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**Program GROUPIE (version 79-1):
calculation of Bondarenko
self-shielded neutron cross sections
and multiband parameters from data
in the ENDF/B format**

D. E. Cullen

MASTER

July 4, 1980

**Lawrence
Livermore
National
Laboratory**

Program GROUPIE (version 79-1): calculation of Bondarenko self-shielded neutron cross sections and multiband parameters from data in the ENDF/B format

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FOREWORD

The total cross-section probability (TCP) system is designed to process evaluated neutron-cross-section data into continuous-energy or multigroup forms. The following figure describes the function of each code in the TCP system by contrasting the form of the data before and after code processing.

Plots of evaluated cross sections in the ENDF/B format can be obtained at any stage of the above processing by using the EVALPLOT program (UCRL-50400, Vol. 17, Part E). Comparisons between evaluated cross sections in the ENDF/E format and experimental data in the ECSIL format can be obtained by using the ECSPLT program (UCRL-50400, Vol. 1, Part 1).

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PROGRAM GROUPIE (VERSION 79-i):
CALCULATION OF BONDARENKO SELF-SHIELDED
NEUTRON CROSS SECTIONS AND MULTIBAND
PARAMETERS FROM DATA IN THE ENDF/B FORMAT

ABSTRACT

Program GROUPIE reads evaluated data in the ENDF/B format and uses these data to calculate Bondarenko self-shielded cross sections and multiband parameters. To give as much generality as possible, the program allows the user to specify arbitrary energy groups and an arbitrary energy-dependent neutron spectrum (weighting function). To guarantee the accuracy of the results, all integrals are performed analytically; in no case is iteration or any approximate form of integration used. The output from this program includes both listings and multiband parameters suitable for use either in a normal multigroup transport calculation or in a multiband transport calculation. A listing of the source deck is available on request.

INTRODUCTION

Program GROUPIE reads evaluated data in the ENDF/B format,¹ calculates Bondarenko self-shielded cross sections,² and uses these to determine multiband parameters.^{3,4,5}

Program GROUPIE is designed to perform all calculations using an arbitrary energy group structure. The user may select one of four built-in group structures (50, 126, 171, or 175 groups), or may specify any set of group boundaries by input.

To evaluate analytically all integrals involved in obtaining Bondarenko self-shielded cross sections, GROUPIE requires that the energy-dependent neutron spectrum and all cross sections be given in tabular form, with linear interpolation between tabulated values.

The user may specify the neutron spectrum to be constant (or "flat") within each group, or may specify any spectrum with linear interpolation between tabulated values. There is no limit to the size of the table used to

describe the spectrum, so the spectrum may be described in as much detail as required.

Cross sections are read using the ENDF/B format. To ensure that all cross sections are linearly interpolable, it may be necessary to use programs LINEAR⁶ and/or RECENT⁷ before using GROUPIE. In addition, if data are required at a temperature other than 0 kelvin, it may be necessary to use program SIGMAL.⁸

PROGRAM LINEAR

Tabulated cross sections in the ENDF/B format may use any of five interpolation laws between any two tabulated points.¹ Program LINEAR reads tabulated cross sections from the ENDF/B format, converts them to linearly interpolable form, and writes the results in the ENDF/B format.

PROGRAM RECENT

Cross sections in the ENDF/B format may be specified by giving a tabulated background cross section and resonance parameters.¹ Program RECENT combines the contribution of the background cross section (linearized, if necessary, using LINEAR) and resonance parameters to obtain linearly interpolable tabulated cross sections, and writes the results in the ENDF/B format.

PROGRAM SIGMAL

The result of running LINEAR and/or SIGMAL will be tabulated, linearly interpolable 0- ∞ cross sections in the ENDF/B format. Program SIGMAL reads these cross sections, Doppler-broadens them⁹ to any user-specified temperature, and outputs them in the ENDF/B format in linearly interpolable form.

GROUPIE reads either the 0-K cross sections output by LINEAR and RECENT or the Doppler-broadened cross sections output by SIGMAL, and uses them to calculate Bondarenko self-shielded cross sections and multiband parameters.

The output from GROUPIE includes both listings and computer-readable forms suitable for use in transport calculations. Specifically, the output includes the following:

1. Listings of Bondarenko self-shielded cross sections and f-factors² for total, elastic, capture, and fission. These quantities are not output in

computer-readable form, because it is more economical and accurate to obtain self-shielded cross sections using multiband parameters than to interpolate in tables of self-shielded cross sections vs Σ_0 .

2. Unshielded, group-averaged cross sections for all reactions, in linearly interpolable (histogram) form in the ENDF/B format. This representation may be used to evaluate the effect of multigrouping cross sections, either graphically¹⁰ or in transport calculations.¹¹

3. Listings and computer-readable multiband parameters for total, elastic, capture, and fission. The binary-form multiband parameter file is designed for use with a Monte Carlo transport code.¹² This file may be used directly in a multiband calculation, or may be used to obtain self-shielded cross sections for use in a multigroup calculation.

METHOD

BONDARENKO SELF-SHIELDED CROSS SECTIONS

Definitions

In any energy group G , the Bondarenko self-shielded cross section is defined as

$$\langle \Sigma_1(\Sigma_0, N) \rangle_G = \frac{\int_{E_G}^{E_{G+1}} \Sigma_1(E) \frac{S(E) dE}{(\Sigma_T(E) + \Sigma_0)^N}}{\int_{E_G}^{E_{G+1}} \frac{S(E) dE}{(\Sigma_T(E) + \Sigma_0)^N}}, \quad (1)$$

where

G = the group index ($G = 1, 2, 3, \dots$),

(E_G, E_{G+1}) = the energy range of group G ,

$\Sigma_1(E)$ = the cross section for reaction 1 (1 = total, elastic, capture, etc.), at energy E , for the material of interest,

$S(E)$ = the energy-dependent neutron spectrum (e.g., Maxwellian, $1/E$, fission, and/or fusion),

$\Sigma_T(E)$ = the total cross section for the material of interest (i.e., it is a particular case of $\Sigma_i(E)$),

Σ_0 = the "background" cross section representing the combined effects of all other isotopes and of leakage, and

N = an integer that differs for each Legendre moment of the flux (e.g., $N = 1$ for scalar flux, $N = 2$ for current, etc.).¹³

The quantity

$$\frac{S(E)}{(\Sigma_T(E) + \Sigma_0)^N}$$

is called the weighting function; it is the product of the neutron spectrum $S(E)$ and the self-shielding factor

$$\frac{1}{(\Sigma_T(E) + \Sigma_0)^N}.$$

The form of the self-shielding factor reflects the fact that peaks in the cross section tend to cause minima in the flux.

Several combinations of Σ_0 and N are of sufficient physical significance to have special names. Among these are the following:

- $(\Sigma_0, N) = (\infty, 1)$ or (arbitrary, 0) corresponds to the unshielded (or infinitely dilute) cross section. In this limit it is assumed that there are so few atoms of the material of interest in the composite mixture that peaks in the total cross section of the material have no appreciable effect on the total cross section of the mixture. In this case self-shielding (or "flux depression") does not occur to any significant degree.

- $(\Sigma_0, N) = (0, 1)$ corresponds to the totally shielded, flux-weighted cross section. This is the case of a pure scatterer, or a narrow-resonance scatterer, in which flux depression is proportional to $1/\Sigma_T(E)$. This cross section is also known as the average distance to collision or the unshielded, current-weighted cross section.¹³

- $(\Sigma_0, N) = (0, 2)$ corresponds to the totally shielded, current weighted cross section.

GROUPIE performs group averages for any arbitrary set of energy-group boundaries; the user may use one of four built-in group structures, or may enter any set of group boundaries he chooses. Therefore the following evaluation of integrals applies for arbitrary group boundaries E_G and E_{G+1} .

Evaluation of the Bondarenko cross section (Eq. (1)) depends on the values of the three functions $\Sigma_1(E)$, $\Sigma_T(E)$, and $S(E)$. Each of these functions is assumed to be given as a table of values $(E_k, f(E_k))$, with linear interpolation between tabulated values. Programs LINEAR,⁶ RECENT,⁷ and SIGMA⁸ can be used to reduce the cross sections $\Sigma_1(E)$ and $\Sigma_T(E)$ to the required linearly interpolable form. Virtually any functional form for the energy-dependent weighting spectrum $S(E)$ can be easily expressed as a linearly interpolable table; e.g., Maxwellian, $1/E$, fission and/or fusion spectra. All data are handled in a paging system, so there is no limit to the number of data points used to represent each function. Therefore there is no limit to the accuracy with which each function may be represented.

Since no approximation is introduced in performing the integrals used to obtain the Bondarenko self-shielded cross sections, the accuracy of the results is guaranteed to be at least as good as the accuracies with which the cross sections $\Sigma_1(E)$ and $\Sigma_T(E)$ and the weighting spectrum $S(E)$ are given by the user.

Evaluation of Integrals (In Normal Forms)

The Bondarenko self-shielded cross section of Eq. (1) can be expressed in terms of a sum over energy intervals,

$$\int_{E_G}^{E_{G+1}} \Sigma_1(E) \frac{S(E) dE}{(\Sigma_T(E) + \Sigma_0)^N} = \sum_j \int_{E_j}^{E_{j+1}} \Sigma_1(E) \frac{S(E) dE}{(\Sigma_T(E) + \Sigma_0)^N}, \quad (2)$$

where the intervals (E_j, E_{j+1}) span the energy group G , and are selected so that $\Sigma_1(E)$, $\Sigma_T(E)$, and $S(E)$ are all linearly interpolable in each interval. (For example, if $\Sigma_1(E)$ and $\Sigma_T(E)$ are tabulated at 5, 15, 25 eV, etc., and $S(E)$ is tabulated at 10, 20, 30 eV, etc., and each is linearly interpolable between tabulated values, then $\Sigma_1(E)$, $\Sigma_T(E)$, and $S(E)$ will

all be linearly interpolable over the intervals 5, 10, 15, 20 eV, etc.) To determine the Bondarenko self-shielded cross section, we need only obtain an algebraic expression for the integral on the right in Eq. (2), which represents a single interval, and then evaluate and sum over all intervals that contribute. (Equation (2) represents only the numerator of Eq. (1); with $\Sigma_1(E)$ set equal to unity, however, it also represents the denominator. Therefore a method for evaluating Eq. (2) will allow us to evaluate Eq. (1).)

We will write the integral on the right-hand side of Eq. (2) in what we call "normal" form, i.e., the form of Eq. (7). We first recognize that if each of the functions Σ_1 , Σ_T , and S is linearly interpolable, each can be written in the form

$$f(E) = \frac{E - E_j}{E_{j+1} - E_j} f_{j+1} + \frac{E_{j+1} - E}{E_{j+1} - E_j} f_j, \quad (3)$$

where f_j and f_{j+1} are the tabulated values of $f(E)$ at E_j and E_{j+1} respectively.

