
C	-----	SIG00740
C	5 OUTPUT REPORT	SIG00750
C	22 RESULT FILE (DATA AT FINAL TEMPERATURE)	SIG00760
C	23 SCRATCH FILE FOR BROADENED DATA	SIG00770
C		SIG00780
C	INPUT CARDS	SIG00790
C	-----	SIG00800
C	CARD COLS. FORMAT DESCRIPTION	SIG00810
C	-----	SIG00820
C	1 1 1 E11.4 FRACTIONAL THINNING CRITERIA	SIG00830
C	(I.E. 0.5 PER-CENT = 0.005)	SIG00840
C	1 12-22 E11.4 FINAL KELVIN TEMPERATURE	SIG00850
C		SIG00860
C	EXAMPLE INPUT	SIG00870
C	-----	SIG00880
C	TO DOPPLER BROADEN TO 293 KELVIN (ROOM TEMPERATURE) AND THIN	SIG00890
C	THE BROADENED DATA TO 0.5 PER-CENT (0.005 AS A FRACTION), THE	SIG00900
C	FOLLOWING INPUT CARD SHOULD BE USED.	SIG00910
C		SIG00920
C	5.0000E-03 2.9300E+02	SIG00930
C		SIG00940
C	THE PROGRAM MAY BE USED TO THIN DATA, WITHOUT DOPPLER	SIG00950
C	BROADENING BY SPECIFYING A TEMPERATURE OF ZERO, AS FOLLOWS.	SIG00960
C		SIG00970
C	5.0000E-03 0.0000E+00	SIG00980
C		SIG00990
C	LINEARIZING AND/OR THINNING DATA CAN BE DONE MORE EFFICIENTLY	SIG01000
C	USING THE PROGRAM LINEAR (UCRL-50400, VOL. 17, PART-B BY D.E. CULLEN)	SIG01010
C		SIG01020
C	***** LTSS *****	SIG01030
C		SIG01040
C	ALL PROGRAM MODIFICATIONS FOR IMPLEMENTATION AT LIVERMORE ARE	SIG01050
C	ENCLOSED IN COMMENT CARDS THAT SAY LTSS (LIVERMORE TIME SHARING	SIG01060
C	SYSTEM). ALL OF THESE MODIFICATIONS ARE RELATED TO THE USE OF	SIG01070
C	DISK FILES AND I/O OPTIMIZATION. THE SUBROUTINES IONAME, FILEIO	SIG01080
C	AND WAIT ARE ONLY REQUIRED FOR OPERATION AT LIVERMORE.	SIG01090
C		SIG01100
C	AS IMPLEMENTED AT LIVERMORE THIS PROGRAM WILL AUTOMATICALLY	SIG01110
C	USE THE FOLLOWING DISK FILE NAMES...	SIG01120
C		SIG01130
C	ENDFIN = SOURCE DATA IN ENDF/B FORMAT	SIG01140
C	ENDFOUT = RESULT DATA IN ENDF/B FORMAT	SIG01150
C	INPUT = INPUT PARAMETERS	SIG01160
C	OUTPUT = OUTPUT REPORT	SIG01170
C	SCRSGMA1 = SCRATCH FILE	SIG01180
C		SIG01190
C	THE SCRATCH FILE WILL BE WRITTEN AND READ USING THE RANDOM ACCESS	SIG01200

C	ROUTINES WJK AND RDK, WHICH AVOID THE INEFFICIENT FORTRAN BINARY	SIG01210
C	WRITE AND READ ROUTINES.	SIG01220
C		SIG01230
C	***** LTSS *****	SIG01240
C		SIG01250
	INTEGER OTAPE,OUTP,SCR	SIG01260
	COMMON/HEADER/CIH,C2H,L1H,L2H,N1H,N2H,MATH,MFH,MTH,NOSEQ	SIG01270
	COMMON/FILLER/DUMMY(17),MATD,MFD,MTD	SIG01280
	COMMON/UNITS/OUTP,INP,ITAPE,OTAPE,SCR	SIG01290
	COMMON/HOTS/ALPHA,TEMPK,TEMPF,ERTHIN,N2TOT1,N2TOT0	SIG01300
	COMMON/MATTOT/MATIN,MATOUT	SIG01310
	COMMON/NORMIT/XNORM(6),KSIGN(6),KEXP(6)	SIG01320
	COMMON/CONTC/CPVI,OVPI2,ATOP	SIG01330
	COMMON/EXTEND/MESS,MEXT,DTMAX	SIG01340
	COMMON/ITCH/IOCH,IAOR,IPAGE,NPOINT(500)	SIG01350
C----	DEFINE ZERO TO FILL MF,MT AND NOSEQ FIELDS OF LABEL RECORD.	SIG01360
	DATA IZER0/0/	SIG01370
C----	DEFINE PORTIONS OF PI TO DEFINE PI ACCURATELY ON VARIOUS	SIG01380
C----	COMPUTERS.	SIG01390
	DATA P11/3.1415/	SIG01400
	DATA P12/9.2653E-5/	SIG01410
	DATA P13/5.6979E-10/	SIG01420
	DATA P14/3.2384E-15/	SIG01430
C	***** LTSS *****	SIG01440
	CALL CHANGE(7H+SIGMA1)	SIG01450
C	***** LTSS *****	SIG01460
C		SIG01470
C	DEFINE ALL I/O UNITS. TO CHANGE UNIT ASSIGNMENTS FOR ANY	SIG01480
C	OTHER INSTALLATION MERELY CHANGE THE FOLLOWING DEFINITIONS	SIG01490
C	TO SUIT YOURSELF, WHERE....	SIG01500
C		SIG01510
C	INP = INPUT CARD	SIG01520
C	OUTP = OUTPUT LISTING FILE	SIG01530
C	ITAPE = DATA IN ENDF/B FORMAT AT ORIGINAL TEMPERATURE	SIG01540
C	OTAPE = DATA IN ENDF/B FORMAT AT FINAL TEMPERATURE	SIG01550
C	SCR = SCRATCH FILE	SIG01560
C		SIG01570
C	IF YOU WISH TO ALLOW FOR VARIABLE UNIT ASSIGNMENTS MERELY	SIG01580
C	ACTIVATE THE SECOND INPUT FORM ALREADY LISTED AS A COMMENT	SIG01590
C	CARD BELOW (THE FORMAT IS ALREADY COMPATIBLE).	SIG01600
C		SIG01610
	INP=5	SIG01620
	OUTP=6	SIG01630
	ITAPE=21	SIG01640
	OTAPE=22	SIG01650
	SCR=23	SIG01660
C----	READ RUN PARAMETERS (2E11,4)	SIG01670
	READ(INP,5000) ERTHIN,TEMPK	SIG01680
C----	VARIABLE UNIT NUMBER INPUT STATEMENT (2E11,4,3111)	SIG01690
C	READ(INP,5000) ERTHIN,TEMPK,ITAPE,OTAPE,SCR	SIG01700
C	***** LTSS *****	SIG01710
C----	DEFINE ALL I/O UNITS AND DISK FILE NAMES.	SIG01720
	CALL IONAME	SIG01730
C	***** LTSS *****	SIG01740
C----	DEFINE REQUIRED CONSTANTS.	SIG01750
	ATOP=4.0	SIG01760
	PI=P11+P12+P13+P14	SIG01770
	OVPI=1.0/SQRT(PI)	SIG01780
	OVPI2=2.0*OVPI	SIG01790
C----	INITIALIZE MAXIMUM ALLOWABLE TEMPERATURE STEP (TO AVOID	SIG01800

C-----CROSS SECTION EXTENSION).	SIG01810
DTMAX=0.0	SIG01820
C----- INITIALIZE OUTPUT SEQUENCE NUMBER.	SIG01830
NOSEQ=0	SIG01840
C-----INITIALIZE TOTAL NUMBER OF FILE3 POINTS READ AND WRITTEN.	SIG01850
N2TOT1=0	SIG01860
N2TOT0=0	SIG01870
C-----LIST RUN PARAMETERS.	SIG01880
CALL NORMAL(ERTHIN,XNORM(1),KSIGN(1),KEXP(1))	SIG01890
CALL NORMAL(TEMPK,XNORM(2),KSIGN(2),KEXP(2))	SIG01900
WRITE(OUTP,6000) (XNORM(L),KSIGN(L),KEXP(L),L=1,2)	SIG01910
C-----DEFINE MAXIMUM ALLOWABLE ENERGY SPACING.	SIG01920
CALL MAXDE	SIG01930
C-----COPY TAPE LABEL TO FROM INPUT TO OUTPUT FILE.	SIG01940
READ(ITAPE,5030) DUMMY,MATD	SIG01950
WRITE(OTAPE,5030) DUMMY,MATD, (ZERO,K=1,3)	SIG01960
C-----LIST TAPE LABEL.	SIG01970
WRITE(OUTP,6010) DUMMY,MATD	SIG01980
C-----READ NEXT CONTROL RECORD.	SIG01990
READ(ITAPE,5000) C1H,C2H,L1H,L2H,N1H,N2H,MATH,MFH,MTM	SIG02000
C-----CHECK FOR SEND, FEND, MEND OR TEND CARDS.	SIG02010
IF(MTH) 20,20,40	SIG02020
C-----OUTPUT SEND, FEND, MEND OR TEND CARD.	SIG02030
20 NOSEQ=NXTSEQ(NSEQ)	SIG02040
C-----SET SEQUENCE NUMBER TO ZERO FOR TEND CARD.	SIG02050
IF(MATH.LT.0) NOSEQ=0	SIG02060
WRITE(OTAPE,5020) MATH,MFH,MTM,NOSEQ	SIG02070
C-----TERMINATE AFTER TEND CARD. RESET SEQUENCE NUMBER AFTER MEND.	SIG02080
IF(MATH) 90,30,10	SIG02090
30 NOSEQ=0	SIG02100
GO TO 10	SIG02110
C-----INCREMENT SEQUENCE NUMBER AND WRITE CONTROL CARD.	SIG02120
40 NOSEQ=NXTSEQ(NSEQ)	SIG02130
CALL NORMAL(C1H,XNORM(1),KSIGN(1),KEXP(1))	SIG02140
CALL NORMAL(C2H,XNORM(2),KSIGN(2),KEXP(2))	SIG02150
WRITE(OTAPE,5010) (XNORM(L),KSIGN(L),KEXP(L),L=1,2).	SIG02160
IF(L1H,L2H,N1H,N2H,MATH,MFH,MTM,NOSEQ	SIG02170
C-----CHECK FOR SECTION OF FILE 3 DATA.	SIG02180
IF(MFH-3) 60,50,60	SIG02190
C-----FILE 3 LOCATED. PROCESS SECTION	SIG02200
50 CALL FILE3	SIG02210
C-----SKIP TO END OF SECTION.	SIG02220
60 READ(ITAPE,5030) DUMMY,MATD,MFD,MTD	SIG02230
NOSEQ=NXTSEQ(NSEQ)	SIG02240
IF(MTD) 80,80,70	SIG02250
70 WRITE(OTAPE,5030) DUMMY,MATD,MFD,MTD,NOSEQ	SIG02260
GO TO 60	SIG02270
80 WRITE(OTAPE,5020) MATD,MFD,MTD,NOSEQ	SIG02280
GO TO 10	SIG02290
C-----TEND CARD READ AND WRITTEN.	SIG02300
C-----WRITE TOTALS FOR LAST MATERIAL.	SIG02310
90 WRITE(OUTP,5040) MATIN,MATOUT	SIG02320
C-----LIST TOTAL NUMBER OF FILE3 POINTS READ AND WRITTEN.	SIG02330
WRITE(OUTP,5050) N2TOT1,N2TOT0	SIG02340
C-----WRITE WARNING MESSAGE IF CROSS SECTION EXTENSION USED.	SIG02350
IF(DTMAX.LE.0.0) GO TO 100	SIG02360
CALL NORMAL(DTMAX,XNORM(1),KSIGN(1),KEXP(1))	SIG02370
WRITE(OUTP,6020) XNORM(1),KSIGN(1),KEXP(1)	SIG02380
C-----CLOSE FILE AND TERMINATE.	SIG02390
100 CONTINUE	SIG02400

```

C***** LYSS *****
C      END FILE OTAPE
C      REWIND ITAPE
C      REWIND OTAPE
C      CALL FILEIO(OTAPE,7HENDFOUT,LLL,3,1ERR,
C      CALL DEVICE(7HDESTROY,9HSCR5IGMA1,1ERR,10CW)
C***** LYSS *****
C      CALL EXIT
5000 FORMAT(2E11.4,4I11.14,12,13,15)
5010 FORMAT(2(F8.5,A1,12),4I11.14,12,13,15)
5020 FORMAT(66X,14,12,13,15)
5030 FORMAT(16A4,A2,14,12,13,15)
5040 FORMAT(2X,54(1H-)/32X,10HMAI TOTALS,217/2X,54(1H-))
5050 FORMAT(2X,54(1H-)/31X,11HTAPE TOTALS,217/2X,54(1H-))
5000 FORMAT(39H1 DOPPLER BROADEN ENDF/B CROSS SECTIONS,
1 14H (SIGMA1 78-1)/2X,54(1H-)/
2 2X,19HTHINNING CRITERIA--F8.5,A1,12/
3 2X,19HTEMPERATURE-----F8.5,A1,12,7H KELVIN/2X,54(1H-))
6010 FORMAT(2X,10HTAPE LABEL/2X,16A4,A2,14/2X,54(1H-))
1 2X,6H      ZA,5H MAT,5H MT,6X,6HKELVIN,5X,7HQ-VALUE,
2 7H POINTS,7H POINTS/
2 28X,2HIN,10X,2HEV,7H      IN,7H      OUT/2X,54(1H-))
6020 FORMAT(///11H EXTENSION/2X,9(1H-))
1 43H CROSS SECTION EXTENSION CAN BE AVOIDED BY/
2 46H THINNING DATA OR DOPPLER BROADENING IN STEPS/
3 14H OF LESS THAN,F8.5,A1,12,74 KELVIN)
END
SUBROUTINE FILE3
C
C      THIS ROUTINE IS DESIGNED TO LOAD DATA INTO THE CORE AND DOPPLER
C      BROADEN IT A PAGE AT A TIME (1 PAGE=1002 POINTS). IF THE SECTION
C      IS 1002 OR LESS POINTS THE ENTIRE OPERATION IS PERFORMED IN CORE.
C      IF THE SECTION IS OVER 1002 POINTS IT IS WRITTEN ONTO A SCRATCH
C      FILE WHICH CAN LATER BE READ BY TABFIN.
C
C      INTEGER DUTP,SCR,TOOH1
C      COMMON/INDEX/JLOW,JHIGH,KLOW,KHIGH,MLOW,MHIGH,NLOW,NHIGH,
1 N2IN,N2MADE,N2OUT,N2LEFT,NPAGE,JJLOW,ILOW
C      COMMON/TERP/NBT(200),INT(200)
C      COMMON/HCTS/ALPHA,TEMPK,TEMPEF,ERTHIN,N2TOT1,N2TOT0
C      COMMON/HEADER/ZA,AWR,11H,L2H,N1H,N2H,MATH,MFH,M1H,NDSO
C      COMMON/LEADER/C1,C2,L1,L2,N1,N2,MAT,MF,MT
C      COMMON/UNITS/OUTP,INP,ITAPE,OTAPE,SCR
C      COMMON/MATTOT/MATIN,MATOUT
C      COMMON/NORMIT/XNORM(6),KSIGN(6),KEXP(6)
C      COMMON/FILLER/IFILL,NFILL,NLEFT,TOOH1,1THRES
C      COMMON/EXTEND/MESS,MEXT,DTMAX
C      COMMON/CONTAC/OVPI,OVPI2,ATOP
C      COMMON X(3006),S(3006),XOUT(255),CK(3006),YOUT(255),YBREF(1002),
1 EIN(255),SIN(255)
C      COMMON/ITCH/10CW,IADR,IPAGE,NPOINT(500)
C      DIMENSION XB(2004),SB(2004),MESSAG(2,2)
C      EQUIVALENCE (CK(2260),SB),(S(2260),XB)
C-----DEFINE BOLTZMANN CONSTANT IN EV/DEGREE KELVIN
C-----ASSUMING ENERGY WILL BE EXPRESSED IN EV AND THE ATOMIC
C-----WEIGHT RATIO WILL BE EXPRESSED IN NEUTRON MASS UNITS,
C-----AS OPPOSED TO ATOMIC MASS UNITS (AMU)).
C      DATA BOLTZM/8.6164E-05/
C---- DEFINE CROSS SECTION EXTENSION MESSAGE.
C      DATA MESSAG/5H      ,5H      ,5HEXTEN,5HSTON /