The integral in Eq. (2) over the energy interval (E_j, E_{j+1}) can be transformed into an integral over the "normal" interval $(-1, 1)$ by changing to the new variable

$$Z = 2 \frac{E - (1/2)(E_j + E_{j+1})}{E_{j+1} - E_j} = \frac{E - E_j}{E_{j+1} - E_j} - \frac{E_{j+1} - E}{E_{j+1} - E_j}; \quad (4)$$

the differential of Z with respect to E is

$$dZ = \frac{2 dE}{E_{j+1} - E_j}. \quad (5)$$

Under this change of variables, each function f becomes

$$f(Z) = (1/2)(1 + Z)f_{j+1} + (1/2)(1 - Z)f_j,$$

or

$$f(Z) = (1/2)(f_{j+1} + f_j) + (1/2)Z(f_{j+1} - f_j). \quad (6)$$

The integral in Eq. (2) can then be written as

$$\begin{aligned}
& \int_{E_j}^{E_{j+1}} \Sigma_1(E) \frac{S(E) dE}{(\Sigma_T(E) + \Sigma_0)^N} \\
&= \frac{(E_{j+1} - E_j)}{2} \int_{-1}^{+1} \left[(1/2)(\Sigma_{1,j+1} + \Sigma_{1,j}) + (1/2)Z(\Sigma_{1,j+1} - \Sigma_{1,j}) \right] \\
&\quad \times \left[(1/2)(S_{j+1} + S_j) + (1/2)Z(S_{j+1} - S_j) \right] \\
&\quad \times \left[(1/2)(\Sigma_{T,j+1} + \Sigma_{T,j}) + (1/2)Z(\Sigma_{T,j+1} - \Sigma_{T,j}) + \Sigma_0 \right]^N dz, \quad (7)
\end{aligned}$$

where the subscripts j and $j+1$ refer to values of $\Sigma_1(E)$, $\Sigma_T(E)$, and $S(E)$ at energies E_j and E_{j+1} .

In this "normal" form the integral has the following properties:

1. Energy has been completely removed from the integral; it appears only as $(E_{j+1} - E_j)$, outside the integral. Therefore points of discontinuity (that is, points at which $E_{j+1} = E_j$, but $\Sigma_{1,j+1} \neq \Sigma_{1,j}$) do not lead to numerical instability because of infinite derivatives in the cross section. In particular, this means that energy intervals of zero length will make zero contribution to the integral.

2. The only variable terms in the integral are the tabulated values of the functions Σ_1 , Σ_T , and S . Therefore, as long as the tabulated values are finite and the total cross section is positive, the value obtained for the integral will be numerically stable and well-defined.

3. If any function is constant over an interval (that is, $f_{j+1} = f_j$), its contribution automatically reduces to its average value $(1/2)(f_{j+1} + f_j)$ without any further differencing. This further improves the numerical stability of the equations.

4. For any positive function f , the average value $(1/2)(f_{j+1} + f_j)$ will always be greater than $(1/2)(f_{j+1} - f_j)$. Therefore the effect of the constant term (the first term in Eq. (6)) in each function is dominant, further improving numerical stability.

The integral of Eq. (7) can now be written in the form

$$\int_{E_j}^{E_{j+1}} \frac{S(E) dE}{(\Sigma_T(E) + \Sigma_0)^N} = \frac{(E_{j+1} - E_j)}{2} \int_{-1}^{+1} \frac{A_j + B_j z + C_j z^2}{(D_j + F_j z)^N} dz$$

$$= \frac{(E_{j+1} - E_j)}{2 D_j^N} \int_{-1}^{+1} \frac{A_j + B_j z + C_j z^2}{(1 + \delta_j z)^N} dz, \quad (8)$$

where

$$A_j = (1/4) (\Sigma_{i,j+1} + \Sigma_{i,j}) (S_{j+1} + S_j),$$

$$B_j = (1/4) (\Sigma_{i,j+1} + \Sigma_{i,j}) (S_{j+1} - S_j) + (S_{j+1} + S_j) (\Sigma_{i,j+1} - \Sigma_{i,j}),$$

$$C_j = (1/4) (\Sigma_{i,j+1} - \Sigma_{i,j}) (S_{j+1} - S_j),$$

$$D_j = (1/2) (\Sigma_{T,j+1} + \Sigma_{T,j}) + \Sigma_0,$$

$$F_j = (1/2) (\Sigma_{T,j+1} - \Sigma_{T,j}),$$

and

$$\delta_j = F_j/D_j.$$

The integral of Eq. (8) can be expressed in terms of the functions

$$F_N^J(\delta) = \int_{-1}^{+1} \frac{z^J dz}{(1 + \delta z)^N}, \quad J = 0, 1, 2; \quad N = 0, 1, 2, 3. \quad (9)$$

These functions satisfy recursion relations that allow functions for higher values of N and J to be expressed in terms of functions for lower values of N and J . Table 1 gives expressions for a number of the F_N^J . Although several of the recursion relations were used to obtain the results given in Table 1, only results will be presented here.

Two cases must be considered in Eq. (9): small δ , and otherwise. By inspection we see that if $\delta = 0$ these functions are independent of N , and depend only on J . (Since $\delta = 0$ corresponds to the total cross section Σ_T being constant across the interval E_j to E_{j+1} , this is what we would expect; i.e., the self-shielding factor will have the same value at all points

TABLE 1. Functional forms (for low values of J and N) of the functions

$$F_N^J(\delta) = \int_{-1}^{+1} \frac{z^J dz}{(1 + \delta z)^N}.$$

J	N	Integral $F_N^J(\delta)$	Expansion for small
0	0	2	--
0	1	$\frac{1}{\delta} \ln\left(\frac{1+\delta}{1-\delta}\right)$	$2\left(1 + \frac{1}{3}\delta^2 + \frac{1}{5}\delta^4 + \frac{1}{7}\delta^6\right)$
0	2	$\frac{2}{1-\delta^2}$	--
0	3	$\frac{2}{(1-\delta^2)^2}$	--
1	0	0	--
1	1	$\frac{1}{\delta} \left[2 - \frac{1}{\delta} \ln\left(\frac{1+\delta}{1-\delta}\right) \right]$	$-2\delta \left(\frac{1}{3} + \frac{1}{5}\delta^2 + \frac{1}{7}\delta^4 + \frac{1}{9}\delta^6 \right)$
1	2	$\frac{1}{\delta} \left[\frac{1}{\delta} \ln\left(\frac{1+\delta}{1-\delta}\right) - \frac{2}{1-\delta^2} \right]$	$\frac{4\delta}{1-\delta^2} \left(\frac{1}{3} + \frac{1}{15}\delta^2 + \frac{1}{35}\delta^4 + \frac{1}{63}\delta^6 \right)$
1	3	$-\frac{2\delta}{(1-\delta^2)^2}$	--
2	0	$\frac{2}{3}$	--
2	1	$\frac{1}{\delta^2} \left[\frac{1}{\delta} \ln\left(\frac{1+\delta}{1-\delta}\right) - 2 \right]$	$2 \left(\frac{1}{3} + \frac{1}{5}\delta^2 + \frac{1}{7}\delta^4 + \frac{1}{9}\delta^6 \right)$
2	2	$\frac{2}{\delta^2} \left[\frac{2-\delta^2}{1-\delta^2} - \frac{1}{\delta} \ln\left(\frac{1+\delta}{1-\delta}\right) \right]$	$\frac{2}{1-\delta^2} \left(\frac{1}{3} + \frac{4}{15}\delta^2 + \frac{4}{35}\delta^4 + \frac{4}{63}\delta^6 \right)$
2	3	$\frac{1}{\delta^2} \left[\frac{1}{\delta} \ln\left(\frac{1+\delta}{1-\delta}\right) - \frac{2-4\delta^2}{(1-\delta^2)^2} \right]$	$\frac{2}{(1-\delta^2)^2} \left(\frac{1}{3} + \frac{8}{35}\delta^2 + \frac{8}{105}\delta^4 + \frac{8}{315}\delta^6 \right)$

in the energy interval, namely $1/D_J^N$, and this has already been factored out in Eq. (8).) Therefore for $\delta = 0$ and for any value of N , evaluation of the integral reduces to averaging the product of the spectrum S and the cross section Σ_i for each reaction i .

Care is needed to obtain a numerically stable algorithm as δ approaches zero. Careful expansion of all those F_N^J that involve natural logarithms shows that as δ approaches zero the functions become insensitive to N , because of a series of exact cancellations of terms in powers of δ . For example, consider

$$F_1^0(\delta) = \frac{1}{\delta} \ln \left(\frac{1 + \delta}{1 - \delta} \right); \quad (10)$$

as δ approaches zero both δ and $\ln [(1 + \delta)/(1 - \delta)]$ approach zero. To obtain a stable algorithm we expand Eq. (10) in powers of δ :

$$F_1^0(\delta) = 2 \left(\delta + \frac{1}{3}\delta^3 + \frac{1}{5}\delta^5 + \frac{1}{7}\delta^7 + \dots \right). \quad (11)$$

For those cases in which $F_N^J(\delta)$ involves differences of natural logarithms, Table 1 shows the function expanded to show its small- δ limit. (All other cases shown in the table are numerically stable and smoothly approach the small- δ limit.) In GROUPIE, for $\delta > 10^{-3}$, the required integrals are expressed in analytic form for the lower-order (small (J, N)) functions, and recursion relations are used for higher-order (J, N) . For $\delta \leq 10^{-3}$, the small- δ expansions are used to obtain the required integrals. The result is an algorithm that is numerically stable over the entire range of δ . For small δ the expansion is accurate through δ^6 ; for $\delta = 10^{-3}$ this yields results accurate to 18 digits. In effect, then, all integrals are performed analytically, in a completely stable manner, and to the maximum accuracy achievable on all present computers.

Selection of Σ_0 and N

For each evaluation, in each group, for each of the reactions (total, elastic, capture, and fission), GROUPIE calculates the Bondarenko self-

shielded cross sections for 25 combinations of Σ_0 and N. The combinations used are as follows:

- (1) $N = 0$ The unshielded cross section. (This is equivalent to $N = 1$, $\Sigma_0 = \infty$.)

- (2-22) $N = 1$ 21 different values of Σ_0 . Bondarenko's approach² is to make Σ_0 equal to powers of 10 (i.e., 10^{-1} barn, 1 barn, 10 barns, etc.). However, because of variation in the magnitude of the total cross section in different isotopes and in different energy ranges, this approach often leads to a poor representation of the self-shielding curve; the values of Σ_0 are too far apart, especially in regions in which the self-shielding curve varies appreciably. Our approach is to make Σ_0 equal to 21 multiples of the unshielded group-averaged total cross section within each group. The multiples we use range from 1/1024 up to 1024 in steps of factors of 2. These values of Σ_0 thus span a range of over six orders of magnitude centered on the unshielded total cross section within each group.

- (23) $N = 1$,
 $\Sigma_0 = 0$ The flux-weighted, totally shielded cross section. These first 23 (Σ_0 , N) pairs span the entire range of Σ_0 from infinity (unshielded) to zero (totally shielded).

- (24) $N = 2$,
 $\Sigma_0 = 0$ The current-weighted, totally shielded cross section.

- (25) $N = 3$,
 $\Sigma_0 = 0$ The next moment in an expansion of the flux in a finite medium.¹³

Treatment of Negative Cross Sections

Cross sections are proportional to probabilities, and are thus positive or zero. Furthermore, neutrons can interact with the nucleus at any energy, so the total cross section Σ_T cannot be zero; thus Σ_T is positive.

Because the weighting function involves reciprocal powers of the total cross section, the weighting function can become infinite if the total cross section is not positive, and the group-averaging process can blow up. This problem does not arise with cross sections in the ENDL library,¹⁴ in which the total cross section is positive at all energies. However, one can obtain negative values when using ENDF/B total cross sections¹ that have been reconstructed from resonance parameters.⁷ This can occur either because of strong resonance-interference effects in the elastic cross section or because of a negative background provided by the evaluator. Regardless of how negative total cross sections arise, they cannot be correct. GROUPE considers any energy interval in which the total cross section is not positive to have zero probability of being correct and ignores such intervals; group averages are obtained using only those portions of the energy range of the group in which the total cross section is positive.