```

```

S1602410
S1602420
S1602430
S1602440
S1602450
S1602460
S1602470
S1602480
S1602490
S1602500
S1602510
S1602520
S1602530
S1602540
S1602550
S1602560
S1602570
S1602580
S1602590
S1602600
S1602610
S1602620
S1602630
S1602640
S1602650
S1602660
S1602670
S1602680
S1602690
S1602700
S1602710
S1602720
S1602730
S1602740
S1602750
S1602760
S1602770
S1602780
S1602790
S1602800
S1602810
S1602820
S1602830
S1602840
S1602850
S1602860
S1602870
S1602880
S1602890
S1602900
S1602910
S1602920
S1602930
S1602940
S1602950
S1602960
S1602970
S1602980
S1602990
S1603000

```

C-----INITIALIZE LAST MAT FOUND	SIG03010
DATA LASMAT/-100000/	SIG03020
C-----INITIALIZE LAST TEMPERATURE READ FOR TOTAL CROSS SECTION	SIG03030
DATA TEMP1/0.0/	SIG03040
C-----DEFINE FIXED POINT ZA.	SIG03050
IZA=ZA	SIG03060
C-----INITIALIZE PAGE COUNT FOR CROSS SECTION EXTENSION TEST.	SIG03070
MEXT=0	SIG03080
C -- -INITIALIZE FLAG NOT TO PRINT OUT MESSAGE WITH SECTION.	SIG03090
MESS=1	SIG03100
C -- -INITIALIZE FLAG TO DOPPLER BRADEN SECTION.	SIG03110
TOOH1=-1	SIG03120
-- -TURN OFF FLAG IF SECTION IS MU-BAR, XI OR GAMMA.	SIG03130
IF (MTH.GE.251.AND.MTH.LE.253) TOOH1=1	SIG03140
C-----DEFINE PAGE SIZE (BY CHANGING DIMENSION, COMMON STATEMENTS	SIG03150
C-----AND THIS NUMBER THE SIZE OF THE CORE TABLES MAY BE CHANGED).	SIG03160
NPAGE=1002	SIG03170
C -- -READ TAB1 LEAD CARD.	SIG03180
READ(ITAPE,5000) C1,C2,L1,L2,N1,N2,MAT,MF,MT	SIG03190
C -- -DEFINE ORIGINAL TEMPERATURE OF SECTION.	SIG03200
IF (L2.LE.0) GO TO 10	SIG03210
TEMPIN=TEMP1	SIG03220
TEMPEF=TEMPK-TEMPIN	SIG03230
GO TO 20	SIG03240
10 TEMPIN=C1	SIG03250
IF (MT.EQ.1) TEMP1=TEMPIN	SIG03260
TEMPEF=TEMPK-TEMPIN	SIG03270
IF (TEMPEF.GT.0.0.AND.TOOTH1.LT.0) C1=TEMPK	SIG03280
-- -SHOULD DATA BE DOPPLER BROADENED....	SIG03290
20 IF (TEMPEF) 30,30,40	SIG03300
C-----NO.	SIG03310
30 TOOH1=1	SIG03320
GO TO 50	SIG03330
C-----YES.	SIG03340
40 ALPHA=AWR/(BCLFZM*TEMPEF)	SIG03350
C-----INITIALIZE TOTAL NUMBER OF POINTS FOR OUTPUT, INPUT AND LEFT	SIG03360
C-----FOR INPUT.	SIG03370
50 N2OUT=0	SIG03380
N2IN=N2	SIG03390
N2LEFT=N2	SIG03400
C-----READ INTERPOLATION LAW.	SIG03410
READ(ITAPE,5010) (NBT(K),INT(K),K=1,N1)	SIG03420
C-----INSURE DATA IS LINEAR-LINEAR INTERPOLABLE.	SIG03430
DO 60 K=1,N1	SIG03440
IF (INT(K).NE.2) GO TO 70	SIG03450
60 CONTINUE	SIG03460
GO TO 80	SIG03470
C-----NOT LINEAR-LINEAR. TERMINATE EXECUTION.	SIG03480
70 WRITE(OUTP,5050) IZA,MATH,MTH	SIG03490
CALL EXIT	SIG03500
C-----SET BROADENING INDICES TO MIDDLE PAGE.	SIG03510
80 NLOW=NPAGE+1	SIG03520
NHIGH=2*NPAGE	SIG03530
C-----SET INDEX TO LOADED POINTS AT BEGINNING OF MIDDLE PAGE.	SIG03540
KLOW=NLOW	SIG03550
C-----SET THINNING CONVERGED INDEX TO FIRST POINT IN CORE.	SIG03560
JJLOW=NLOW	SIG03570
C-----SET INDICES TO LOAD MIDDLE AND LAST PAGE.	SIG03590
MLOW=NLOW	SIG03590
MHIGH=3*NPAGE	SIG03600

C-----INITIALIZE SECTION FLAGS.	SIG03610
NFILL=240	SIG03620
IFILL=NFILL+1	SIG03630
NLEFT=N2	SIG03640
N2MADE=0	SIG03650
C-----LOAD NEXT PAGE OF DATA AT ORIGINAL TEMPERATURE.	SIG03660
90 CALL FILLUP	SIG03670
C-----SET INDEX TO LOADED POINTS TO LAST POINT LOADED.	SIG03680
KHIGH=MHIGH	SIG03690
IF (NHIGH.GT.MHIGH) NHIGH=MHIGH	SIG03700
C-----SHOULD DATA BE DOPPLER BROADENED....	SIG03710
100 IF (TOOH.LE.0) GO TO 120	SIG03720
C-----COPY UNBROADENED DATA TO BROADENED LOCATIONS (NO BROADENING).	SIG03730
C-----NOTE...ENERGY HAS NOT BEEN CONVERTED TO SPEED AND THEREFORE	SIG03740
C-----SHOULD NOT BE RE-CONVERTED DURING THIS STEP.	SIG03750
DO 110 K=NLOW,NHIGH	SIG03760
XB(K)=X(K)	SIG03770
110 SB(K)=S(K)	SIG03780
GO TO 130	SIG03790
C-----BROADEN POINTS IN MIDDLE PAGE	SIG03800
120 CALL BROADN	SIG03810
C-----THIN BROADENED POINTS.	SIG03820
130 CALL THINB	SIG03830
C-----DEFINE NUMBER OF POINTS LEFT IN PAGE AFTER THINNING.	SIG03840
NB=JHIGH-JLOW+1	SIG03850
C-----IF ORIGINAL DATA IS ONE PAGE OR LESS OUTPUT SECTION	SIG03860
C-----DIRECTLY FROM CORE.	SIG03870
IF (NHIGH.LT.KHIGH) GO TO 140	SIG03880
IF (N2MADE.LE.NPAGE) GO TO 200	SIG03890
C-----OTHERWISE OUTPUT TO SCRATCH.	SIG03900
140 IF (NB.LE.0) GO TO 150	SIG03910
C-----INCREASE SCRATCH PAGE COUNT AND SAVE NUMBER OF POINTS IN PAGE.	SIG03920
IPAGE=IPAGE+1	SIG03930
IF (IPAGE.LE.500) GO TO 150	SIG03940
WRITE(OUTP,5060) 1ZA,MATH,MTH	SIG03950
CALL EXIT	SIG03960
150 NPOINT(IPAGE)=NB	SIG03970
C-----INCREASE COUNT OF POINTS TO OUTPUT.	SIG03980
N2OUT=N2OUT+NB	SIG03990
C***** LTSS *****	SIG04000
C WRITE(SCR) (XB(K),SB(K),K=JLOW,JHIGH)	SIG04010
CALL WDK(IOCW,IADR,XB(JLOW),NB)	SIG04020
CALL WAIT(IOCW,IERR)	SIG04030
IADR=IADR+NB	SIG04040
CALL WDK(IOCW,IADR,SB(JLOW),NB)	SIG04050
CALL WAIT(IOCW,IERR)	SIG04060
IADR=IADR+NB	SIG04070
C***** LTSS *****	SIG04080
C-----HAS THE LAST POINT BEEN BROADENED....	SIG04090
160 IF (NHIGH.GE.KHIGH) GO TO 210	SIG04100
C-----NO. SAVE UNCONVERGED THINNING POINTS (IF ANY) IN THE LOCATIONS	SIG04110
C-----IMMEDIATELY IN FRONT OF THE NEXT PAGE TO BE BROADENED (AFTER NEXT)	SIG04120
C-----PAGE IS BROADENED THESE REMAINING POINTS PLUS THE BROADENED PAGE	SIG04130
C-----MAY BE TREATED AS ONE SET OF POINTS FOR THINNING).	SIG04140
IF (ILOW.GT.NHIGH) GO TO 180	SIG04150
KK=NLOW-1-(NHIGH-ILOW)	SIG04160
JJLOW=KK	SIG04170
DO 170 K=ILOW,NHIGH	SIG04180
XB(KK)=XB(K)	SIG04190
SB(KK)=SB(K)	SIG04200

170 KK=KK+1	SIG04210
C-----SHIFT REMAINING UNBROADENED POINTS ONE PAGE FORWARD IN CORE.	SIG04220
180 KK=0	SIG04230
DO 180 K=NLOW,KHIGH	SIG04240
KK=KK+1	SIG04250
X(KK)=X(K)	SIG04260
S(KK)=S(K)	SIG04270
190 CK(KK)=CK(K)	SIG04280
C-----SET INDEX TO LOADED POINTS TO BEGINNING OF TABLE.	SIG04290
KLOW=1	SIG04300
C--- SET INDEX TO NEXT AVAILABLE LOCATION FOR LOADING.	SIG04310
MLOW=KK+1	SIG04320
-----ARE THERE ANY MORE POINTS STILL TO READ.....	SIG04330
IF(N2LEFT.GT.0) GO TO 90	SIG04340
C-----NO SET INDEX TO LAST LOADED POINT.	SIG04350
KHIGH=KK	SIG04360
C-----SET INDEX TO BROADEN ALL REMAINING POINTS.	SIG04370
NHIGH=KHIGH	SIG04380
GO TO 100	SIG04390
C-----DEFINE SIZE OF ENTIRELY CORE RESIDENT TABLE.	SIG04400
200 N2OUT=NB	SIG04410
C-----ENTIRE TABLE BROADENED. COPY FROM CORE OR SCRATCH TO OUTPUT	SIG04420
C-----DEVICE.	SIG04430
210 CALL TABFIN	SIG04440
C-----WRITE REPORT OF SECTION.	SIG04450
IF(MATH.EQ.LASMAT) GO TO 220	SIG04460
IF(LASMAT.GT.0) WRITE(OUTP,5040) MATIN,MATOUT	SIG04470
MATIN=0	SIG04480
MATOUT=0	SIG04490
LASMAT=MATH	SIG04500
220 MATIN=MATIN+N2IN	SIG04510
MATOUT=MATOUT+N2OUT	SIG04520
CALL NORMAL(TEMPIN,XNORM(1),KSIGN(1),KEXP(1))	SIG04530
CALL NORMAL(C2,XNORM(2),KSIGN(2),KEXP(2))	SIG04540
WRITE(OUTP,5030) IZA,MATH,MTH,	SIG04550
1 (XNORM(1),KSIGN(1),KEXP(1)),L=1,2,N2IN,N2OUT,	SIG04560
2 MESSAG(1,MESS),MESSAG(2,MESS)	SIG04570
N2TOT1=N2TOT1+N2IN	SIG04580
N2TOT0=N2TOT0+N2OUT	SIG04590
RETURN	SIG04600
5000 FORMAT(2E11.4,4I11,14,12,13,15)	SIG04610
5010 FORMAT(6I11)	SIG04620
5030 FORMAT(2X,16,215,2(1X,F8.5,A1,12),217,2X,2A5)	SIG04630
5040 FORMAT(2X,54(1H-)/32X,10HMAT TOTALS,217/2X,54(1H-))	SIG04640
5050 FORMAT(2X,54(1H-)/2X,16,215//	SIG04650
1 2X,38HINTERPOLATION LAW IS NOT LINEAR-LINEAR/	SIG04660
2 6X,30H**** EXECUTION TERMINATED ****)	SIG04670
5060 FORMAT(2X,54(1H-)/2X,16,215//	SIG04680
1 2X,35HSCRATCH MAXIMUM PAGE COUNT EXCEEDED/	SIG04690
2 4X,30H**** EXECUTION TERMINATED ****)	SIG04700
END	SIG04710
SUBROUTINE FILLUP	SIG04720
C	SIG04730
C LOAD NEXT PAGE OR PAGES OF CROSS SECTIONS AT THE ORIGINAL	SIG04740
C TEMPERATURE INTO CORE. INSURE THAT THE MAXIMUM ENERGY	SIG04750
C SPACING REQUIRED FOR LINEAR-LINEAR INTERPOLATABLE DOPPLER	SIG04760
C BROADENED DATA IS NOT EXCEEDED.	SIG04770
C	SIG04780
INTEGER TOOH	SIG04790
COMMON/HOTS/ALPHA,TEMPK,TEMPEF,ERTHIN,N2TOT1,N2TOT0	SIG04800


```

COMMON/UNITS/GUTP,INP,ITAPE,OTAPE,SCR                SIG04810
COMMON/INDEX/JLOW,JHIGH,KLOW,KHIGH,MLOW,MHIGH,NLOW,NHIGH. SIG04820
I N2IN,N2MADE,N2OUT,N2LEFT,NPAGE,JJLOW,ILOW          SIG04830
COMMON/FILLER/IFILL,NFILL,NLEFT,TOOH1,ITHRES         SIG04840
COMMON/CONTACT/OVP1,OVP12,ATOP                       SIG04850
COMMON: X(3006),S(3006),XOUT(255),CK(3006),YOUT(255),YBREAL(1002), SIG04860
I EIN(255),SIN(255)                                  SIG04870
DIMENSION XIN(240),YIN(240)                          SIG04880
C-----DEFINE MINIMUM ENERGY (EFFECTIVE THRESHOLD WILL NOT BE SHIFTED SIG04890
C-----TO AN ENERGY LOWER THAN THIS).              SIG04900
DATA XM1N/1.0E-05/                                    SIG04910
C-----SET UP LOOP OVER POINTS TO LOAD INTO ORIGINAL TEMPERATURE ARRAY. SIG04920
DO 70 K=MLOW,MHIGH                                    SIG04930
C-----IF NO MORE POINTS IN CORE READ NEXT PAGE (IF ANY). SIG04940
IF(1FILL.LE.NFILL) GO TO 20                          SIG04950
IF(NLEFT.GT.NFILL) GO TO 10                          SIG04960
IF(NLEFT.LE.0) GO TO 80                               SIG04970
NFILL=NLEFT                                           SIG04980
10 NLEFT=NLEFT-NFILL                                  SIG04990
READ(ITAPE,5000) (XIN(I),YIN(I),I=1,NFILL)          SIG05000
IFILL=1                                               SIG05010
C-----DETERMINE IF DATA WILL BE DOPPLER BROADENED (IF NOT MAXIMUM SIG05020
C-----ENERGY SPACING IS NOT REQUIRED).              SIG05030
20 IF(TOOH1) 30,40,50                               SIG05040
C-----NO DOPPLER BROADENING IF THRESHOLD OVER 1,000,000*KT/A. SIG05050
30 TOOHI=1                                           SIG05060
ITHRES=0                                             SIG05070
AX=ALPHA*XIN(1)                                     SIG05080
IF(AX.GE.1000000.0) GO TO 50                       SIG05090
TOOH1=0                                              SIG05100
C-----IF THIS IS A THRESHOLD REACTION DOPPLER BROADENING WILL SHIFT THE SIG05110
C-----THRESHOLD TO A LOWER ENERGY EFFECTIVE THRESHOLD. CREATE EXTRA DATA SIG05120
C-----POINTS BELOW THE ORIGINAL THRESHOLD AT WHICH THE INITIAL CROSS SIG05130
C-----SECTION IS ZERO. POSITION THE SUB-THRESHOLD POINTS TO INSURE THE SIG05140
C-----CROSS SECTION AT THE LOWEST ENERGY WILL BE ZERO AFTER DOPPLER SIG05150
C-----BROADENING (NEW EFFECTIVE THRESHOLD).          SIG05160
IF(XIN(1).LT.1.0) GO TO 50                          SIG05170
ITHRES=1                                           SIG05180
V=SQRT(AX)-ATOP                                     SIG05190
XNEXT=V*V/ALPHA                                     SIG05200
IF(XNEXT.LT.XM1) XNEXT=XM1                          SIG05210
X(K)=XNEXT                                           SIG05220
S(K)=0.0                                             SIG05230
GO TO 60                                             SIG05240
C-----CHECK FOR MAXIMUM ALLOWABLE ENERGY SPACING. SIG05250
40 IF(XIN(1FILL).LE.XNEXT) GO TO 50                SIG05260
C-----INTERPOLATE TO INSERT POINT AT MAXIMUM ALLOWABLE ENERGY SPACING. SIG05270
X(K)=XNEXT                                           SIG05280
S(K)=SKM1+(XNEXT-XKM1)*(YIN(1FILL)-SKM1)/(XIN(1FILL)-XKM1) SIG05290
GO TO 60                                             SIG05300
C-----ENERGY SPACING O.K.                          SIG05310
50 X(K)=XIN(1FILL)                                  SIG05320
S(K)=YIN(1FILL)                                     SIG05330
IFILL=1FILL+1                                       SIG05340
60 XKM1=X(K)                                         SIG05350
SKM1=S(K)                                           SIG05360
70 XNEXT=DEMAX*XKM1                                 SIG05370
IF(NLEFT.LE.0.AND.1FILL.GT.NFILL) N2LEFT=0         SIG05380
GO TO 90                                             SIG05390
C-----END OF DATA TABLE.                        SIG05400

```

```

80 MHIGH=K-1                                SIG05410
   NZLEFT=0                                SIG05420
90 NZMADE=NZMADE+(MHIGH-MLOW)*1             SIG05430
   RETURN                                   SIG05440
   ENTRY MAXDE                               SIG05450
C                                           SIG05460
C   ENTRY POINT TO DEFINE MAXIMUM ALLOWABLE ENERGY SPACING. SIG05470
C                                           SIG05480
   CON=2.0*SQRT(1.0/3.0)/3.0               SIG05490
   T=1.2                                    SIG05500
   DT=0.1                                    SIG05510
   PUSE=ERTHIN                               SIG05520
   IF (ERTHIN.LT.0.001) ERUSE=0.001         SIG05530
100 T=T-DT                                    SIG05540
   BOTTOM=T*T*T                               SIG05550
   TOP=BOTTOM+1.0                             SIG05560
   ERS=ABS(1.0-CON*TOP*SQRT(TOP)/BOTTOM)     SIG05570
   IF (ERS.ERUSE) 110,120,100               SIG05580
110 IF (DT.LT.1.0E-06) GO TO 120           SIG05590
   T=T+DT                                       SIG05600
   DT=0.1*DT                                   SIG05610
   GO TO 100                                   SIG05620
120 DEMAX=T*T                                   SIG05630
   RETURN                                       SIG05640
5000 FORMAT(6E11.4,                          SIG05650
   END                                         SIG05660
   SURROUTINE BROADEN                        SIG05670
                                           SIG05680
   GIVEN A CROSS SECTION THAT IS DESCRIBED BY A TABLE OF
   X'S VS. X AND LINEAR-LINEAR INTERPOLATION BETWEEN POINTS
   THIS ROUTINE WILL EXACTLY DOPPLER BROADENING THE CROSS
   SECTION AT A PORTION OF THE ENERGIES CORRESPONDING TO THE
   ORIGINAL CROSS SECTION (APPROXIMATELY THE MIDDLE THIRD).
                                           SIG05690
   INPUT PARAMETERS                           SIG05700
   KLOW =INDEX TO FIRST POINT LOADED IN CORE. SIG05710
   KHIGH =INDEX TO LAST POINT LOADED IN CORE. SIG05720
   NLOW =INDEX TO FIRST POINT TO BROADEN.    SIG05730
   NHIGH =INDEX TO LAST POINT TO BROADEN.    SIG05740
   MLOW =INDEX TO FIRST POINT JUST LOADED.   SIG05750
   MHIGH =INDEX TO LAST POINT JUST LOADED.   SIG05760
   X =TABLE OF ENERGIES CORRESPONDING TO S.  SIG05770
   S =TABLE OF CROSS SECTIONS AT INITIAL TEMPERATURE. SIG05780
   CK =SCRATCH ARRAY TO USE FOR SLOPE BETWEEN POINTS IN (X,S). SIG05790
   EB =TABLE OF ENRGIES CORRESPONDING TO SB. SIG05800
   SB =TABLE OF CROSS SECTIONS BROADENED TO TEMPF. SIG05810
   ALPHA =DOPPLER WIDTH (11505.3*AWR/TEMPEF) SIG05820
                                           SIG05830
   THE POINTS JUST LOADED (MLOW,MHIGH) ARE CONVERTED TO SPEED
   LIKE TERMS AND SLOPES BETWEEN POINTS COMPUTED. THE TABLE OF
   POINTS (KLOW,KHIGH) IS USED TO BROADEN THE RESULT TABLE
   (NLOW,NHIGH).                             SIG05840
                                           SIG05850
   THE CORE TABLES MAY BE CONSIDERED TO BE COMPOSED OF PAGES OF
   1000 POINTS EACH. THREE PAGES ARE USED FOR THE DATA AT THE
   ORIGINAL TEMPERATURE (X,S,CK) (9018 WORDS) AND ONE PAGE
   IS USED FOR THE BROADENED CROSS SECTION (SB). SIG05860
                                           SIG05870
   DURING ONE PASS OF THIS ROUTINE A PAGE OF DOPPLER BROADENED
   CROSS SECTIONS WILL BE CREATED AT THE ENERGIES CORRESPONDING
   SIG05880
   SIG05890
   SIG05900
   SIG05910
   SIG05920
   SIG05930
   SIG05940
   SIG05950
   SIG05960
   SIG05970
   SIG05980
   SIG05990
   SIG06000