Output of Self-Shielded Cross Sections

Boncharenko self-shielded cross sections are calculated for 25 combinations of Σ_0 and N, and all of these cross sections are used to obtain multiband parameters. In the output listing, however, only 12 combinations of Σ_0 and N are represented; these are ($N = 0$, $\Sigma_0 = \text{arbitrary}$) (the unshielded case), ($N = 1$, $\Sigma_0 = x \langle \Sigma_T(0, 0) \rangle_G$, for $x = 256, 64, 16, 4, 1, 1/4, 1/16, 1/64, 1/256$, and 0), where $\langle \Sigma_T(0, 0) \rangle_G$ is the unshielded total cross section), and ($N = 2$, $\Sigma_0 = 0$).

The unshielded cross sections ($N = 0$, $\Sigma_0 = \text{arbitrary}$) are output directly, in barns. For each of the last 11 combinations of N and Σ_0 the output is not the corresponding self-shielded cross section itself, but rather an f-factor--the ratio of self-shielded to unshielded cross section:

$$f_i(\Sigma_0, N)_G = \frac{\langle \Sigma_i(\Sigma_0, N) \rangle_G}{\langle \Sigma_i(0, 0) \rangle_G} . \quad (12)$$

It requires an extra step for the user to obtain $\langle \Sigma_i(\Sigma_0, N) \rangle_G$ from the f-factor and the unshielded cross section, but tabulating the results in this form makes it easy to see the effect of self shielding, since f-factors of unity represent no self shielding at all. See Example Output Listings for details.

MULTIBAND PARAMETERS

Definitions

In the multiband method,³⁻⁵ each group is subdivided into a number of ranges, or bands, of total cross section. Unlike the probability-table method,¹⁵ which preassigns ranges of total cross section and explicitly determines the probability, or measure, of each range, the multiband method attempts to minimize the number of cross-section bands and at the same time to guarantee exact solutions to certain limiting transport cases.

If we examine the form taken by the neutron flux in real applications, we find that the extremes of narrow, intermediate, and wide resonances, and of optically thin, intermediate, or thick media can be described by a flux of the form

$$\frac{1}{(\Sigma_T(E) + \Sigma_0)^N}, \text{ for } \Sigma_0 \geq 0 \text{ and } N = 0, 1, 2, \dots$$

Therefore, to guarantee that multiband parameters can be used in a wide variety of applications and will exactly reproduce results in any system in which the flux can be described by the above expression, GROUPIE defines multiband weights and cross sections in an integral sense so that they exactly reproduce the previously calculated Bondarenko self-shielded cross sections.

To explain this procedure, we first transform the definition of the group-averaged cross section (Eq. (1)) from a Riemann integral over energy to a Lebesgue integral over the range of the total cross section. This is accomplished by first multiplying Eq. (1) by unity in the form of an integral, over total cross section, of a Dirac delta function:

$$\langle \Sigma_1(\Sigma_0, N) \rangle_G = \frac{\int_{E_G}^{E_{G+1}} \int_{\Sigma_T^*} \delta(\Sigma_T^* - \Sigma_T(E)) \Sigma_1(E) \frac{S(E)}{(\Sigma_T(E) + \Sigma_0)^N} dE d\Sigma_T^*}{\int_{E_G}^{E_{G+1}} \int_{\Sigma_T^*} (\Sigma_T^* - \Sigma_T(E)) \frac{S(E)}{(\Sigma_T(E) + \Sigma_0)^N} dE d\Sigma_T^*}. \quad (13)$$

Equation (13) represents a multiplication by unity in the sense that if the integral over Σ_T^* (the entire range of total cross section in the group) is performed first, Eq. (1) is recovered.

However, if integration over energy is carried out first, we obtain the equation

$$\langle \Sigma_i(\Sigma_0, N) \rangle = \frac{\int_{\Sigma_T^*} \Sigma_i(\Sigma_T^*) \frac{P(\Sigma_T^*)}{(\Sigma_T^* + \Sigma_0)^N} d\Sigma_T^*}{\int_{\Sigma_T^*} \frac{P(\Sigma_T^*)}{(\Sigma_T^* + \Sigma_0)^N} d\Sigma_T^*}, \quad (14)$$

where

$$P(\Sigma_T^*) = \frac{\int_{E_G}^{E_{G+1}} \delta(\Sigma_T^* - \Sigma_T(E)) S(E) dE}{\int_{E_G}^{E_{G+1}} S(E) dE} \quad (15)$$

and

$$\Sigma_i(\Sigma_T^*) P(\Sigma_T^*) = \int_{E_G}^{E_{G+1}} \delta(\Sigma_T^* - \Sigma_T(E)) \Sigma_i(E) S(E) dE. \quad (16)$$

(We have dropped the group index G in Eqs. (14), (15), and (16) to simplify the notation, but it is still implied.) From Eq. (15) it can be seen that the quantity $P(\Sigma_T^*) d\Sigma_T^*$ is a normalized probability distribution, representing the probability that the total cross section is within $d\Sigma_T^*$ of Σ_T^* in energy group G . Similarly, $\Sigma_i(\Sigma_T^*)$ is the average cross section for reaction i , obtained by averaging over all energy intervals in group G in which the total cross section is within $d\Sigma_T^*$ of Σ_T^* . Equation (14) can be rewritten compactly in the form

$$\langle \Sigma_i(\Sigma_0, N) \rangle = \frac{\left\langle \frac{\Sigma_i p}{(\Sigma_T + \Sigma_0)^N} \right\rangle}{\left\langle \frac{p}{(\Sigma_T + \Sigma_0)^N} \right\rangle}. \quad (17)$$

Rather than working with the continuous probability density $p(\Sigma_T^*)$ and the continuous cross section $\Sigma_i(\Sigma_T^*)$ we introduce a quadrature that is equivalent to the assumption that the total cross section takes on only certain discrete values. This is equivalent to the assumption that $p(\Sigma_T^*)$ can be represented by a weighted sum of B Dirac delta functions:

$$p_i(\Sigma_T^*) = \sum_{b=1}^B p_b \delta(\Sigma_{Tb} - \Sigma_T^*). \quad (18)$$

With this assumption, the integral in Eq. (14) can be replaced by a sum:

$$\langle \Sigma_i(\Sigma_0, N) \rangle = \frac{\sum_b \frac{\Sigma_{ib} p_b}{(\Sigma_{Tb} + \Sigma_0)^N}}{\sum_b \frac{p_b}{(\Sigma_{Tb} + \Sigma_0)^N}}. \quad (19)$$

(This procedure is analogous to that used in the multigroup method, in which the continuous energy is replaced by a number of discrete energy values, i.e., the average energies of the groups.) The new quantities p_b , Σ_{ib} , and Σ_{Tb} are the so-called multiband parameters; p_b is the band weight, Σ_{Tb} is the band average total cross section, and Σ_{ib} is the band average cross section for reaction i , for each of the B bands into which the range of total cross section is divided.

Determination of Multiband Parameters as a Moment Problem

If we know the band cross sections Σ_{ib} and Σ_{Tb} and the band weights p_b , we can use Eq. (19) to determine the self-shielded cross section corresponding to any (Σ_0, N) combination. On the other hand, if we know

values of the self-shielded cross section, Eq. (19) represents a system of coupled, nonlinear algebraic equations that must be solved for the band cross sections Σ_{ib} and Σ_{Tb} and for the band weights P_b .

This latter problem is a classic moment problem: for $\Sigma_0 = 0$ and various values of N , it becomes the Hausdorff moment problem,¹⁶ while for $N = 1$ and various values of Σ_0 it becomes the Stieltjes-Hilbert moment problem.¹⁶ Both of these problems have been widely studied, and only pertinent results will be given here.

First take $i = \text{Total}$. In this case, for B bands we have $2B$ unknowns: they are P_b and Σ_{Tb} , for $b = 1, 2, \dots, B$. Given $2B$ values of the self-shielded total cross section (arising from $2B$ different combinations of Σ_0 and N), the system of Eq. (19) can be solved uniquely for the P_b and the Σ_{Tb} . Given more than $2B$ values of the self-shielded total cross section, the system can be solved in some "best-fit" sense (e.g., least-squares or min-max).

Once the P_b and the Σ_{Tb} are known, the system of Eq. (19) is linear in the B unknowns Σ_{ib} , for $i = \text{elastic, capture, or fission}$; given B or more values of the self-shielded cross sections for reaction i , the system is easy to solve uniquely or in some "best fit" sense.

How Many Bands are Required?

If the multiband approach is to be a practical alternative to the multigroup method in all energy ranges, it must be demonstrated that only a few bands are needed to reproduce correctly the self-shielding effects that we expect to encounter in a wide variety of applications; clearly, if several hundred bands were required in each energy group, the method would not be economically feasible.

In a wide variety of applications, the neutron flux is of the form

$$\frac{1}{(\Sigma_T(L) + \Sigma_0)^N}, \quad \text{with } \Sigma_0 \geq 0 \text{ and } N = 1.$$

If we allow for all transport situations, so that Σ_0 can assume any value between 0 and ∞ , how many bands are required to reproduce the entire self-shielding curve to within some acceptable error? GROUPIE answers this

question by finding the smallest number of bands that can reproduce the 23 Bondarenko self-shielded total cross sections for which $N = 1$, which include values of Σ_0 between 0 and ∞ (the first cross section, for which $N = 0$, corresponds to $N = 1$, $\Sigma_0 = \infty$), to within a fractional error $\epsilon_{\max}$ chosen by the user. That is, GROUPIE finds the minimum number of bands such that

$$\left| \langle \Sigma_T(\Sigma_0, N) \rangle - \frac{\sum_b \frac{\Sigma_{Tb} P_b}{\Sigma_{Tb} + \Sigma_0}}{\sum_b \frac{P_b}{\Sigma_{Tb} + \Sigma_0}} \right| < \epsilon_{\max} \langle \Sigma_T(\Sigma_0, N) \rangle. \quad (20)$$

Table 2 presents results for the entire ENDL library¹⁴ using the TART 175-group structure. The table shows that the entire curve of self-shielded total cross sections can be reproduced within 0.1% accuracy for every material in the library with two or three (or occasionally four) bands. These results indicate that the multiband approach can be used in all energy groups and will be both accurate and economical of computer time.

Solution of the Multiband Equations

GROUPIE calculates multiband parameters for from one to five bands per energy group (one band per group is just the multigroup method). The user can specify the maximum number of bands per group. The program starts from one band per group, and increases the number of bands in any group until the entire self-shielding curve can be reproduced to within some allowable error or until the maximum is reached. (The output for any given material will have the same number of bands in each group, namely, the largest number of bands required in any group in the material. However, since fewer bands may be adequate in some groups, the weights of unused bands will be zero. For example, if three bands is the largest number required to reproduce the self-shielding in any group in ²³⁸U, but group 112 requires only two bands, the weight of the third band in group 112 will be zero.)

The most difficult point in solving the system of Eq. (19) for the band total cross sections and weights Σ_{Tb} and P_b is the fact that the equations are nonlinear in the Σ_{Tb} . In our solution, we use the fact that the solution to the system is not unique, in the sense that if we interchange the

TABLE 2. Maximum percent error in multiband fitting of self-shielded neutron total cross section using one, two, three, and four bands. Results are given for each evaluation in the ENDL library. (The TART 175-group structure was used in generating the self-shielded cross sections.)

Target	1 band ^a	2 band	3 band	4 band	Target	1 band	2 band	3 band	4 band
0-n-1	0.29	0.00			63-Eu-nat	132.52	0.71	0.01	
1-H-1	0.16	0.00			64-Gd-nat	456.50	2.25	0.05	
1-H-2	0.04	0.00			67-Ho-165	1825.96	6.73	0.43	0.02
1-H-3	0.03	0.00			73-Ta-181	1807.27	13.12	0.59	0.04
2-He-3	3.70	0.00			74-W-nat	2316.44	8.43	0.66	0.03
2-He-4	1.75	0.00			75-Re-185	1261.69	6.92	0.38	0.02
3-Li-6	3.97	0.01			75-Re-187	2104.84	9.00	0.37	0.06
3-Li-7	14.79	0.02			78-Pt-nat	260.57	2.36	0.05	
4-Be-7	4.01	0.00			79-Au-197	466.87	4.30	0.10	
4-Be-9	8.13	0.00			82-Pb-nat	4.15	0.01		
5-B-10	3.70	0.00			90-Th-231	8.18	0.01		
5-B-11	5.11	0.00			90-Th-232	5658.84	14.09	0.89	0.10
6-C-12	6.00	0.01			90-Th-233	3.69	0.00		
7-N-14	10.83	0.01			92-U-233	152.01	1.22	0.01	
8-O-16	73.31	0.40	0.00		92-U-234	3.42	0.00		
9-F-19	116.98	0.68	0.01		92-U-235	236.94	1.47	0.03	
11-Na-23	66.86	0.48	0.00		92-U-236	2818.67	5.44	0.15	0.01
12-Mg-nat	44.37	0.16	0.00		92-U-237	3.62	0.00		
13-Al-27	63.93	2.32	0.09		92-U-238	2990.51	8.23	0.44	0.03
14-Si-nat	174.90	0.77	0.01		92-U-239	18.42	0.04		
15-P-31	17.46	0.06			92-U-240	1.44	0.00		
16-S-32	32.72	0.28	0.00		93-Np-237	798.30	7.65	0.25	0.02
17-Cl-nat	89.16	0.93	0.02		94-Pu-238	1615.13	8.50	0.41	0.02
18-Ar-nat	17.11	0.01			94-Pu-239	623.01	3.57	0.08	
19-K-nat	165.07	1.53	0.07		94-Pu-240	6892.58	10.65	0.58	0.07
20-Ca-nat	89.78	0.54	0.01		94-Pu-241	87.37	0.18	0.00	
22-Ti-nat	314.87	3.04	0.11	0.00	94-Pu-242	2678.86	7.73	0.51	0.07
23-V-51	686.72	4.28	0.13	0.01	94-Pu-243	487.05	2.89	0.08	
24-Cr-nat	131.70	0.92	0.01		95-Am-241	322.40	2.01	0.07	
25-Mn-55	1155.01	2.89	0.11	0.01	95-Am-242	61.96	0.25	0.00	
26-Fe-nat	77.36	0.89	0.02		95-Am-243	532.32	2.61	0.06	
27-Co-59	225.18	3.02	0.10		96-Cm-242	991.85	6.06	0.30	0.01
28-Ni-nat	185.98	0.91	0.01		96-Cm-243	128.77	0.90	0.01	
28-Ni-58	190.58	1.18	0.01		96-Cm-244	1273.68	7.30	0.48	0.02
29-Cu-nat	19.90	0.06			96-Cm-245	132.99	0.95	0.01	
31-Ga-nat	43.36	0.12	0.00		96-Cm-246	669.11	3.46	0.13	0.00
40-Zr-nat	161.08	2.95	0.07		96-Cm-247	341.71	2.32	0.06	
41-Nb-93	274.08	3.91	0.10		96-Cm-248	847.79	5.41	0.15	0.01
42-Mo-nat	80.95	0.26	0.00		97-Bk-249	946.69	3.65	0.12	0.01
47-Ag-107	829.74	5.97	0.16	0.01	98-Cf-249	263.58	1.48	0.04	
47-Ag-109	1723.35	8.80	0.31	0.02	98-Cf-250	499.59	2.09	0.10	
48-Cd-nat	63.37	0.47	0.01		98-Cf-251	102.48	0.44	0.01	
50-Sn-nat	94.49	0.43	0.00		98-Cf-252	986.71	4.79	0.16	0.01
56-Ba-138	21.23	0.04			Th-232 Prod.	4.23	0.00		

^a1 band = unshielded multigroup cross sections.

parameters for any two bands we again obtain a solution. The solution becomes unique when we introduce an ordering into the parameters such as $\Sigma_{T1} < \Sigma_{T2} < \dots < \Sigma_{TB}$. The fact that the band cross sections are indistinguishable without ordering leads us to conclude that for B bands the B total cross sections will be the roots of a Bth-order polynomial. Since polynomials of order four or less have analytic solutions that can be obtained by a change of variables, which essentially introduces an ordering, we expect that there is an analytic solution for the multiband parameters for the case of four or fewer bands. Since polynomials of order five or higher are irreducible, only iterative solutions exist for five or more bands.

GROUPIE uses an analytic solution for two bands and an iterative solution for more than two bands. Table 2 shows that few isotopes require more than two bands per group; for these isotopes, only a few groups require more than two bands. Therefore the approach used in GROUPIE is extremely economical, since most solutions will be analytical, and yet extremely accurate, because of the use of iteration to calculate band parameters accurately in any group that requires more than two bands.

The next section describes the solution for two bands; the section following that describes the solution for three, four, or five bands (the "multiband" problem).

Two Bands. For two bands, the total cross section equations (Eq. (19), with $i = \text{Total}$) have four unknowns: P_1 , P_2 , Σ_{T1} , and Σ_{T2} . The user may choose either of two sets of four coupled equations to be solved analytically for these two-band parameters. The first three equations are, in either case,

$$1 = P_1 + P_2, \quad (21)$$

$$\langle \Sigma_T \rangle = P_1 \Sigma_{T1} + P_2 \Sigma_{T2}, \quad (22)$$

and

$$\frac{1}{\Sigma_T} = \frac{P_1}{\Sigma_{T1}} + \frac{P_2}{\Sigma_{T2}}. \quad (23)$$

For the fourth equation, what we call Method 1 uses

$$\frac{1}{\Sigma_T} = \frac{P_1}{\Sigma_{T1}} + \frac{P_2}{\Sigma_{T2}}, \quad (24)$$

and Method 2 uses

$$\frac{1}{\Sigma_T + \Sigma_0} = \frac{P_1}{\Sigma_{T1} + \Sigma_0} + \frac{P_2}{\Sigma_{T2} + \Sigma_0}. \quad (25)$$

By taking ratios, one can show Eq. (21) to be equivalent to a normalized probability distribution, Eq. (22) to conservation of the unshielded, flux-weighted cross section, and Eq. (23) to conservation of the distance to collision, or totally shielded, flux-weighted cross section. Equation (24) (method 1) is equivalent to conservation of the totally shielded, current-weighted cross section, and Eq. (25) (method 2) to conservation of the partially shielded, flux-weighted cross section. If method 2 is used, the program will take Σ_0 equal to the unshielded total cross section for that group (i.e., $\Sigma_0 = \langle \Sigma_T \rangle$).

The discussion at the end of the preceding section indicates that the parameters we seek are the roots of second-order polynomials--that is, solutions of quadratic equations. The standard change of variables used to solve quadratic equations is, in this case,

$$\begin{aligned} P_1 &= 1/2 + D, & \Sigma_{T1} &= 1/X_1, & X_1 &= A + B, \\ P_2 &= 1/2 - D, & \Sigma_{T2} &= 1/X_2, & X_2 &= A - B. \end{aligned} \quad (26)$$

This change of variables immediately satisfies Eq. (21); the remaining equations can be readily solved for A, B, and D. The equations of method 1 yield

$$A = \frac{1}{2} \frac{\frac{1}{\Sigma_T^2}}{\frac{1}{\Sigma_T}} \left[\frac{\langle \Sigma_T \rangle - \frac{\frac{1}{\Sigma_T}}{\frac{1}{\Sigma_T^2}}}{\langle \Sigma_T \rangle - \frac{1}{\frac{1}{\Sigma_T}}} \right],$$

$$B^2 = \frac{\langle \Sigma_T \rangle A^2 - 2A + \frac{1}{\Sigma_T}}{\langle \Sigma_T \rangle},$$

$$D = \frac{\frac{1}{\Sigma_T} - A}{2B}. \quad (27a)$$

Similarly, the equations of method 2 yield

$$A = \frac{1}{2} \frac{1}{\Sigma_T} \left\{ 1 + \frac{\langle \Sigma_T \rangle}{\Sigma_0} \left[\frac{\langle \Sigma_T(\Sigma_0, 1) \rangle - \frac{1}{\frac{1}{\Sigma_T}}}{\langle \Sigma_T \rangle - \langle \Sigma_T(\Sigma_0, 1) \rangle} \right] \right\},$$

$$B^2 = A^2 - \frac{\frac{1}{\Sigma_T}}{\Sigma_0} \left[\frac{\langle \Sigma_T(\Sigma_0, 1) \rangle - \frac{1}{\frac{1}{\Sigma_T}}}{\langle \Sigma_T \rangle - \langle \Sigma_T(\Sigma_0, 1) \rangle} \right],$$

$$D = \frac{\frac{1}{\Sigma_T} - A}{2B}. \quad (27b)$$

As expected, the solutions are not unique, since the equations for B have both positive and negative roots. From the definitions of Σ_1 , Σ_2 , and D, it can be seen that changing the sign of B yields the same band parameters with the band numbers interchanged. Since the choice is arbitrary, for definiteness we use the positive root for B; this introduces the ordering $\Sigma_{T1} < \Sigma_{T2}$, and makes the solution unique. The parameters A, B, and D have all been expressed in terms of quantities normally available in a library of Bondarenko self-shielded cross sections. These quantities are

$$\langle \Sigma_T \rangle = \langle \Sigma_T(\text{arb}, 0) \rangle$$

(the unshielded (or infinitely dilute) total cross section),

$$\frac{1}{\langle \frac{1}{\Sigma_T} \rangle} = \langle \Sigma_T(0, 1) \rangle$$

(the totally shielded, flux-weighted total cross section), and (for Eq. (27a))

$$\frac{\frac{1}{\Sigma_T}}{\langle \frac{1}{\Sigma_T^2} \rangle} = \langle \Sigma_T(0, 2) \rangle$$

(the totally shielded, current-weighted total cross section) or (for Eq. (27b))

$$\Sigma_0 \text{ and } \langle \Sigma_T(\Sigma_0, 1) \rangle$$

(the partially shielded, flux-weighted total cross section). In this last case the value of Σ_0 used by GROUPIE is $\langle \Sigma_T \rangle$.

Once the band weights P_b and the band total cross sections Σ_{Tb} are known, we may proceed to solve Eq. (19) for each reaction i . Equation (19) is linear in the band cross sections Σ_{ib} for the remaining reactions (elastic, capture, and fission). There are just two unknowns for each reaction, Σ_{i1} and Σ_{i2} ; these are solved for exactly rather than by a fitting procedure, using equations resulting from the insertion of $N = 0$, Σ_0 arbitrary and $N = 1$, $\Sigma_0 = 0$ in Eq. (19).