```

C	TO THOSE IN THE MIDDLE PAGE OF THE DATA AT THE ORIGINAL	SIG06010
C	TEMPERATURE.	SIG06020
C		SIG06030
C	ONCE THE BROADENED DATA ARE CREATED THE DATA AT THE	SIG06040
C	ORIGINAL TEMPERATURE IN THE FIRST PAGE IS NO LONGER NEEDED	SIG06050
C	AND THE ENERGIES CORRESPONDING TO THE BROADENED CROSS	SIG06060
C	SECTIONS ARE STORED IN THE FIRST PAGE OF (CK) FOR LATER	SIG06070
C	THINNING IN ROUTINE THINB.	SIG06080
C		SIG06090
C	IN ORDER TO ALLOW THE SAME INDICES TO BE USED FOR BOTH	SIG06100
C	THE ORIGINAL AND BROADENED DATA TWO DUMMY ARRAYS (EB,SB)	SIG06110
C	ARE DEFINED ONE PAGE IN FRONT OF THE LOCATIONS THAT WILL	SIG06120
C	BE USED TO STORE THE BROADENED DATA.	SIG06130
C		SIG06140
	COMMON/INDEX/JLOW,JHIGH,KLOW,KHIGH,MLOW,MHIGH,NLOW,NHIGH.	SIG06150
	1 N2:IN,N2MADE,N2OUT,N2LEFT,NPAGE,JJLOW,JLOW	SIG06160
	COMMON/HEADER/C1H,AHR,L1H,L2H,N1H,N2H,MATH,MFH,MTH,NOSEQ	SIG06170
	COMMON/LEADER/C1,C2,L1,L2,N1,N2,MAT,MF,MT	SIG06180
	COMMON/HOTS/ALPHA,TEMPK,TEMPEF,ERTHIN,N2TOT1,N2TOT0	SIG06190
	COMMON/ERFEXP/EXPERF	SIG06200
	COMMON/CONTACT/DVP1,DVP12,ATOP	SIG06210
	COMMON/INDICE/KNOW,LNOW,KLP1,KHM1	SIG06220
	COMMON/EXTEND/MESS,MEXT,DTMAX	SIG06230
	COMMON X13006),S13006),EOUT(255),CK(3006),SOUT(255),SBREAL(1002),	SIG06240
	1 E1N(255),S1N(255)	SIG06250
	DIMENSION EB(2004),SB(2004)	SIG06260
	EQUIVALENCE (S12260),EB),CK(2260),SB)	SIG06270
C		SIG06280
C	CONVERT FROM ENERGY TO SPEED AND DEFINE SLOPES BETWEEN POINTS.	SIG06290
C		SIG06300
C	-----CONVERT ENERGIES TO SPEED LIKE TERMS.	SIG06310
	DO 10 N=MLOW,MHIGH	SIG06320
	10 X(N)=SQRT(ALPHA*X(N))	SIG06330
C	-----DEFINE THE NUMBER OF INTERVALS AND COMPUTE SLOPE IN	SIG06340
C	-----EACH INTERVAL.	SIG06350
	KLP1=KLOW+1	SIG06360
	KHM1=KHIGH-1	SIG06370
	ML=MLOW	SIG06380
	IF(MLOW.GT.KLOW) ML=ML-1	SIG06390
	MHM1=MHIGH-1	SIG06400
	XXLAST=X(ML)**2	SIG06410
	DO 30 KNOW=ML,MHM1	SIG06420
	XXNOW=X(KNOW+1)**2	SIG06430
	DX=XXNOW-XXLAST	SIG06440
	IF(DX.LE.0.0) GO TO 20	SIG06450
	CK(KNOW)=(S(KNOW+1)-S(KNOW))/DX	SIG06460
	GO TO 30	SIG06470
	20 CK(KNOW)=0.0	SIG06480
	30 XLAST=XXNOW	SIG06490
C		SIG06500
C	TEST FOR CROSS SECTION EXTENSION	SIG06510
C		SIG06520
C	-----TEST LOWER LIMIT FOR ALL PAGES BEYOND SECOND.	SIG06530
	MEXT=MEXT+1	SIG06540
	IF(MEXT.LE.3) GO TO 40	SIG06550
	DX=X(1003)-X(1)	SIG06560
	IF(DX.LE.ATOP) GO TO 50	SIG06570
C	-----TEST UPPER LIMIT FOR ALL PAGES BUT LAST ONE.	SIG06580
	40 IF(N2LEFT.LE.0) GO TO 60	SIG06590
	DX=X13006)-X12004)	SIG06600

```

      IF(DX.GT.ATOP) GO TO 60
C-----DEFINE MAXIMUM ALLOWABLE TEMPERATURE CHANGE TO AVOID
C-----CROSS SECTION EXTENSION.
      50 DX=DX/ATOP
      DTMAX2=TEMPEF*DX*DX
      IF(DTMAX.LE.0.0.OR.DTMAX2.LT.DTMAX) DTMAX=DTMAX2
C-----SET FLAG TO PRINT OUT MESSAGE WITH SECTION
      MESS=2
C
C      BROADEN DATA. SPECIAL TREATMENT FOR LOW ENERGY.
C
      5. KNOW=NLOW
      IF(X(NLOW).GT.ATOP) GO TO 70
      CALL BROADL
      IF(KNOW.GT.NHIGH) RETURN
      70 CALL BROADH
      RETURN
      END
      SUBROUTINE BROADL
C
C      LOW ENERGY DOPPLER BROADENING ROUTINE. THIS ROUTINE WILL
C      BE USED TO DOPPLER BROADEN ALL CROSS SECTIONS AT ENERGIES
C      WHERE AE/KT IS LESS THAN OR EQUAL TO 16. ANY POINT WITH A
C      HIGHER ENERGY WILL BE PASSED ON TO ROUTINE BROADH.
C
C      THE ROUTINE HAS BEEN DESIGNED WITH NO SUBROUTINE CALLS
C      IN ORDER TO MINIMIZE RUNNING TIME. THE ARITHMETIC
C      STATEMENT FUNCTIONS RATION(A) AND ERFC(R,EXPERF) WILL
C      BE COMPILED AS IN LINE CODING BY VIRTUALLY ANY FORTRAN
C      COMPILER, AND AS SUCH DO NOT REPRESENT FUNCTION CALLS.
C
      COMMON/INDEX/JLOW,JHIGH,KLOW,KHIGH,MLOW,MHIGH,NLOW,NHIGH,
      I,N2IN,N2MADE,N2OUT,N2LEFT,NPAGE,JJLOW,ILOW
      COMMON/HEADER/C1H,AWR,L1H,L2H,N1H,N2H,MATH,MFH,MTH,NOSEQ
      COMMON/LEADER/C1,C2,L1,L2,N1,N2,MAT,MF,MT
      COMMON/HOTS/ALPHA,TEHPK,TEMPEF,ERTHIN,N2TOT1,N2TOT0
      COMMON/ERFEXP/L:PERF
      COMMON/CONTACT/OVP1,OVP12,ATOP
      COMMON/INDEX/KNOW,LNOW,KLPI,KHMI
      COMMON X(3006),S(3006),EOUT(255),CK(3006),SOUT(255),SBREAL(1002),
      I,EIN(255),SIN(255)
      DIMENSION EB(2004),SB(2004)
      EQUIVALENCE (S(2260),EB),(CK(2260),SB)
C
C      COMPLEMENTARY ERROR FUNCTION DEFINITION.
C
C-----DEFINE CONSTANTS FOR COMPLEMENTARY ERROR FUNCTION
      DATA A1,A2,A3,A4,A5/0.254829592,-0.284496736,1.421413741,
      1-1.453152027,1.061405429/
C-----DEFINE ARITHMETIC STATEMENT FUNCTION FOR RATIONAL ARGUMENT
C-----OF COMPLEMENTARY ERROR FUNCTION.
      RATION(A)=1./(1.+0.3275911*A)
C-----DEFINE ARITHMETIC STATEMENT FUNCTION FOR COMPLEMENTARY
C-----STATEMENT FUNCTION.
      ERFC(R,EXPERF)=((((A5*R+A4)*R+A3)*R+A2)*R+A1)*R*EXPERF
C
C      SET UP LOOP TO DOPPLER BROADEN CROSS SECTIONS.
C
      DO 150 KNOW=NLOW,NHIGH
C-----INITIALIZE INTEGRAL AND CONSTANTS.

```

```

SIG06610
SIG06620
SIG06630
SIG06640
SIG06650
SIG06660
SIG06670
SIG06680
SIG06690
SIG06700
SIG06710
SIG06720
SIG06730
SIG06740
SIG06750
SIG06760
SIG06770
SIG06780
SIG06790
SIG06800
SIG06810
SIG06820
SIG06830
SIG06840
SIG06850
SIG06860
SIG06870
SIG06880
SIG06890
SIG06900
SIG06910
SIG06920
SIG06930
SIG06940
SIG06950
SIG06960
SIG06970
SIG06980
SIG06990
SIG07000
SIG07010
SIG07020
SIG07030
SIG07040
SIG07050
SIG07060
SIG07070
SIG07080
SIG07090
SIG07100
SIG07110
SIG07120
SIG07130
SIG07140
SIG07150
SIG07160
SIG07170
SIG07180
SIG07190
SIG07200