For $N = 0$ (unshielded cross section),

$$\frac{\sum \Sigma_{ib} P_b}{\sum P_b} = \sum \Sigma_{ib} P_b = \Sigma_{i1} P_1 + \Sigma_{i2} P_2 = \langle \Sigma_i(\text{arb}, 0) \rangle \equiv \langle \Sigma_i \rangle. \quad (28)$$

For $N = 1$, $\Sigma_0 = 0$ (totally shielded cross section),

$$\frac{\sum \frac{\Sigma_{ib} P_b}{\Sigma_{Tb}}}{\sum \frac{P_b}{\Sigma_{Tb}}} = \frac{\sum \frac{\Sigma_{ib} P_b}{\Sigma_{Tb}}}{\langle \frac{1}{\Sigma_T} \rangle} = \langle \Sigma_i(0, 1) \rangle;$$

we rewrite this as

$$\sum \frac{\Sigma_{ib} P_b}{\Sigma_{Tb}} = \frac{\Sigma_{i1} P_1}{\Sigma_{T1}} + \frac{\Sigma_{i2} P_2}{\Sigma_{T2}} = \langle \Sigma_i(0, 1) \rangle \langle \frac{1}{\Sigma_T} \rangle \equiv \left\langle \frac{\Sigma_i}{\Sigma_T} \right\rangle. \quad (29)$$

We change variables to

$$\begin{aligned}\Sigma_{i1} &= \langle \Sigma_i \rangle - \frac{C_i}{P_1} \\ \Sigma_{i2} &= \langle \Sigma_i \rangle + \frac{C_i}{P_2},\end{aligned}\quad (30)$$

which immediately satisfies Eq. (28). We substitute Eqs. (30) into Eq. (29), solve for C_i ,

$$C_i = \frac{\langle \Sigma_i \rangle \left\langle \frac{1}{\Sigma_T} \right\rangle - \left\langle \frac{\Sigma_i}{\Sigma_T} \right\rangle}{\frac{1}{\Sigma_{T1}} - \frac{1}{\Sigma_{T2}}}, \quad (31)$$

and all band parameters are completely determined.

Three or More Bands. If the user allows more than two bands, the program will automatically determine the minimum number of bands required in each group to reproduce the entire self-shielding curve ($N = 1$, $\Sigma_0 = 0$ to ∞) to within some user-specified tolerance. The program will start with the two-band solution (method 2) and determine the maximum fractional error at any of the 23 values of Σ_0 . If all errors are less than that specified by the user, two bands are enough. If the self-shielded cross section for one or more values of Σ_0 has a larger fractional error than that allowed by the user, the program will increase the number of bands to three, solve for the total band cross sections and weights, and again check for convergence. The program will continue to increase the number of bands until either convergence occurs or the maximum number of bands specified by the user is reached.

For more than two bands, the system of Eq. (19) is solved by iteration (as opposed to the analytical solution for two bands). If we know the self-shielded cross section $\langle \Sigma_T(\Sigma_0, N) \rangle$ for 25 combinations of (Σ_0, N) , approximating the total cross section probability by B bands leads to a fractional error

$$\varepsilon_T(\varepsilon_0, N) = \left| \frac{\langle \varepsilon_T(\varepsilon_0, N) \rangle - \frac{\sum_b \frac{\varepsilon_{Tb} P_b}{(\varepsilon_{Tb} + \varepsilon_0)^N}}{\sum_b \frac{P_b}{(\varepsilon_{Tb} + \varepsilon_0)^N}}}{\langle \varepsilon_T(\varepsilon_0, N) \rangle} \right|. \quad (32)$$

Upon multiplying and adding and subtracting terms, this becomes

$$\varepsilon_T(\varepsilon_0, N) = \frac{(\langle \varepsilon_T(\varepsilon_0, N) \rangle + \varepsilon_0) \sum_b \frac{P_b}{(\varepsilon_{Tb} + \varepsilon_0)^N} - \sum_b \frac{P_b}{(\varepsilon_{Tb} + \varepsilon_0)^{N-1}}}{\langle \varepsilon_T(\varepsilon_0, N) \rangle \sum_b \frac{P_b}{(\varepsilon_{Tb} + \varepsilon_0)^N}}. \quad (33)$$

From Eq. (33), we see that to have $\varepsilon_T = 0$ we require

$$(\langle \varepsilon_T(\varepsilon_0, N) \rangle + \varepsilon_0) \sum_b \frac{P_b}{(\varepsilon_{Tb} + \varepsilon_0)^N} = \sum_b \frac{P_b}{(\varepsilon_{Tb} + \varepsilon_0)^{N-1}}. \quad (34)$$

We solve this expression for the sum on the left, and, setting $N = 0, 1, 2, \dots$, obtain approximate expressions for the sum in the denominator of Eq. (33) and for the sum with the $N-1$ exponent. For $N = 0$ we obtain

$$Q_0 \equiv \sum_b P_b = 1;$$

for $N = 1, 2, 3, \dots$, we obtain

$$Q_1 = \sum_b \frac{P_b}{\varepsilon_{Tb} + \varepsilon_0} \approx \frac{1}{\langle \varepsilon_T(\varepsilon_0, 1) \rangle + \varepsilon_0},$$

$$Q_2 = \sum_b \frac{P_b}{(\varepsilon_{Tb} + \varepsilon_0)^2} \approx \frac{1}{(\langle \varepsilon_T(\varepsilon_0, 1) \rangle + \varepsilon_0) (\langle \varepsilon_T(\varepsilon_0, 2) \rangle + \varepsilon_0)},$$

etc., and finally

$$Q_N = \sum_b \frac{P_b}{(\varepsilon_{Tb} + \varepsilon_0)^N} \approx \frac{1}{(\langle \varepsilon_T(\varepsilon_0, 1) \rangle + \varepsilon_0) \times \dots \times (\langle \varepsilon_T(\varepsilon_0, N) \rangle + \varepsilon_0)}. \quad (35)$$

Substitution of this approximation into Eq. (33) leads to a coupled set of nonlinear equations, in which the unknowns P_b and Σ_{Tb} are in separable form:

$$\epsilon_T(\Sigma_0, N) = \left| \frac{(\langle \Sigma_T(\Sigma_0, N) \rangle + \Sigma_0) \sum_b \frac{P_b}{(\Sigma_{Tb} + \Sigma_0)^N} - Q_{N-1}}{\langle \Sigma_T(\Sigma_0, N) \rangle Q_N} \right|. \quad (36)$$

"Separable" implies that the unknowns appear in the form $\sum_i a_i f_i(x)$; here $a_i = P_b$, $x = \Sigma_0$, and

$$f_i(x) = \frac{1}{(\Sigma_{Tb} + \Sigma_0)^N}.$$

The resulting set of equations (Eq. (36)), for 25 combinations of (Σ_0, N) is then solved by using a standard set of linear (for P_b) and non-linear (for Σ_{Tb}) matrix routines, MLR¹⁷ and ZXSSQ,¹⁸ which use an iterative algorithm originally proposed by F. N. Fritsch.¹⁹

As in most iterative schemes, the speed of convergence depends crucially on making a good initial guess, so that one can start close to the solution. In GROUPIE, this is done by keeping track of the range of the total cross section (maximum and minimum) while computing the Bondarenko self-shielded cross sections. The initial guesses for the band weights and total cross sections are supplied by Gaussian quadrature points distributed about the unshielded total cross section in such a way that the system will start out exactly conserving both the sum of the band weights and the unshielded total cross sections. After each non-linear iteration, the results are renormalized to again exactly conserve these two quantities.

Once the band weights P_b and the total cross sections Σ_{Tb} are known, for each other reaction i the error associated with using B bands is

$$\epsilon_i(\Sigma_0, N) = \left| \frac{\langle \Sigma_i(\Sigma_0, N) \rangle - \frac{\sum_b \frac{\Sigma_{ib} P_b}{(\Sigma_{Tb} + \Sigma_0)^N}}{\sum_b \frac{P_b}{(\Sigma_{Tb} + \Sigma_0)^N}}}{\langle \Sigma_i(\Sigma_0, N) \rangle} \right|. \quad (37)$$

This system is linear in the band cross sections Σ_{ib} , and is solved for each reaction i (i = elastic, capture or fission) by using the standard matrix solver MLR¹⁷ (Minimize Linear Residuals), which minimizes the maximum error associated with each of the corresponding 25 self-shielded cross sections.

Physically and Mathematically Acceptable Parameters

The physical basis of the quantities P_b and Σ_{ib} leads us to impose constraints on their values. Furthermore, the fact that in the calculation of multi-band parameters a set of integrals is replaced by a set of sums--that is,

$$\frac{\bar{\Sigma}_i}{(\Sigma_T + \Sigma_0)^N} = \int_{T_{\min}}^{T_{\max}} \frac{\bar{\Sigma}_i(\Sigma_T) p(\Sigma_T) d\Sigma_T}{(\Sigma_T + \Sigma_0)^N} = \sum_b \frac{\Sigma_{ib} P_b}{(\Sigma_{Tb} + \Sigma_0)^N}, \quad (38)$$

leads us to impose additional mathematical constraints on the multi-band parameters.

Since $p(\Sigma_T)$ is a normalized probability density, each of the band weights P_b should be positive and no greater than unity, and the weights should sum to unity:

$$0 \leq P_b \leq 1$$

and

$$\sum_b P_b = 1. \quad (39)$$

For each reaction i (i = total, elastic, etc.), the multiband cross section Σ_{ib} should lie in the range between the minimum and maximum values reached by the corresponding cross section in each energy group. This condition is particularly important: if it is not met, it is possible to obtain erroneous solutions in which the equivalent group-averaged cross section for one or more reactions lies outside of the cross section range for those reactions.

The algorithms presented in the preceding sections for the calculation of the multiband parameters will satisfy both these criteria as long as consistent cross section moments are used. For example, in the two-band

algorithms presented in the preceding section it may be seen from Eq. (26) that the two band weights will always sum to unity. However, they will be positive only if $|D| \leq 1/2$. By substituting for A and B in the equation for D (Eq. (31a)) we can express the condition $|D| \leq 1/2$ as

$$\left\langle \frac{1}{\Sigma_T^2} \right\rangle \geq \left\langle \frac{1}{\Sigma_T} \right\rangle^2, \quad (40)$$

this is true for any function, and in particular for $1/\Sigma_T$. Therefore, in principle, this condition should always be satisfied; indeed, it is always satisfied when the Bondarenko self-shielded cross sections are calculated using analytic integrals. However, when iterative integration is used, the condition is not always satisfied. Obviously if both integrals are performed to within some accuracy ϵ , and if the integrals differ by less than 2ϵ , this inequality may be violated, resulting in physically unacceptable multiband parameters.