```

Y=X(KNOW)	S1G07210
IF(Y.GT.ATOP) RETURN	S1G07220
C-----INITIALIZE INTEGRALS TO ZERO DISTANCE VALUES.	S1G07230
C-----DEFINE ALL REQUIRED CONSTANTS FOR POINT.	S1G07240
Y2=2.0*Y	S1G07250
YY=Y*Y	S1G07260
YYA=0.5*YY	S1G07270
C-----INITIALIZE INTEGRALS.	S1G07280
DUMMY1=0.0	S1G07290
IF(Y2.LE.ATOP) GO TO 10	S1G07300
ERFCY2=0.0	S1G07310
F2B=YYA*OVPI2*Y	S1G07320
GO TO 20	S1G07330
10 R=RATION(Y2)	S1G07340
EXPERF=EXP(-Y2*Y2)	S1G07350
ERFCY2=ERFC(R,EXPERF)	S1G07360
F2B=YYA*(1.0-ERFCY2)*OVPI2*Y	S1G07370
C*	S1G07380
C* INTEGRATE OVER ALL ENERGY INTERVALS ABOVE THE CURRENT ENERGY	S1G07390
C* POINT.	S1G07400
C*	S1G07410
C-----NO INTERVALS ABOVE THE LAST POINT.	S1G07420
20 IF(KNOW.EQ.KHIGH) GO TO 70	S1G07430
C-----SET UP LOOP OVER INTERVALS ABOVE CURRENT ONE.	S1G07440
DO 60 LNOW=KNOW,KHMI	S1G07450
B=X(LNOW+1)	S1G07460
C-----TEST FOR END OF RANGE OF INTEGRATION.	S1G07470
BMY=B-Y	S1G07480
IF(BMY.LE.ATOP) GO TO 30	S1G07490
C-----EXTEND INTEGRAL FROM CURRENT POINT TO INFINITY.	S1G07500
DUMMY1=DUMMY1+0.5*(S(LNOW+1)+S(LNOW))*F2B	S1G07510
GO TO 80	S1G07520
C-----SAVE VALUES FROM LAST INTERGAL.	S1G07530
30 F2A=F2B	S1G07540
RBMY=RATION(BMY)	S1G07550
EXBMY=EXP(-BMY*BMY)	S1G07560
C-----TEST FOR END OF RANGE OF INTEGRATION OF SECOND INTEGRAL	S1G07570
BPY=B+Y	S1G07580
RBPY=RATION(BPY)	S1G07590
IF(BPY.LE.ATOP) GO TO 40	S1G07600
EXBPY=0.0	S1G07610
GO TO 50	S1G07620
40 EXBPY=EXP(-BPY*BPY)	S1G07630
50 F2B=YYA*(ERFC(RBMY,EXBMY)-ERFC(RBPY,EXBPY))*	S1G07640
1 OVPI*(B*(EXBMY-EXBPY)+Y*(EXBMY+EXBPY))	S1G07650
60 DUMMY1=DUMMY1+0.5*(S(LNOW+1)+S(LNOW))*(F2A-F2B)	S1G07660
C-----CONTINUE CROSS SECTION AS CONSTANT TO X=INFINITY.	S1G07670
70 DUMMY1=DUMMY1+S(KHIGH)*F2B	S1G07680
C-----RE-INITIALIZE INTEGRALS TO ZERO DISTANCE VALUES	S1G07690
80 F2A=YYA*(1.0+ERFCY2)*OVPI2*Y	S1G07700
C*	S1G07710
C* INTEGRATE OVER ALL ENERGY INTERVALS BELOW THE CURRENT ENERGY	S1G07720
C* POINT.	S1G07730
C*	S1G07740
C-----NO INTERVALS BELOW FIRST POINT.	S1G07750
IF(KNOW.EQ.KLOW) GO TO 130	S1G07760
C---SET UP LOOP OVER INTERVALS BELOW CURRENT POINT.	S1G07770
LNOW=KNOW	S1G07780
DO 120 LL=KLP1,KNOW	S1G07790
LNOW=LNOW-1	S1G07800

```

      A=X(LNOW)
C-----TEST FOR END OF RANGE OF INTEGRATION.
      YMA=Y-A
      IF(YMA.LE.ATOP) GO TO 90
C-----DEFINE REMAINING INTEGRAL AS ZERO.
      DUMMY1=DUMMY1-0.5*(S(LNOW+1)+S(LNOW))*F2A
      GO TO 150
C-----SAVE VALUES FROM LAST INTEGRAL.
      90 F2B=F2A
C-----DEFINE EXPONENTIAL FOR FIRST INTEGRAL.
      EXYMA=RATION(YMA)
      EXYMA=EXP(-YMA*YMA)
C-----DEFINE CONTRIBUTION FROM SECOND INTEGRAL.
      YMA=Y+A
      EXYMA=RATION(YMA)
      IF(YMA.LE.ATOP) GO TO 100
      EXYPA=0.0
      GO TO 110
100 EXYPA=EXP(-YPA*YPA)
C-----ADD CONTRIBUTION FROM CURRENT INTERVAL.
110 F2A=-YYA*(ERFC(RYMA,EXYMA)+ERFC(RYPA,EXYPA))+
      1 OVPI*(A*(EXYMA-EXYPA)+Y*(EXYMA*EXYPA))
120 DUMMY1=DUMMY1+0.5*(S(LNOW+1)+S(LNOW))*(F2A-F2B)
C-----CONTINUE CROSS SECTION AS CONSTANT TO X=0.0
130 IF(Y.LE.ATOP) GO TO 140
      DUMMY1=DUMMY1-S(KLOW)*F2A
      GO TO 150
140 R=RATION(Y)
      EXPERF=EXP(-YY)
      DUMMY1=DUMMY1+S(KLOW)*((-YYA*2.0*ERFC(R,EXPERF)
      1 OVPI2*Y*EXPERF)-F2A)
C-----DEFINE BROADENED CROSS SECTION.
150 SB(KNOW)=0.5*DUMMY1/YY
C-----CONVERT SPEED LIKE TERMS BACK TO ENERGY.
      DO 160 N=LOW,NHIGH
160 EB(N)=X(N)**2/ALPHA
      KNOW=NHIGH+1
      RETURN
      END
      SUBROUTINE BROADC:
C
C      HIGH ENERGY DOPPLER BROADENING ROUTINE. THIS ROUTINE WILL
C      BE USED TO DOPPLER BROADEN ALL CROSS SECTIONS AT ENERGIES
C      WHERE AE/KT IS GRATER THAN 16. ANY POINT WITH A LOWER
C      ENERGY WILL ALREADY HAVE BEEN DOPPLER BROADENED BY
C      ROUTINE BROADL.
C
C      THE ROUTINE HAS BEEN DESIGNED WITH NO SUBROUTINE CALLS
C      IN ORDER TO MINIMIZE RUNNING TIME. THE ARITHMETIC
C      STATEMENT FUNCTIONS RATION(A) AND ERFC(R,EXPERF) WILL
C      BE COMPILED AS IN LINE CODING BY VIRTUALLY ANY FORTRAN
C      COMPILER, AND AS SUCH DO NOT REPRESENT FUNCTION CALLS.
C
      COMMON/INDEX/JLOW,JHIGH,KLOW,KHIGH,MLOW,MHIGH,NLOW,NHIGH,
      1 N2IN,N2MADE,N2OUT,N2LEFT,NPAGE,JJLOW,JJHIGH
      COMMON/HEADER/CIH,AWR,L1H,L2H,N1H,N2H,MATH,MFH,MTH,NOSEQ
      COMMON/LEADER/C1,C2,L1,L2,N1,N2,MAT,MF,MT
      COMMON/HOTS/ALPHA,TEMPK,TEMPF,ERTHIN,N2TOT1,N2TOT0
      COMMON/ERFEXP/EXPERF
      COMMON/CONTACT/OVPI,OVPI2,ATOP

```

```

SIG07810
SIG07820
SIG07830
SIG07840
SIG07850
SIG07860
SIG07870
SIG07880
SIG07890
SIG07900
SIG07910
SIG07920
SIG07930
SIG07940
SIG07950
SIG07960
SIG07970
SIG07980
SIG07990
SIG08000
SIG08010
SIG08020
SIG08030
SIG08040
SIG08050
SIG08060
SIG08070
SIG08080
SIG08090
SIG08100
SIG08110
SIG08120
SIG08130
SIG08140
SIG08150
SIG08160
SIG08170
SIG08180
SIG08190
SIG08200
SIG08210
SIG08220
SIG08230
SIG08240
SIG08250
SIG08260
SIG08270
SIG08280
SIG08290
SIG08300
SIG08310
SIG08320
SIG08330
SIG08340
SIG08350
SIG08360
SIG08370
SIG08380
SIG08390
SIG08400

```

```

COMMON/INDICE/KNOW,LNOW,KLP1,KHM1
COMMON X(3006),S(3006),EOUT(255),CK(3006),SOUT(255),SREAL(1002),
1 E1N(255),S1N(255)
DIMENSION EB(2004),SB(2004)
EQUIVALENCE (S(2260),EB),(CK(2260),SB)
C
C COMPLEMENTARY ERROR FUNCTION DEFINITION.
C
C-----DEFINE CONSTANTS FOR COMPLEMENTARY ERROR FUNCTION
DATA A1,A2,A3,A4,A5/0.254829592,0.284496736,1.4214137,1.,
1 -1.433152027,1.05405429/
C-----DEFINE ARITHMETIC STATEMENT FUNCTION FOR RATIONAL ARGUMENT
C-----OF COMPLEMENTARY ERROR FUNCTION.
A10N(A)=1./((1.+1.3275911*A)
C-----DEFINE ARITHMETIC STATEMENT FUNCTION FOR COMPLEMENTARY
C-----STATEMENT FUNCTION.
ERFCL(R,EXPERF)=((((A5*R+A4)*R+A3)*R+A2)*R+A1)*R*EXPERF
C
C SET UP LOOP TO DOPPLER BROADEN CROSS SECTIONS.
C
NNLOW=KNOW
DO 90 KNOW=NNLOW,NHIGH
C-----INITIALIZE INTEGRAL AND CONSTANTS.
Y=X(KNOW)
C-----INITIALIZE INTEGRALS TO ZERO DISTANCE VALUES.
C-----DEFINE ALL REQUIRED CONSTANTS FOR POINT.
YY=Y*Y
BB=YY
YYA=0.5*YY
YYB=YY*(YY+3.0)+0.75
YYC=2.0*(YY+1.0)
YYD=YY+1.5
C-----INITIALIZE INTEGRALS.
DUMMY1=0.0
DUMMY2=0.0
F2B=YYA*OVP12*Y
F4B=YYB*OVP12*Y*YYC
C*
C* INTEGRATE OVER ALL ENERGY INTERVALS ABOVE THE CURRENT ENERGY
C* POINT.
C*
C-----NO INTERVALS ABOVE THE LAST POINT.
IF(KNOW.EQ.KHIGH) GO TO 30
C-----SET UP LOOP OVER INTERVALS ABOVE CURRENT ONE.
DO 20 LNOW=KNOW,KHM1
B=X(LNOW+1)
BMY=B-Y
IF(BMY.LE.ATOP) GO TO 10
DUMMY1=DUMMY1+S(LNOW)*F2B
DUMMY2=DUMMY2+CK(LNOW)*(F4B-BB*F2B)
GO TO 40
C-----SAVE VALUES FROM LAST INTERVAL.
10 F2A=F2B
F4A=F4B
C-----DEFINE CONSTANTS FOR THIS POINT.
AA=BB
BB=B*B
BPY=B*Y
R=RATION(BMY)
EXPERF=EXP(-BMY*BMV)

```

```

S1G08410
S1G08420
S1G08430
S1G08440
S1G08450
S1G08460
S1G08470
S1G08480
S1G08490
S1G08500
S1G08510
S1G08520
S1G08530
S1G08540
S1G08550
S1G08560
S1G08570
S1G08580
S1G08590
S1G08600
S1G08610
S1G08620
S1G08630
S1G08640
S1G08650
S1G08660
S1G08670
S1G08680
S1G08690
S1G08700
S1G08710
S1G08720
S1G08730
S1G08740
S1G08750
S1G08760
S1G08770
S1G08780
S1G08790
S1G08800
S1G08810
S1G08820
S1G08830
S1G08840
S1G08850
S1G08860
S1G08870
S1G08880
S1G08890
S1G08900
S1G08910
S1G08920
S1G08930
S1G08940
S1G08950
S1G08960
S1G08970
S1G08980
S1G08990
S1G09000

```

S0=ERFC(R,EXPERF)	SIG09010
F2B=YYA*S0+OVP1*BPY*EXPERF	SIG09020
F4B=YYB*S0+OVP1*(BPY*(BB+YYD)+Y)*EXPERF	SIG09030
S1=F2A-F2B	SIG09040
DUMMY1=DUMMY1+S(LNOW)*S1	SIG09050
20 DUMMY2=DUMMY2+CK(LNOW)*((F4A-F4B)-AA*S1	SIG09060
C-----CONTINUE CROSS SECTION AS CONSTANT TO X=INFINITY.	SIG09070
30 DUMMY1=DUMMY1+S(KHIGH)*F2B	SIG09080
C-----RE-INITIALIZE INTEGRALS TO ZERO DISTANCE VALUES	SIG09090
40 AA=YY	SIG09100
F2A=-YYA+OVP12*Y	SIG09110
F4A=-YYB+OVP12*Y*YYC	SIG09120
	SIG09130
INTEGRATE OVER ALL ENERGY INTERVALS BELOW THE CURRENT ENERGY	SIG09140
C* POINT.	SIG09150
C*	SIG09160
C-----NO INTERVALS BELOW CURRENT FIRST POINT.	SIG09170
IF(KNOW.EQ.KLOW) GO TO 70	SIG09180
C- SET UP LOOP OVER INTERVALS BELOW CURRENT POINT.	SIG09190
LNOW=KNOW	SIG09200
DO 60 LL=KLP1,KNOW	SIG09210
LNOW=LNOW-1	SIG09220
A=X(LNOW)	SIG09230
YMA=Y-A	SIG09240
IF(YMA.LE.ATOP) GO TO 50	SIG09250
DUMMY1=DUMMY1-S(LNOW+1)*F2A	SIG09260
DUMMY2=DUMMY2-CK(LNOW)*(F4A-AA*F2A)	SIG09270
GO TO 90	SIG09280
C- --SAVE VALUES FROM LAST INTEGRAL.	SIG09290
50 F2B=F2A	SIG09300
F4B=F4A	SIG09310
C-----DEFINE CONSTANTS FOR THIS POINT.	SIG09320
BB=AA	SIG09330
AA=A*A	SIG09340
YPA=Y+A	SIG09350
R=RATION(YMA)	SIG09360
EXPERF=EXP(-YMA*YMA)	SIG09370
S0=-ERFC(R,EXPERF)	SIG09380
F2A=YYA*S0+OVP1*YPA*EXPERF	SIG09390
F4A=YYB*S0+OVP1*(YPA*(AA+YYD)+Y)*EXPERF	SIG09400
S1=F2A-F2B	SIG09410
DUMMY1=DUMMY1+S(LNOW+1)*S1	SIG09420
60 DUMMY2=DUMMY2+CK(LNOW)*((F4A-F4B)-BB*S1)	SIG09430
C-----CONTINUE CROSS SECTION AS CONSTANT TO X=0.0	SIG09440
70 IF(Y.LE.ATOP) GO TO 80	SIG09450
DUMMY1=DUMMY1-S(KLOW)*F2A	SIG09460
GO TO 90	SIG09470
80 R=RATION(Y)	SIG09480
EXPERF=EXP(-YY)	SIG09490
DUMMY1=DUMMY1+S(KLOW)*((-YYA*ERFC(R,EXPERF)	SIG09500
+OVP1*Y*EXPERF)-F2A)	SIG09510
C-----DEFINE BROADENED CROSS SECTION.	SIG09520
90 SB(KLOW)=0.5*(DUMMY1+DUMMY2)/YY	SIG09530
C-----CONVERT SPEED LIKE TERMS BACK TO ENERGY.	SIG09540
DO 100 N=NLOW,NHIGH	SIG09550
100 EB(N)=X(N)**2/ALPHA	SIG09560
RETURN	SIG09570
END	SIG09580
SUBROUTINE THINB	SIG09590
C	SIG09600

C	GIVEN A FUNCTION REPRESENTED BY X AND S COORDINATES	SI609610
C	AND LINEAR-LINEAR INTERPOLATION BETWEEN POINTS, THIS	SI609620
C	ROUTINE WILL REMOVE ALL EXTRANEIOUS POINTS THAT LIE WITHIN A	SI609630
C	GIVEN ACCURACY OF THE FUNCTION BASED UPON INTERPOLATION	SI609640
C	FROM SURROUNDING POINTS.	SI609650
C		SI609660
C	DURING ONE PASS THIS ROUTINE WILL THIN ANY UNCONVERGED POINTS	SI609670
C	FROM THE LAST BROADENED PAGE PLUS THE CURRENT BROADENED PAGE.	SI609680
C	AT THE END OF THE CURRENT PAGE THE LAST CONVERGED POINT AND ALL	SI609690
C	UNCONVERGED POINTS WILL BE LEFT IN THE CORE TO BE THINNED WITH	SI609700
C	THE NEXT PAGE (UNLESS THE END OF THE TABLE IS REACHED IN WHICH	SI609710
C	CASE THE LAST POINT IS CONVERGED).	SI609720
C		SI609730
	COMMON/INDEX/JLOW,JHIGH,KLOW,KHIGH,MLOW,MHIGH,NLOW,NHIGH,	SI609740
	1 N2IN,N2MADE,N2OUT,N2LEFT,NPAGE,JJLOW,ILOW	SI609750
	COMMON/LEADER/C1,C2,L1,L2,N1,N2,PAT,MF,MT	SI609760
	COMMON/HOTS/ALPHA,TEMPK,TEMPEF,ERTHIN,N2TOT1,N2TOT0	SI609770
	COMMON X(3006),S(2259),XB(3006),YOUT(255),SB(2004),	SI609780
	1 EIN(255),SIN(255)	SI609790
C-----	IF ALLOWABLE ERROR IS NOT POSITIVE NO THINNING CAN BE	SI609800
C-----	PERFORMED ON THE TABLE.	SI609810
	IF(ERTHIN.LE.0.0) GO TO 10	SI609820
C-----	AT LEAST 3 POINTS REQUIRED FOR THINNING.	SI609830
	IF(NHIGH-NLOW.GE.2) GO TO 20	SI609840
C-----	SET THINNED INDICES EQUAL TO ORIGINAL INDICES AND RETURN.	SI609850
	10 JL/I=JJLOW	SI609860
	JHIGH=NHIGH	SI609870
	ILOW=NHIGH+1	SI609880
	RETURN	SI609890
C-----	INITIALIZE THINNED INDICES TO AUTOMATICALLY ACCEPT FIRST POINT.	SI609900
	20 JLOW=JJLOW	SI609910
	JHIGH=JJLOW	SI609920
C-----	INITIALIZE INDEX TO NEXT CANDIDATE FOR THINNING.	SI609930
	ILOW=JJLOW+1	SI609940
C-----	SET UP LOOP OVER ALL OTHER POINTS.	SI609950
	NBOT=JJLOW+2	SI609960
	DO 60 N=NBOT,NHIGH	SI609970
C-----	DEFINE INDEX TO LAST CANDIDATE FOR THINNING.	SI609980
	NM1=N-1	SI609990
C-----	DEFINE CHANGE IN ENERGY AND CHECK FOR THREE (OR MORE)	SI610000
C-----	SUCCESSIVE POINTS ALL WITH THE SAME ENERGY.	SI610010
	DXB=XB(N)-XB(JHIGH)	SI610020
	IF(DXB.LE.0.0) GO TO 40	SI610030
C-----	DEFINE SLOPE BETWEEN LAST ACCEPTED POINT AND END OF	SI610040
C-----	INTERVAL.	SI610050
	SLOPE=(SB(N)-SB(JHIGH))/DXB	SI610060
C-----	TEST ALLOWABLE ERROR AT ALL INTERVENING POINTS.	SI610070
	DO 30 K=ILOW,NM1	SI610080
	YP=SB(JHIGH)+SLOPE*(XB(K)-XB(JHIGH))	SI610090
	IF(ABS(YP-SB(K)).GT.ERTHIN*SB(K)) GO TO 50	SI610100
	30 CONTINUE	SI610110
C-----	ALL INTERVENING POINTS CAN BE THINNED. EXTEND INTERVAL TO	SI610120
C-----	THIN BY ONE MORE POINT.	SI610130
	GO TO 60	SI610140
C-----	THREE OR MORE POINTS ALL WITH THE SAME ENERGY. KEEP NEXT	SI610150
C-----	POINT IF NOT THE SAME CROSS SECTION AS LAST POINT.	SI610160
	40 IF(SB(JHIGH).EQ.SB(ILOW)) GO TO 60	SI610170
C-----	AT LEAST ONE POINT IN INTERVAL FAILS TEST. SAVE LAST POINT	SI610180
C-----	WITHIN THE INTERVAL.	SI610190
	50 JHIGH=JHIGH+1	SI610200

XB(JHIGH)=XB(NMI)	SIG10210
SB(JHIGH)=SB(NMI)	SIG10220
C-----RESET LOWER LIMIT OF INTERVAL THAT CAN BE THINNED.	SIG10230
ILOW=N	SIG10240
60 CONTINUE	SIG10250
C-----IS THIS THE END OF THE ENTIRE TABLE (ALL POINTS BROADENED)....	SIG10260
IF(NHIGH.LT.KHIGH) GO TO 70	SIG10270
C----YES. MOVE LAST POINT IN TABLE TO THINNED TABLE.	SIG10280
JHIGH=JHIGH+1	SIG10290
XB(JHIGH)=XB(NHIGH)	SIG10300
SB(JHIGH)=SB(NHIGH)	SIG10310
RETURN	SIG10320
C----NO. DETERMINE NUMBER OF UNCONVERGED POINTS LEFT OVER FROM	SIG10330
C-----THINNING.	SIG10340
70 KLEFT=NHIGH-ILOW+1	SIG10350
C----WILL REMAINING POINTS FIT INTO (XOUT,YOUT)	SIG10360
IF(KLEFT.LE.255) GO TO 80	SIG10370
C----NO. THIN INTERMEDIATE POINTS BETWEEN ILOW AND NHIGH BY SIMPLY	SIG10380
C----RESETTING LOWER THINNING INDEX.	SIG10390
ILOW=NHIGH	SIG10400
RETURN	SIG10410
C-----YES. SAVE LAST CONVERGED POINT IN CORE TO SERVE AS PIVOT FOR	SIG10420
C-----THINNING OF NEXT PAGE OF DATA.	SIG10430
80 ILOW=ILOW-1	SIG10440
JHIGH=JHIGH-1	SIG10450
RETURN	SIG10460
END	SIG10470
SUBROUTINE TABFIN	SIG10480
C	SIG10490
C THIS ROUTINE IS DESIGNED TO COPY THE SECTION OF BROADENED AND/OR	SIG10500
C THINNED DATA FROM THE CORE OR SCRATCH FILE TO THE RESULT FILE IN	SIG10510
C THE ENDF/B FORMAT.	SIG10520
C	SIG10530
INTEGER OTAPE,OUTP,SCR	SIG10540
COMMON/UNITS/OUTP,INP,ITAPE,OTAPE,SCR	SIG10550
COMMON/TERP/NBT(200),INT(200)	SIG10560
COMMON/HEADER/C1H,C2H,L1H,L2H,N1H,N2H,MATH,MFH,MTH,N0SEQ	SIG10570
COMMON/LEADER/C1,C2,L1,L2,N1,N2,MAT,MF,MT	SIG10580
COMMON/INDEX/JLOW,JHIGH,KLOW,KHIGH,MLOW,MHIGH,NLOW,NHIGH,	SIG10590
N2IN,N2MADE,N2OUT,N2LEFT,NPAGE,JJLOW,ILOW	SIG10600
COMMON X(3006),S(3006),XOUT(255),CK(3006),YOUT(255),YREAL(1002),	SIG10610
E1N(255),SIN(255)	SIG10620
COMMON/NORMIT/XNORM(6),KSIGN(1),KEXP(6)	SIG10630
COMMON/FILLER/IFILL,NFILL,NLEFT,TOOHI,ITHRES	SIG10640
COMMON/ITCH/IOCH,IAOR,IPAGE,NPOINT(500)	SIG10650
DIMENSION XP(1257),YF(1257),XB(2259),SB(2259)	SIG10660
EQUIVALENCE (S(2260),XB),(CK(2260),SB),(XB(1003),XP),(SB(1003),YF)	SIG10670
C----DEFINE NUMBER OF POINTS TO OUTPUT.	SIG10680
N2=N2OUT	SIG10690
C----SET INTERPOLATION LAW TO LINEAR LINEAR OVER ENTIRE TABLE.	SIG10700
NBT(1)=N2OUT	SIG10710
INT(1)=2	SIG10720
NI=1	SIG10730
C----INCREMENT SEQUENCE NUMBER AND WRITE LEAD AND INTERPOLATION LAW.	SIG10740
NOSEQ=NXSEQ(N0SEQ)	SIG10750
CALL NORMAL(C1,XNORM(1),KSIGN(1),KEXP(1))	SIG10760
CALL NORMAL(C2,XNORM(2),KSIGN(2),KEXP(2))	SIG10770
WRITE(OTAPE,5000) (XNORM(L),KSIGN(L),KEXP(L),L=1,2),	SIG10780
1 L1,L2,N1,N2,MAT,MF,MT,NOSEQ	SIG10790
NOSEQ=NXSEQ(N0SEQ)	SIG10800