To illustrate the set of inequalities that the Bondarenko self-shielded cross sections must satisfy to be mathematically acceptable, consider what happens when we fix N and vary Σ_0 , or fix Σ_0 and vary N. Starting from the definition of the Bondarenko self-shielded total cross section,

$$\langle \Sigma_T(\Sigma_0, N) \rangle = \frac{\left\langle \frac{\Sigma_T}{(\Sigma_T + \Sigma_0)^N} \right\rangle}{\left\langle \frac{1}{(\Sigma_T + \Sigma_0)^N} \right\rangle}, \quad (41)$$

what happens when we fix N and vary Σ_0 ? The answer is obtained by examination of the partial derivative

$$\frac{\partial}{\partial \Sigma_0} \langle \Sigma_T(\Sigma_0, N) \rangle = N \frac{\left\langle \frac{1}{(\Sigma_T + \Sigma_0)^{N-1}} \right\rangle \left\langle \frac{1}{(\Sigma_T + \Sigma_0)^{N+1}} \right\rangle - \left\langle \frac{1}{(\Sigma_T + \Sigma_0)^N} \right\rangle^2}{\left\langle \frac{1}{(\Sigma_T + \Sigma_0)^N} \right\rangle^2}. \quad (42)$$

What happens when we fix Σ_0 and vary N ? In this case, we examine the difference

$$\begin{aligned} & \langle \Sigma_T(\Sigma_0, N) \rangle - \langle \Sigma_T(\Sigma_0, N+1) \rangle \\ &= \frac{\left\langle \frac{1}{(\Sigma_T + \Sigma_0)^{N-1}} \right\rangle \left\langle \frac{1}{(\Sigma_T + \Sigma_0)^{N+1}} \right\rangle - \left\langle \frac{1}{(\Sigma_T + \Sigma_0)^N} \right\rangle^2}{\left\langle \frac{1}{(\Sigma_T + \Sigma_0)^N} \right\rangle \left\langle \frac{1}{(\Sigma_T + \Sigma_0)^{N+1}} \right\rangle}. \end{aligned} \quad (43)$$

Note that the numerators of both expressions are identical. By use of the Cauchy-Schwarz inequality,²⁰ it can be shown that this numerator is always greater than or equal to zero, with equality only in the case of a constant total cross section across the entire energy group. Therefore, for fixed N , increasing Σ_0 cannot decrease the self-shielded cross section:

$$\langle \Sigma_T(\Sigma_1, N) \rangle \geq \langle \Sigma_T(\Sigma_2, N) \rangle, \quad (\Sigma_1 > \Sigma_2).$$

Similarly, for fixed Σ_0 , decreasing N cannot decrease the self-shielded cross section:

$$\langle \Sigma_T(\Sigma_0, M) \rangle \geq \langle \Sigma_T(\Sigma_0, N) \rangle, \quad (M < N). \quad (44)$$

The moments of a total cross section must satisfy these inequalities to be physically and mathematically acceptable. If a set of moments used to generate multiband parameters does not satisfy these conditions, one should not be surprised to obtain physically unacceptable multiband parameters (e.g., negative band weights or cross sections); such a result merely indicates that no physical cross section distribution corresponds to those moments. Therefore it is recommended that any multigroup processor that generates self-shielded cross sections ensure that the above inequalities are satisfied.

Since GROUPIE performs all integrals analytically, these inequalities are always satisfied. However, care must still be exercised when there is very little self-shielding. For example, in the limit of a constant total cross section, all self-shielded cross sections will be exactly equal. In this case the moment equations (Eq. (19)) used to determine the multiband parameters will no longer be linearly independent, and the solution will no longer be

unique. In particular, the band weights are not unique since the equations can be satisfied by setting all band cross sections equal to the unshielded total cross section, and using any set of band weights that sum to unity.

GROUPIE avoids this problem by recognizing that, when there is little or no self-shielding, the total cross section will be almost constant across the energy group, and that it can be represented by a single band (one band per group is the normal multigroup method). Since $\langle \Sigma_T(\Sigma_0, N) \rangle$ will be monotonically increasing for increasing Σ_0 and fixed N , this condition of nearly constant cross section can be found by comparing the unshielded and totally shielded cross sections; if

$$\langle \Sigma_T(0, 0) \rangle - \langle \Sigma_T(0, 1) \rangle < \epsilon \langle \Sigma_T(0, 0) \rangle, \quad (15)$$

a single band of weight unity and cross section $\langle \Sigma_T(0, 0) \rangle$ is adequate to represent the group.

Output of Multiband Parameters

Multiband parameters are output in both listed and computer-readable form. The listing is designed for desk-top use so that one can see where multiband effects are important (see Example Output Listings). The computer-readable multiband parameters can either be used directly in transport calculations,^{4,21} or to calculate Bondarenko self-shielded cross sections for use in the usual multigroup calculations (i.e., use Eq. (19) to determine the self-shielded cross section for any (Σ_0, N) combination).

USE OF MULTIBAND PARAMETERS

USE OF THE MULTIBAND METHOD IN TRANSPORT CALCULATIONS

Starting from G energy groups and using B bands in each group results in a coupled set of $G \times B$ multigroup, multiband equations.^{3,4} Mathematically these equations are identical to a set of $G \times B$ multigroup equations, which can be solved for the neutron flux by existing transport codes.²² Once the

multiband cross sections are determined a multigroup processor must provide only the source and transfer matrices to describe the multigroup, multiband equations completely.^{3,4}

The multiband parameters are output by GROUPIE in a form that can be used directly in transport calculations to account for self-shielding effects due to elastic scattering, capture, and fission. The parameters output by GROUPIE are weights and cross sections for total, elastic, capture, and fission. For the 175 energy groups usually used at Livermore⁵ it is an excellent approximation to ignore self-shielding in other reactions. If one is using a significantly smaller number of groups this approximation may not be valid, and self-shielding should be considered, particularly for (n, charged particle) reactions in light nuclides. For each reaction except elastic, capture, and fission, the cross section in all bands within a group should be equal to its group-averaged value, indicating no self-shielding. For consistency, it is recommended that the total cross section for each band be calculated by summing the partial cross sections for all reactions, i.e., the band elastic, capture, and fission cross sections, and the group-averaged cross sections for all other reactions.

A multigroup source can be converted into a group-band source by distributing the group source between bands within each group according to the weight of each band. That is, set

$$S_{G,B} = P_{G,B} S_G, \quad (46)$$

where

$S_{G,B}$ = the source for band B in group G,

$P_{G,B}$ = the weight for band B in group G, and

S_G = the source for group G (normal multigroup source).

In distributing the source between bands in this manner, one assumes that there is no correlation between the value of the source at any energy, $S(E)$, and the value of the total cross section at that energy, $\Sigma_T(E)$; this assumption is almost always correct.

A multigroup (group-to-group) transfer matrix can be written in the form

$$f_L(G' \rightarrow G) = \sum_i m_i \langle \Sigma \rangle_{iG} g_{iL}(G' \rightarrow G), \quad (47)$$

where

- $f_l(G' \rightarrow G)$ = the total transfer probability for Legendre component l from group G' to group G ,
 i = identifies reactions (elastic, fission, etc.),
 m_i = the multiplicity (number of emitted particles) for reaction i ($m = 1$ for elastic scattering, $m = \nu(E)$ for fission, $m = 2$ for $(n, 2n)$ reactions),
 $\langle \Sigma \rangle_{iG}$ = the group-averaged cross section for reaction i in group G , and
 $g_{il}(G' \rightarrow G)$ = the probability (normalized when summed over G) of transfer from G' to G due to reaction i .

The equivalent multiband transfer matrix can be obtained from this expression by recognizing that the multiplicity m_i and probability of transfer from one energy group to another $g_{il}(G \rightarrow G')$ are independent of the magnitude of the cross section. Therefore m_i and $g_{il}(G \rightarrow G')$ should be the same for all bands in group G' . The probability of interaction in band B' of group G' is represented by the group-band cross section $\langle \Sigma_i \rangle_{G'B}$, instead of the group-averaged cross section $\langle \Sigma_i \rangle_G$. The probability of arriving in band B of group G is merely the probability of arriving in group G (represented by $g_{il}(G' \rightarrow G)$) times the probability of arriving in band B (represented by P_{GB}). The group-band transfer matrix can thus be written as

$$f_l(G'B' \rightarrow GB) = P_{GB} \sum_i m_i \langle \Sigma_i \rangle_{G'B} g_{il}(G' \rightarrow G), \quad (48)$$

where m_i and $g_{il}(G' \rightarrow G)$ are the terms in the group-to-group transfer matrix, and P_{GB} and $\langle \Sigma_i \rangle_{G'B}$ are the multiband parameters just defined. Therefore, starting from a multigroup transfer matrix for G groups in which each reaction is represented separately, the multiband transfer matrix for GB group bands can be determined immediately. If only the total multigroup transfer matrix is available, the above arguments lead to the excellent approximation^{3,4}

$$f_l(G'B' \rightarrow GB) = P_{GB} \frac{\langle \Sigma_T \rangle_{G'B'}}{\langle \Sigma \rangle_{TG}} f_l(G' \rightarrow G), \quad (49)$$

where $\langle \Sigma \rangle_{TG}$, and $f_g(G' \rightarrow G)$ are the group-to-group expressions and P_{GB} and $\langle \Sigma_T \rangle_{G'B'}$ are multiband parameters.

SELF-SHIELDED CROSS SECTIONS FROM MULTI-BAND PARAMETERS

Cross Sections for Single Materials

From their definition, it is obvious that once the multiband parameters are known they can be used to determine Bondarenko self-shielded cross sections for any given values of Σ_0 and N :

$$\Sigma_i(\Sigma_0, N) = \frac{\sum_b \frac{\Sigma_{ib} P_b}{(\Sigma_{Tb} + \Sigma_0)^N}}{\sum_b \frac{P_b}{(\Sigma_{Tb} + \Sigma_0)^N}}. \quad (50)$$

The fact that all 25 values of the self-shielded cross section can be reproduced using only a few bands indicates that the use of multiband parameters, which are valid for all values of Σ_0 , is faster and more accurate than interpolating in tables of $\langle \Sigma_i(\Sigma_0, N) \rangle$ to obtain the cross section between tabulated values.

To see what functional form is being assumed when multiband parameters are used to determine Bondarenko self-shielded cross sections, let us examine the case $N = 1$. Upon multiplying by the product of terms

$$\prod_b (\Sigma_{Tb} + \Sigma_0)$$

and collecting terms in like powers of Σ_0 , we find that a rational approximation in Σ_0 is being used, namely

$$\langle \Sigma_i(\Sigma_0, 1) \rangle = \frac{\langle \Sigma_i(\infty, 1) \rangle \Sigma_0^{B-1} + A_{n-1} \Sigma_0^{B-2} + \dots + A_1 \Sigma_0 + A_0}{\Sigma_0^{B-1} + B_{n-1} \Sigma_0^{B-2} + \dots + B_1 \Sigma_0 + A_0 / \langle \Sigma_i(0, 1) \rangle}, \quad (51)$$

where B is the number of bands. In this form, the equation explicitly defines the limit for $\Sigma_0 = 0$ ($\langle \Sigma_i(0, 1) \rangle$), and the limit as Σ_0 approaches infinity

$\langle \sigma_i(\infty, 1) \rangle$). All the coefficients A_i and C_i can be shown to be positive, so that the polynomials in the numerator and denominator have no real roots. Therefore the rational approximation is well behaved over the entire range of Σ_0 (from 0 to ∞).

Cross Sections for Constituents of Mixtures

Normally, when tabulated Bondarenko self-shielded cross sections are used for a mixture of materials, one must iterate to obtain the correct value of Σ_0 for each material. With multiband parameters, the self-shielded cross section for any reaction i in any constituent isotope j of a mixture of M materials can be written directly, without iteration, as²³

$$\frac{\Sigma_i}{(\Sigma_T + \Sigma_0)^N} G_{i,j} = \sum_{b1} \sum_{b2} \dots \sum_{bM} \frac{\Sigma_{ibj} p_{b1} p_{b2} \dots p_{bM}}{(\Sigma_{Tb1} + \Sigma_{Tb2} + \dots + \Sigma_{TbM} + \Sigma_0)^N} \quad (52)$$

(divided by the appropriate normalization factor), where

Σ_{ibj} = the band cross section for band b , reaction i , in isotope j ,
($j = 1, 2, \dots, M$),

Σ_{Tbk} = the band total cross section for band b , isotope k ,

Σ_0 = the effect of all nonresonant isotopes (if any), and

p_{bk} = the band weight for isotope k .

INTERMEDIATE RESONANCES

The procedures described above involve the use of multiband parameters with an assumed self-shielding factor of the Bondarenko form,

$$\frac{1}{(\Sigma_T + \Sigma_0)^N} \quad (53)$$

Although the quadrature points for the bands were selected to reproduce exactly the effect of Bondarenko self-shielding, the resulting quadrature set yields excellent approximations to the effects of other self-shielding

models. (Gaussian quadrature gives another example of this phenomenon: it is constructed to give exact results for polynomials, but it yields excellent results for other functions.)

For example, the multiband parameters can be used to obtain self-shielded cross sections using an intermediate-resonance model,²⁴ which is equivalent to using a self-shielding factor of the form^{4,25}

$$\frac{\Sigma_m + \lambda \Sigma_s}{\Sigma_m + \Sigma_a + \lambda \Sigma_s},$$

where

Σ_m = the moderator cross section,

Σ_s = the elastic scattering cross section,

Σ_a = the absorption cross section, and

λ = the intermediate resonance parameter (group-averaged value).^{4,25}

With B bands and known intermediate-resonance parameter λ , it is possible to define group-average cross sections using the intermediate-resonance model:

$$\langle \Sigma_i \rangle = \frac{\sum_b \Sigma_{ib} w_b}{\sum_b w_b},$$

where w_b is merely the intermediate-resonance weighting function

$$w_b = \frac{\Sigma_{mb} + \lambda \Sigma_{sb}}{\Sigma_{mb} + \Sigma_{ab} + \lambda \Sigma_{sb}}.$$

In many cases of interest, this weighting function is very simple; for example, if the moderator cross section is constant, the self-shielding factor in each band is simply

$$\frac{\Sigma_m + \lambda \Sigma_{sb}}{\Sigma_m + \Sigma_{ab} + \lambda \Sigma_{sb}} \quad (\Sigma_m \text{ is independent of } b).$$

To see how to include intermediate-resonance effects directly in multiband transport calculations, see refs. 4 and 25.

Where the absorption and scattering cross sections are approximately proportional to the total, i.e., where

$$\Sigma_{ab} \approx A\Sigma_{Tb}$$

and

$$\Sigma_{sb} \approx S\Sigma_{Tb} + \Sigma_p, \quad (54)$$

the intermediate-resonance weighting function is equivalent to

$$\frac{\Sigma_m + \lambda\Sigma_p + \lambda S\Sigma_{Tb}}{\Sigma_m + \Sigma_p + (A + \lambda S)\Sigma_{Tb}} = \frac{\Sigma_0 + c\Sigma_{Tb}}{\Sigma_0 + \Sigma_{Tb}}, \quad (55)$$

where

$$\Sigma_0 = \frac{\Sigma_m + \lambda\Sigma_p}{A + \lambda S} \quad (56)$$

and

$$c = \frac{\lambda S}{A + \lambda S}.$$

From Eq. (55), we see that the weight for intermediate resonances is a linear combination of the unshielded and shielded weights, since

$$\frac{\Sigma_0 + c\Sigma_{Tb}}{\Sigma_0 + \Sigma_{Tb}} = c + \frac{(1 - c)\Sigma_0}{\Sigma_0 + \Sigma_{Tb}}. \quad (57)$$

Therefore, in general, when Eq. (54) holds, we expect the intermediate-resonance result to be expressible in terms of unshielded and shielded results. In particular, when the absorption resonance contribution is much greater than the scattering resonance contribution (as in the resonance region of most fissile isotopes), the quantity c becomes small, and the weighting becomes identical to the Bondarenko weighting of $(\Sigma_T + \Sigma_0)^{-1}$ with an equivalent Σ_0 given by Eq. (56).

PROGRAM USE--GENERAL

LIMITATIONS AND ASSUMPTIONS

GROUPIC uses only the ENDF/B BCD format (as opposed to binary). It copies all sections except File 3 as Hollerith. Since the ENDF/B format is the same for File 3 in all versions of ENDF/B, this program can be used to process data in the ENDF/B-I, II, III, IV, or V formats.

If ENDF/B-formatted output is requested, this program outputs the entire ENDF/B evaluation, not just the cross sections treated in the program. Thus the output from this program is complete and in a form suitable for direct use in subsequent processing codes.

All File 3 cross sections (see Ref. 1) must be linearly interpolable over their entire energy range. The program checks the interpolation law for each cross section and aborts if any cross section is not linearly interpolable. Therefore it is recommended that ENDF/B tapes be linearized using program LINEAR⁶ as soon as they are received.

Because all data handling in this code is performed in pages²⁶ there is no limit to the number of data points used to represent any given reaction.

Evaluations can be in MAT or ZA order.¹ When data are requested using MAT (or ZA) the program assumes the data are ordered by MAT (or ZA). Once the program finds an evaluation with a MAT or ZA value larger than the largest value requested, it assumes that all requested evaluations have been processed and does not search any further.

The algorithms in this program are designed to handle any number of energy groups. The present core allocation is for a maximum of 175 energy groups; this limit can easily be extended if the user wishes to allocate additional core storage.

GROUPIC can create a multiband library, including random-access pointers, for up to 100 evaluations. If there are more than 100 evaluations for inclusion in your multiband library, process up to 100 at a time and combine them using the multiband library maintenance program CROSSUP (see Related Programs).

The multigroup cross sections output by this program will be in linearly interpolable form. The output will consist of a series of steps, one step per group, with a repeated energy and a jump in cross section between groups. In other words, the cross section will be discontinuous at group boundaries. (For example, to represent value $\langle \sigma \rangle_1$ between energies E_1 and E_2 , value $\langle \sigma \rangle_2$ between E_2 and E_3 , etc., the output would have the form

$$\begin{array}{ll}
 E_1 & \langle \sigma \rangle_1 \\
 E_2 & \langle \sigma \rangle_1 \\
 E_2 & \langle \sigma \rangle_2 \\
 E_3 & \langle \sigma \rangle_2 \\
 E_3 & \langle \sigma \rangle_3 ,
 \end{array}$$

etc.)

The cross section for each reaction (each section of File 3) can be given on its own energy structure. In particular, the total cross section need not be given at every energy at which one or more other reactions is given, but only at those energies needed to give linear interpolability in the total cross section itself to the accuracy desired.

Floating-point output will be in standard six-digit-accuracy form.⁸ The variable nine-digit-accuracy output used in LINEAR, RECENT, and SIGMAL is not required to represent the energies of group boundaries.

REQUIREMENTS

The I/O units used are as follows:

<u>Filename*</u>	<u>Unit</u>	<u>Description</u>
INPUT	5	Input cards.
OUTPUT	6	Output cards.
ENDFIN	20	Evaluated data in ENDF/B format.
LSTMG	21	Listing of multigroup cross sections (optional).
LSTBANDS	22	Listing of multiband parameters (optional).
CROSS	24	Multiband library (computer readable multiband parameters--optional).
ENDFOUT	25	Unshielded multigroup cross sections in the ENDF/B format.
SCR100	26	Scratch file for neutron energy spectrum.
SCR200	27	Scratch file for total cross section.
SCR300	28	Scratch file for elastic cross section.
SCR400	29	Scratch file for fission cross section.
SCR500	30	Scratch file for capture cross section.

* The names in the filename column only apply to the program used at Livermore. Disk files by these names are automatically assumed by the program.

All read, write, and buffered I/O statements use variable I/O units. To convert to any other set of unit numbers, redefine the unit numbers on the program card and at the beginning of the program.

The program requires approximately 42 000 words of core storage on the LLL CDC-7600 or CRAY-1. On the CRAY-1, the program requires 3.6 min to calculate 175 group constants and multiband parameters for all of the 88 evaluations in the ENDF¹⁴ library, or about 2.5 s per evaluation. The results of this calculation are given in Ref. 5. The program executes approximately twice as fast on the CRAY-1 as on the CDC-7600.

PROGRAM USE--DETAILS

REQUESTING EVALUATED DATA

Evaluations may be requested either by MAT number (see Ref. 1) or by ZA, where ZA = 1000Z + A for an isotope and ZA = 1000Z for a natural element. Up to 100 MAT or ZA ranges can be requested. The ENDF/B data must be in MAT or ZA order, whichever criterion the user specifies for retrieval; this is because the program searches the library and processes evaluations that meet the retrieval criteria only until a MAT (or ZA) greater than the largest value specified is found. (For example, if the user specifies the two MAT ranges 1000-1100 and 1200-1300, processing is ended as soon as a MAT larger than 1300 is found.)

To simplify requests for individual evaluations, as opposed to evaluations in ranges of MAT or ZA, GROUPIE has been written so that if only a minimum MAT or ZA is specified, only an evaluation with that MAT or ZA will be searched for. For example, to process ²³⁸U, searching by ZA, one need only specify the lower limit ZA = 92238 and make no entry for the upper limit. If the upper limit is blank or zero it will automatically be set equal to the lower limit. (See Input Cards for details.)

ENERGY GROUPS

GROUPIE allows the user to specify an arbitrary energy-group structure. Although the algorithms in this code can be used with any number of groups, the present core allocation allows no more than 175 groups (given by up to 176 energy boundaries). This limit can easily be extended if the user wishes to allocate more core storage.

Alternatively, the user can choose any of four built-in group structures, with 50, 126, 171, or 175 energy groups. Appendix A lists the energy boundaries of these group structures.

If the user inputs energy-group boundaries, the values must be in eV and in monotonically increasing order.

NEUTRON SPECTRUM

GROUPIE allows the user to specify an arbitrary energy-dependent neutron weighting spectrum, in the form of tabulated values with linear interpolation between tabulated values, or to use an energy-independent ("flat") weighting. There is no limit to the size of the tabulated spectrum, so it can represent a spectrum to any accuracy the user requires.

If the user inputs a tabulated spectrum, energies must be in ascending order, in eV, and all values for the spectrum must be zero or positive.

INPUT CARDS

<u>Card</u>	<u>Columns</u>	<u>Format</u>	<u>Description</u>
1	1-11	I11	Retrieval criterion (0 indicates MAT, 1 indicates ZA).
	12-22	I11	Number of groups chosen by user, or selection of a built-in group structure. A number N greater than zero causes N + 1 arbitrary group boundaries to be read from input file. (Remember N groups require N + 1 boundaries.) Current program maximum is 175 groups (read 176 boundaries).

0 indicates the 175 TART groups. }
 -1 indicates the 50 ORNL groups. } See Appendix A for
 -2 indicates the 126 ORNL groups. } group boundaries.
 -3 indicates the 171 ORNL groups. }

1 23-33 I11 Type of multiband calculation.
 0 indicates no multiband calculation.
 1 indicates 2-band calculation, conserving

$$\langle E_T \rangle, \langle 1/E_T \rangle, \text{ and } \langle 1/E_T^2 \rangle \text{ (Method 1).}$$

2 indicates 2-band calculation, conserving

$$\langle E_T \rangle, \langle 1/E_T \rangle, \text{ and}$$

$$\langle 1/(E_T + E_0) \rangle \text{ (Method 2).}$$

3-5 indicates maximum number of bands in multiband calculation, conserving $\langle E_T \rangle$, and min-max fit to self-shielding curve ($E_0 = 0$ to ∞).