WRITE(OTAPE,5010) NBT(1),INT(1),MAT,MF,MT,NOSEQ	SIG10810
C-----IF TABLE LESS THAN ONE PAGE IT IS ALREADY CORE RESIDENT.	SIG10820
IF(N2MADE GT,NPAGE) GO TO 10	SIG10830
C-----INDICES (JLOW,JHIGH) ARE ALREADY SET FOR CORE RESIDENT TABLE.	SIG10840
C-----DEFINE NUMBER OF POINTS ON SCRATCH AS ZERO AND OUTPUT CORE	SIG10850
C-----RESIDENT TABLE.	SIG10860
N2=0	SIG10870
GO TO 40	SIG10880
C-----END SCRATCH FILE AND POSITION FOR READING.	SIG10890
10 IPAGE=0	SIG10900
C***** LTSS *****	SIG10910
C END FILE SCR	SIG10920
C REWIND SCR	SIG10930
IADR=0	SIG10940
C***** LTSS *****	SIG10950
C-----RESET BASE LOCATION FOR POINTS TO OUTPUT.	SIG10960
20 JLOW=NPAGE+1	SIG10970
C-----INCREASE SCRATCH PAGE INDEX AND DEFINE NUMBER OF POINTS IN PAGE.	SIG10980
30 IPAGE=IPAGE+1	SIG10990
NPT=NPOINT(IPAGE)	SIG11000
C-----LOAD NEXT THINNED PAGE INTO CORE.	SIG11010
C***** LTSS *****	SIG11020
C READ(SCR) (XP(K),YP(K),K=1,NPT)	SIG11030
CALL RDK(10CW,IADR,XP,NPT)	SIG11040
CALL WAIT(10CW,IERR)	SIG11050
IADR=IADR+NPT	SIG11060
CALL RDK(10CW,IADR,YP,NPT)	SIG11070
CALL WAIT(10CW,IERR)	SIG11080
IADR=IADR+NPT	SIG11090
C***** LTSS *****	SIG11100
C-----DEFINE NUMBER OF POINTS REMAINING ON SCRATCH.	SIG11110
N2=N2-NPT	SIG11120
C-----SET INDEX TO TOP OF CORE TABLE.	SIG11130
JHIGH=NPAGE+NPT	SIG11140
C-----IF THRESHOLD REPLACED DUE TO DOPPLER BROADENING INSURE	SIG11150
C-----FIRST TABULATED POINT IS A THRESHOLD.	SIG11160
40 IF(1THRES) 60,60,50	SIG11170
50 1THRES=0	SIG11180
YP(1)=0.0	SIG11190
C-----SET UP LOOP TO OUTPUT CARD IMAGES.	SIG11200
60 DO 80 K=JLOW,JHIGH,3	SIG11210
C-----INCREMENT SEQUENCE NUMBER	SIG11220
NOSEQ=NXTSEQ(NOSEQ)	SIG11230
C-----SET INDEX TO END OF CARD.	SIG11240
KK=K+2	SIG11250
C-----IF FULL CARD CANNOT BE WRITTEN BRANCH TO SAVE POINTS OR	SIG11260
C-----WRITE LAST PARTIALLY FILLED CARD.	SIG11270
IF(KK,GT,JHIGH) GO TO 90	SIG11280
C-----OUTPUT FULL CARD IMAGE.	SIG11290
LL=0	SIG11300
DO 70 L=K,KK	SIG11310
LL=LL+1	SIG11320
CALL NORMAL(XB(LL),XNORM(LL),KSIGN(LL),KEXP(LL))	SIG11330
LL=LL+1	SIG11340
70 CALL NORMAL(SB(LL),XNORM(LL),KSIGN(LL),KEXP(LL))	SIG11350
80 WRITE(OTAPE,5020) (XNORM(LL),KSIGN(LL),KEXP(LL),L=1,6),	SIG11360
1 MAT,MF,MT,NOSEQ	SIG11370
C-----NO MORE POINTS LEFT IN CORE. ANY MORE POINTS TO READ....	SIG11380
IF(N2) 160,160,20	SIG11390
C-----ONE OR TWO POINTS LEFT IN CORE. SAVE IF MORE POINTS TO READ OR	SIG11400

C-----WRITE PARTIALLY FILLED RECORD IF THIS IS END OF TABLE.	SIG11410
90 IF(N2) 120,120,100	SIG11420
C-----SAVE ONE OR TWO POINTS IMMEDIATELY IN FRONT OF PAGE THAT WILL	SIG11430
C-----BE READ NEXT.	SIG11440
100 JLOW=NPAGE-(JHIGH-K)	SIG11450
KK=JLOW	SIG11460
DO 110 L=K,JHIGH	SIG11470
SB(KK)=SB(L)	SIG11480
XB(KK)=XB(L)	SIG11490
110 KK=KK+1	SIG11500
GO TO 30	SIG11510
C-----LAST CARD OF TABLE IS PARTIALLY FULL.	SIG11520
120 KLEFT=JHIGH-K+1	SIG11530
L=0	SIG11540
DO 130 L=K,JHIGH	SIG11550
LL=LL+1	SIG11560
CALL NORMAL(XB(LL),XNORM(LL),KSIGN(LL),KEXP(LL))	SIG11570
LL=LL+1	SIG11580
140 CALL NORMAL(SB(L),XNORM(LL),KSIGN(LL),KEXP(LL))	SIG11590
GO TO (140,150),KLEFT	SIG11600
140 WRITE(OTAPE,5030) (XNORM(L),KSIGN(L),KEXP(L),L=1,2),	SIG11610
1 MAT,MF,MT,NOSEQ	SIG11620
GO TO 160	SIG11630
150 WRITE(OTAPE,5040) (XNORM(L),KSIGN(L),KEXP(L),L=1,4),	SIG11640
1 MAT,MF,MT,NOSEQ	SIG11650
C-----IF SCRATCH FILE WAS USED RE-POSITION FOR NEXT TABLE.	SIG11660
150 IF(N2MADE.LE.NPAGE) RETURN	SIG11670
IPAGE=0	SIG11680
C***** LTSS *****	SIG11690
C REWIND SCR	SIG11700
IADR=0	SIG11710
C***** LTSS *****	SIG11720
RETURN	SIG11730
5000 FORMAT(2(F8.5,A1,I2),4I11,I4,I2,I3,I5)	SIG11740
5010 FORMAT(2I11,44X,I4,I2,I3,I5)	SIG11750
5020 FORMAT(6(F8.5,A1,I2),I4,I2,I3,I5)	SIG11760
5030 FORMAT(2(F8.5,A1,I2),44X,I4,I2,I3,I5)	SIG11770
5040 FORMAT(4(F8.5,A1,I2),22X,I4,I2,I3,I5)	SIG11780
END	SIG11790
SUBROUTINE NORMAL(X,XNORM,KSIGN,KEXP)	SIG11800
C	SIG11810
C CONVERT FLOATING POINT NUMBER TO NORMAL FORM FOR OUTPUT.	SIG11820
C OUTPUT WILL BE IN THE FORM X.XXXXX+/-NN, WHICH GIVES	SIG11830
C AN ADDITIONAL DIGIT OF ACCURACY WHEN COMPARED TO E11.4	SIG11840
C FORTRAN OUTPUT. IN ADDITION THE OUTPUT WILL BE COMPUTER	SIG11850
C INDEPENDENT (I.E. SAME ON IBM, CD, UNIVAC ETC.)	SIG11860
C	SIG11870
INTEGER PLUS	SIG11880
C-----DEFINE TWO POSSIBLE SIGNES FOR EXPONENT.	SIG11890
DATA PLUS/'H+/'	SIG11900
DATA MINUS/'H-/'	SIG11910
C-----COMPUTE SIGNED EXPONENT FROM ABSOLUTE VALUE.	SIG11920
XABS=ABS(X)	SIG11930
C-----IF NUMBER IS 0.0 DEFINE 0.00000+ 0	SIG11940
IF(XABS) 50,50,10	SIG11950
C-----DEFINE EXPONENT TO NORMALIZE MANTISSA.	SIG11960
10 KEXP=ALOG10(XABS)	SIG11970
SHIFT=10.0**KEXP	SIG11980
XNORM=XABS/SHIFT	SIG11990
IF(XNORM.GE.0.999995) GO TO 20	SIG12000

KEXP=KEXP-1	SIG12010
SHIFT=SHIFT/10.0	SIG12020
GO TO 30	SIG12030
20 IF(XNORM.LT.9.999995) GO TO 30	SIG12040
KEXP=KEXP+1	SIG12050
SHIFT=10.0*SHIFT	SIG12060
C-----COMPUTE SIGNED MANTISSA.	SIG12070
30 XNORM=X/SHIFT	SIG12080
C-----DEFINE SIGN OF EXPONENT AND INSURE EXPONENT IS POSITIVE.	SIG12090
IF(KEXP) 40,60,70	SIG12100
40 KSIGN=MINUS	SIG12110
KEXP=-KEXP	SIG12120
RETURN	SIG12130
C-----X IS 0.0. DEFINE AS 0.00000+ 0	SIG12140
50 XNORM=0.0	SIG12150
60 KEXP=0	SIG12160
70 KSIGN=PLUS	SIG12170
RETURN	SIG12180
END	SIG12190
FUNCTION NXTSEQ(NDSEQ)	SIG12200
C	SIG12210
C DEFINE NEXT SEQUENCE NUMBER FOR ENDF/B OUTPUT. ALLOW FOR	SIG12220
C MORE THAN 10000 CARDS PER EVALUATION BY RESETTNG NUMBER	SIG12230
C TO 1 EVERY TIME 100000 IS REACHED.	SIG12240
C	SIG12250
NN=NOSEQ+1	SIG12260
IF(NN.EQ.100000) NN=1	SIG12270
NXTSEQ=NN	SIG12280
RETURN	SIG12290
END	SIG12300
SUBROUTINE IONAME	SIG12310
C	SIG12320
C DEFINE ALL I/O UNITS AND DISK FILE NAMES.	SIG12330
C	SIG12340
INTEGER OUTP,OTAPE	SIG12350
COMMON/UNITS/OUTP,INP,ITAPE,OTAPE,SCR	SIG12360
COMMON/ITCH,IOCW,IADR,IPAGE,NPOINT(500)	SIG12370
C-----RE-DEFINE OUTPUT REPORT UNIT FOR TELETYPE WHEN I/O UNITS ARE	SIG12380
C-----BEING DEFINED (ANY ERROR MESSAGES WILL THEN APPEAR ON LINE).	SIG12390
OUTP=59	SIG12400
C-----DEFINE ENDF/B FORMAT FILE TO BE LINEARIZED.	SIG12410
CALL FILEIO(ITAPE,GHENDFIN,LLL,1,IERR)	SIG12420
IF(IERR.NE.0) CALL EXIT	SIG12430
C-----DEFINE ENDF/B FORMAT FILE FOR LINEARIZED DATA.	SIG12440
LLL=3*LLL	SIG12450
IF(LLL.LT.100000) LLL=100000	SIG12460
CALL FILEIO(ITAPE,7HENDFOUT,LLL,2,IERR)	SIG12470
IF(IERR.NE.0) CALL EXIT	SIG12480
C-----DEFINE SCRATCH UNIT FOR LINEARIZED DATA.	SIG12490
LLL=500000	SIG12500
IADR=0	SIG12510
ERRA CALL DEVICE(7HDESTROY,9HSCRSIGMA1,IERR,IOCW)	SIG12520
CALL DEVICE(6HCREATE,9HSCRSIGMA1,LLL,IERR,IOCW)	SIG12530
C-----IF ANY PROBLEM DELAY AND THEN TRY AGAIN.	SIG12540
IF(IERR.LE.0) GO TO ERB	SIG12550
CALL FROST(2500B,0,5000000,ERRA)	SIG12560
GO TO ERRA	SIG12570
C-----RE-DEFINE OUTPUT REPORT UNIT FOR PRINTER.	SIG12580
ERRB OUTP=6	SIG12590
RETURN	SIG12600

END	SIG12610
SUBROUTINE FILEIO(UNIT,NAME,LENGTH,IWAY,IERR)	SIG12620
C*	SIG12630
C* THIS ROUTINE IS DESIGNED TO HANDLE ALL DEVICE ASSIGNMENTS.	SIG12640
C* FILE OPENING AND CLOSING AS WELL AS END OF FILES AND LAST	SIG12650
C* BUFFER UNLOADING (EMPTY).	SIG12660
C*	SIG12670
C* THE TYPE OF OPERATION IS DEFINED BY IWAY AS FOLLOWS....	SIG12680
C* IWAY =1 OPEN FILE	SIG12690
C* =2 CREATE FILE	SIG12700
C* =3 END FILE, EMPTY BUFFER, TRUNCATE SIZE AND CLOSE FILE.	SIG12710
C* =4 END FILE, TRUNCATE SIZE AND CLOSE FILE.	SIG12720
C* =5 CLOSE FILE.	SIG12730
C* =6 RENAME FILES (DELETE UNIT, RENAME NAME TO UNIT	SIG12740
C* (AS BACKUP) RENAME LENGTH TO UNIT)	SIG12750
C* =7 OPEN TAPE.	SIG12760
C* =8 DESTROY FILE (USUALLY SCRATCH AT END OF EXECUTION)	SIG12770
C*	SIG12780
INTEGER TTY,UNIT,BLANK	SIG12790
COMMON/UNITS/TTY	SIG12800
COMMON/Q100789/ICBLK(8,16)	SIG12810
DIMENSION IBETA(2),NBETA(2),MAXWAIT(2)	SIG12820
DATA BLANK/1H /	SIG12830
C-----DEFINE SUSPEND TIMES (IN MICROSECONDS) TO SUSPEND FOR 5 MINUTES	SIG12840
C----FOR AN OPEN OR 5 SECONDS FOR A CREATE.	SIG12850
DATA NBETA/30000000,5000000/	SIG12860
C----DEFINE SUSPEND COUNTS FOR A TOTAL OF 5 HOURS.	SIG12870
DATA MAXWAIT/60,3600/	SIG12880
C----INITIALIZE SUSPEND WAIT COUNT.	SIG12890
NWAIT=0	SIG12900
C-----BRANCH TO PROPER OPERATION.	SIG12910
GO TO (10,10,90,90,140,160,10,200).IWAY	SIG12920
C-----DEFINE CORRESPONDENCE BETWEEN UNIT AND FILENAME (OPEN OR CREATE)	SIG12930
10 CALL ASSIGN(UNIT,NAME)	SIG12940
CALL NOPAGE(UNIT)	SIG12950
C-----BRANCH TO OPEN, CREATE OR TAPE.	SIG12960
IF(IWAY=2) 20,40,30	SIG12970
C-----OPEN FILE.	SIG12980
20 CALL DEVICE(4HOPEN,NAME,LENGTH,IERR)	SIG12990
IF(IERR.LE.0.OR.IERR.EQ.2) GO TO 150	SIG13000
IF(TTY.EQ.-59) RETURN	SIG13010
GO TO 50	SIG13020
C-----OPEN TAPE	SIG13030
30 CALL DEVICE(4HTAPE,NAME,IERR)	SIG13040
C-----CHECK FOR ERROR (ALLOW WRITE PROTECTED FILE,IERR=2).	SIG13050
IF(IERR.LE.0.OR.IERR.EQ.2) GO TO 150	SIG13060
C-----ERROR DURING OPEN OR TAPE. BRANCH TO ERROR MESSAGE.	SIG13070
GO TO 50	SIG13080
C-----CREATE FILE (FIRST DESTROY ANY FILE OF SAME NAME).	SIG13090
40 CALL DEVICE(7HDESTROY,NAME,IERR)	SIG13100
CALL DEVICE(6HCREATE,NAME,LENGTH,IERR)	SIG13110
C-----CHECK FOR ERROR DURING FILE CREATION.	SIG13120
IF(IERR.LE.0) GO TO 150	SIG13130
C-----ERROR DURING OPE, TAPE OR CREATE. PRINT ERROR MESSAGE FIRST TIME	SIG13140
C-----AND DETERMINE IF SUSPEND RE-TRY LOOP SHOULD BE ENTERED.	SIG13150
50 IF(NWAIT,GT.0) GO TO 60	SIG13160
IF(TTY,GT.0) WRITE(TTY,5900) NAME	SIG13170
GO TO 70	SIG13180
C-----ALREADY IN SUSPEND LOOP. TEST IF MAXIMUM NUMBER OF SUSPENDS	SIG13190
C-----HAS BEEN EXCEEDED.	SIG13200

60 IF(NWAIT.LE.MAXWAIT*IWAY)) GO TO 80	SIG13210
WRITE(TTY,5960)	SIG13220
IF(TTY.NE.59) RETURN	SIG13230
NWAIT=0	SIG13240
GO TO 70	SIG13250
C-----NO SUSPEND LOOP FOR TAPE INITIALIZATION (OPERATORS WOULD	SIG13260
C-----GO BANANAS)	SIG13270
70 IF(IWAY.GT.2) RETURN	SIG13280
C-----SUSPEND UNTIL FILE OR DISK SPACE AVAILABLE.	SIG13290
IF(TTY.GT.0) WRITE(TTY,5940)	SIG13300
C-----INCREMENT SUSPEND COUNT, SUSPEND AND AFTER SUSPEND RE-TRY.	SIG13310
80 NWAIT=NWAIT+1	SIG13320
CALL FROST(2500B,0,NBETA*IWAY),ERRA)	SIG13330
ERRA GO TO (20,40),IWAY	SIG13340
RETURN	SIG13350
C-----WRITE END OF FILE.	SIG13360
90 END FILE UNIT	SIG13370
C-----EMPTY BUFFER IF REQUESTED.	SIG13380
IF(IWAY.EQ.3) CALL EMPTY(UNIT)	SIG13390
C-----TRUNCATE SIZE OF FILE. LOOK UP FILENAME IN ORDERLIB TABLE.	SIG13400
DO 100 I=1,16	SIG13410
IF((ICBLK(I,1)-NAME) .100,110,100	SIG13420
100 CONTINUE	SIG13430
C-----FILENAME NOT FOUND. TRUNCATION NOT POSSIBLE.	SIG13440
IF(TTY.GT.0) WRITE(TTY,3930) NAME	SIG13450
GO TO 140	SIG13460
C-----RIGHT ADJUST FILENAME FOR FROST CALL.	SIG13470
110 INAME=NAME	SIG13480
DO 120 K=1,10	SIG13490
IF((INAME.INT.77B).NE.0) GO TO 130	SIG13500
120 INAME=INAME.SHL.54	SIG13510
C-----FILENAME IS COMPLETELY ZERO	SIG13520
IF(TTY.GT.0) WRITE(TTY,5930) NAME	SIG13530
GO TO 140	SIG13540
C-----LOAD RIGHT ADJUSTED FILENAME AND FILE LENGTH FOR FROST CALL	SIG13550
130 IBETA(1)=INAME	SIG13560
IBETA(2)=(ICBLK(4,1).SHR.36).INT.3777777B	SIG13570
CALL FROST(1200B,0,IBETA,ERRB)	SIG13580
GO TO 140	SIG13590
C-----ERROR DURING FILE LENGTH TRUNCATION.	SIG13600
ERRB IF(TTY.GT.0) WRITE(TTY,5930) NAME	SIG13610
C-----CLOSE FILE (WRITE PROTECTED).	SIG13620
140 CALL DEVICE(6HCLUSER,NAME,IERR)	SIG13630
C-----CHECK FOR ERROR DURING CLOSING.	SIG13640
IF(IERR.LE.0) GO TO 150	SIG13650
C-----CLOSING ERROR. WRITE ERROR MESSAGE.	SIG13660
IF(TTY.GT.0) WRITE(TTY,5910) NAME	SIG13670
RETURN	SIG13680
C-----SET ERROR FLAG TO STANDARD O. K. RETURN.	SIG13690
150 IERR=0	SIG13700
RETURN	SIG13710
C-----IS THERE A BACKUP FILENAME.....	SIG13720
160 IF(UNIT.NE.BLANK) GO TO 170	SIG13730
C-----NO. DESTROY FILE AND DO RENAME WITHOUT BACKUP FILE.	SIG13740
CALL DEVICE(7HDESTROY,NAME,IERR)	SIG13750
GO TO 190	SIG13760
C-----YES. DESTROY BACKUP FILE.	SIG13770
170 CALL DEVICE(7HDESTROY,UNIT,IERR)	SIG13780
C-----IS THERE A SECOND FILENAME.....	SIG13790
IF(NAME.NE.BLANK) GO TO 180	SIG13800

C--- NO. USE THIRD FILENAME AND BACKUP FILENAMES.	SIG13810
CALL CHN(LENGTH,UNIT,IERR)	SIG13820
IF(IERR.GT.0.AND.TTY.GT.0) WRITE(TTY,5920) LENGTH,UNIT	SIG13830
RETURN	SIG13840
C--- YES. CHANGE SECOND FILENAME TO BACKUP FILENAME.	SIG13850
180 CALL CHN(NAME,UNIT,IERR)	SIG13860
IF(IERR.GT.0.AND.TTY.GT.0) WRITE(TTY,5920) NAME,UNIT	SIG13870
C--- IF NO THIRD FILENAME OPERATION WAS JUST SECOND FILENAME TO BACKUP.	SIG13880
IF(LENGTH.EQ.BLANK) RETURN	SIG13890
C--- CHANGE THIRD FILENAME TO SECOND FILENAME.	SIG13900
190 CALL CHN(LENGTH,NAME,IERR)	SIG13910
IF(IERR.GT.0.AND.TTY.GT.0) WRITE(TTY,5920) LENGTH,NAME	SIG13920
RETURN	SIG13930
C--- DESTROY FILE.	SIG13940
200 CALL DEVICE(7HDESTROY,NAME,IERR)	SIG13950
RETURN	SIG13960
5900 FORMAT(IX,A10,26H FILE INITIALIZATION ERROR)	SIG13970
5910 FORMAT(IX,A10,19H FILE CLOSING ERROR)	SIG13980
5920 FORMAT(IX,A10,4H TO ,A10,22H FILENAME CHANGE ERROR,16)	SIG13990
5930 FORMAT(IX,A10,34H ERROR DURING FILE SIZE TRUNCATION)	SIG14000
5940 FORMAT(IX,A10,12HWILL SUSPEND)	SIG14010
5950 FORMAT(IX,A10,24H CANNOT PERFORM OPERATION)	SIG14020
END	SIG14030
SUBROUTINE WAIT(LCIOC,IERR)	SIG14040
	SIG14050
C	SIG14060
DELAY UNTIL ALL I/O IS COMPLETED ON UNIT DEFINED BY LCIOC	SIG14070
C	SIG14080
INTEGER TTY,TESTDK	SIG14090
COMMON/UNIT5/TTY	SIG14100
10 NOC=TESTDK	SIG14110
IF(NOC) 20,40,30	SIG14120
20 CALL DELAY(LCIOC)	SIG14130
GO TO 10	SIG14140
30 IERR=1	SIG14150
IF(TTY.GT.0) WRITE(TTY,5900)	SIG14160
RETURN	SIG14170
40 IERR=0	SIG14180
RETURN	SIG14190
5900 FORMAT(29HWAIT...TROUBLE WITH DISK I/O)	SIG14200
END	SIG14210

Acknowledgments

Many people contributed to the development of the SIGMAL code. The author would particularly like to acknowledge the contributions of R. J. LaBauve, R.E. MacFarlane and P. Soran of Los Alamos Scientific Laboratory, and C. R. Weisbin, J. White and R. Q. Wright of Oak Ridge National Laboratory.

1978 Edition

Many people contributed useful suggestions for improving and correcting the 1977 version of program SIGMAL; in particular the author would like to acknowledge the contributions of W. Rathenstein, the Technicon, Haifa, Israel, L. B. Levitt, Brookhaven National Laboratory, and the staff of the Argonne Code Center.

References

1. D. E. Cullen and C. R. Weisbin, *Nuc. Sci. and Eng.* 60, 199-229 (1976).
2. R. V. Meghreblian and D. K. Holmes, *Statistical Analysis* (McGraw-Hill Book Company, New York, 1960), p. 137.
3. D. Garber, et al., *Data Format and Procedures for the Evaluated Nuclear Data File*, ENDF, Brookhaven National Laboratory, Upton, New York, Rept. BNL-NCS-50496 (ENDF-102) (1975).
4. D. E. Cullen, *Program LINEAR: Linearize Evaluated Data in the Evaluated Nuclear Data File/Version B (ENDF/B) Format Version 76-2*, Lawrence Livermore Laboratory, Rept. UCRL-50400, Vol. 17, Part A (1978).
5. R. J. Howerton, et al., *The LLL Evaluated Nuclear Data Library (ENDL)*, Lawrence Livermore Laboratory, Rept. UCRL-50400, Vol. 15, Parts A, B, and C (1976).