1 34-44 I11 Number of points used to describe energy-dependent neutron spectrum $S(E)$.
<1 indicates energy-independent (flat) spectrum. No data are read from input file.
 >1 indicates the number of points to be read from the input file to describe the weighting spectrum $S(E)$.

1 45-55 E11.4 Multiband convergence criterion. Used only for calculations for 3 or more bands. The number of bands in each group is selected so that the entire self-shielding curve (all 23 values of E_0 between 0 and ∞) can be reproduced to within this fractional error.

1 56-66 I11 Constant cross section in all bands. This option is used only if one wishes to determine the

importance of using multiband data as opposed to multigroup data. This can be accomplished by having the program prepare a machine-readable multiband file with the same cross section in each band. This library can then be used with a transport calculation. Multiband effects are important if the results of such a transport calculation differ significantly from those of a true multiband calculation.

0 indicates normal multiband calculation.
 1-25 indicates use of the same self-shielded cross section in all bands of each group. The index selects one of the 25 self-shielded cross sections generated in each group (see Selection of Σ_0 and N for a description of these 25 cross sections).

The second input card is used to select desired output modes. Each output device may be turned off (indicated by a 0) or on (+1); the value +1 corresponds to input data from ENDL, and -1 corresponds to input data from ENDF. Appropriate titles for the output data will identify the data source as ENDL or ENDF. (Note, however, that all data are read in the ENDF format.)

<u>Card</u>	<u>Columns</u>	<u>Format</u>	<u>Description</u>
2	1-11	I11	Self-shielded cross section (listing).
	12-22	I11	Multiband parameters (listing).
	23-33	I11	Multiband parameters (computer-readable).
	34-44	I11	Unshielded averages in ENDF/B format.
3	1-80	20A4	Library identification: any text (up to 80 characters) that the user wishes to use to identify the computer-readable multiband data file.
vary	1-11	I11	Minimum MAT or ZA.
	12-22	I11	Maximum MAT or ZA.

TABLE 3. Sample output report from GROUPIE. Lists user's input parameters (with explanations), the number of data points given in File 3 of the ENDF/B format for each reaction, the maximum percent error in fitting the self-shielded neutron total cross section (for fits using all numbers of bands up to the maximum number specified by the user), and the percent error for each of the 25 combinations of (Σ_0 , N) used in the determination of the multiband parameters.

MULTI-GROUP AND MULTI-BAND PARAMETERS FROM ENDF/B CROSS SECTIONS (GROUPIE 79-1)						
RETRIEVAL CRITERIA-----			MAT			
NUMBER OF ENERGY GROUPS-----			175 (TART)			
MAXIMUM NUMBER OF BANDS/GROUP-----			4			
POINTS IN WEIGHTING SPECTRUM-----			2 (FLAT WEIGHTED)			
BAND SELECTION CRITERIA-----			1 0000E-03 (0.100 PER-CENT)			
CONSTANT CROSS SECTION OPTION-----			0			
SELF-SHIELDED LISTING-----			YES			
MULTI-BAND LISTING-----			YES			
MULTI-BAND FILE-----			YES			
ENDF/B MULTI-GROUP FILE-----			YES			
MULTI-BAND LIBRARY IDENTIFICATION						

TWO BAND TEST PROBLEM						
MAT RANGES-----			MINIMUM		MAXIMUM	
			0		9999	

ENDF/B TAPE LABEL						
ENDL TOTAL, ELASTIC, CAPTURE AND FISSION CREATED BY ENDL2FNDF						800

ISOTOPE	MAT	KELVIN	TOTAL POINTS	ELASTIC POINTS	CAPTURE POINTS	FISSION POINTS
1001	0001	0.	301	99	219	0
1002	8002	0.	109	40	72	0
3006	8003	0.	350	55	271	0
5010	8004	0.	420	44	56	0
5011	8005	0.	84	55	35	0
6012	8006	0.	157	123	11	0
7014	8007	0.	658	409	50	0
8016	8008	0.	329	264	0	0
13027	8009	0.	1958	1713	158	0
14000	8010	0.	953	871	46	0
67165	8011	0.	7027	3372	4662	0
79197	8012	0.	3715	126	3583	0
90232	8013	0.	6261	2983	5535	34
92235	8014	0.	2294	235	767	1511
92238	8015	0.	1744	453	1473	41

MAXIMUM PER-CENT ERROR DURING SIGMA-0 INTERPOLATION						

ZA	1 BAND	2 BANDS	3 BANDS	4 BANDS	5 BANDS	
1001	0.16	0.00				
1002	0.04					
3006	8.97	0.01				
5010	3.70	0.00				
5011	5.11	0.00				
6012	6.00	0.01				
7014	10.83	0.02				
8016	73.31	0.36	0.01			
13027	68.93	1.27	0.03			
14000	174.90	0.10	0.02			
67165	1825.95	6.45	0.36		0 01	
79197	466.87	3.28	0.09			
90232	5658.87	13.45	0.83		0 06	
92235	236.94	1.46	0.06			
92238	2990.50	8.22	0.44		0 03	

TABLE 3 (Continued.)

MAXIMUM PER-CENT ERROR VS SIGMA-0 FOR ENTIRE FILE					
INDEX	1 BAND	2 BANDS	3 BANDS	4 BANDS	5 BANDS
1	0	0	0	0	0
2	1 40	0 28	0 04	0 00	0 00
3	2 77	0 54	0 07	0 01	0 01
4	5 37	1 02	0 14	0 01	0 01
5	10 24	1 83	0 24	0 02	0 02
6	19 77	3 13	0 36	0 03	0 03
7	37 21	5 11	0 45	0 05	0 05
8	67 69	7 20	0 68	0 05	0 05
9	118 35	8 22	0 83	0 02	0 02
10	198 73	7 02	0 70	0 04	0 04
11	321 20	5 63	0 42	0 06	0 06
12	499 89	2 01	0 09	0 00	0 00
13	745 46	3 62	0 42	0 06	0 06
14	1055 97	8 25	0 42	0 02	0 02
15	1408 19	11 82	0 74	0 06	0 06
16	1758 13	13 45	0 67	0 04	0 04
17	2057 80	13 09	0 40	0 04	0 04
18	2748 49	11 08	0 35	0 06	0 06
19	3575 47	8 10	0 57	0 02	0 02
20	4317 70	5 08	0 52	0 02	0 02
21	4871 87	2 89	0 36	0 03	0 03
22	5227 11	1 12	0 20	0 02	0 02
23	5658 87	0 83	0 03	0 00	0 00
24	14179 19	15 32	1 56	0 24	0 24
25	15875 22	49 44	7 35	0 74	0 74

EXAMPLE OUTPUT

Table 3 is an example output report obtained by creating self-shielded cross sections and multiband parameters for a variety of materials.

For example output listings, see Appendix B.

ERROR MESSAGES

1. SCRATCH I/O ERROR--EXECUTION TERMINATED

This can only occur if the amount of data for any reaction exceeds the current scratch file sizes or if there is a computer problem. Since the scratch files are configured so that each reaction can contain up to 500 000 points, it is unlikely that this size will be exceeded. If there is a computer problem, wait and try again.

2. ENDFIN INITIALIZATION ERROR

3. ENDFOUT CLOSING ERROR

4. SCR200 DESTROY ERROR

These errors indicate that the program is having trouble locating, creating, or destroying a disk file. If the program cannot initialize ENDFIN, the message indicates the ENDF/B format data are either not on disk or that the disk has the wrong filename. If the program cannot initialize ENDFOUT, SCR100,..., SCR500, it is having trouble locating disk space in order to create a file; it will keep trying.

5. INTERPOLATION LAW IS NOT LINEAR-LINEAR

```
MAT/MF/MT/N1 = 1261 3 1 2
- - NBT - - INT
    37      5
    1502    2
EXECUTION TERMINATED
```

The ENDF/B-format data must be run through LINEAR⁶ and RECENT⁷ (if any materials have resonance parameters) before this program is used.

6. GROUP BOUNDARY NOT IN ENERGY ORDER--GROUP 2 1.302+2 1.000+2.

The user-supplied group boundaries as read from the INPUT file must be in increasing numerical order.

7. NUMBER OF GROUPS = 225 MUST BE -3 to 175

The user can select one of four built-in group structures (-3 to 0), or can input group boundaries for up to 175 groups (up to 176 energy boundaries)

8. SPECTRUM ENERGIES ARE NOT IN ENERGY ORDER--POINT 2 1.302+2 1.000+2

9. SPECTRUM CANNOT BE NEGATIVE--POINT 2 1.00+2 -1.000+ 0

10. ENERGY SPECTRUM FROM 1.000+2 to 1.000+6 EV DOES NOT SPAN THE GROUP RANGE FROM 1.000-3 to 2.000+7 EV

If the user chooses to input a spectrum, energies must be in ascending numerical order and the tabulated spectrum values must be zero or positive. The spectrum must be given over an energy range that at least spans the energy range of the group structure.

11. $\text{BA}^* \gamma$ FACTOR IN ZA 26056 GROUP 12

The f-factors for the 25 self-shielded total cross sections must be monotonically decreasing as the index goes from 1 (unshielded) to 25 ($\langle 1/\Sigma_A^2 \rangle$ -weighted). This error message cannot occur unless the present coding is changed.

12. XPAGES...INDEX = 0 (MUST BE 1 TO 1053)

13. YPAGES...INDEX = 0 (MUST BE 1 TO 1053)

The paging system retrieves data by use of a table index with values between 1 and the size of the table. This error message cannot occur unless the present coding is changed.

14. BAD WEIGHTS IN ZA 26056 GROUP 12

Band weights must be non-negative. This error message cannot occur unless the present coding is changed.

OPERATION

OPERATION AT LLL

At Livermore, compiled, loaded, ready-to-execute versions of this program are available from the photostore for either the CDC-7600, with the command

.193026:PROGRAMS [GROUPIE IGROUPIE] ,

or the CRAY-1, with the command

RD .193026:PROGRAMS:CRAY1 [GROUPIE IGROUPIE] .

After these files are read from photostore file, IGROUPIE should be renamed INPUT and edited to select the options that the user requires.

The program is small enough (40 000 words) to run at a low priority during the day.

The program will automatically use the disk filenames shown in the following diagram:

The program is designed to be compiled using the CHAT compiler for the CDC-7600 or the CIVIC compiler for the CRAY-1.

CONVERSION TO OTHER INSTALLATIONS

This edition of the code is designed for use either on a LLL CDC-7600 or a CRAY-1, or for export to any other installation that uses Fortran IV. Most of the coding is in standard Fortran. When an instruction takes different forms for the CDC-7600 or CRAY-1, it is present in three different forms—one for each of the LLL computers and one in standard Fortran. Each card in the group of three is inserted as a comment card and is labelled "CDC-7600," "CRAY-1," or "EXPORT" (this last label designates any machine using standard Fortran). To use the code on any given computer, activate the appropriate instruction in each set by eliminating the comment-card identifier "C" and the label, and leave the other two instructions in the set as inactive comment cards.

In particular see the following subroutines, which contain machine-dependent coding:

- DROPIT At LLL this subroutine creates a copy of the loaded program, which is then executed; the original program is not affected. On other computers the subroutine simply returns.
- IBLOCK This subroutine does the scratch I/O. In Fortran IV this is equivalent to binary I/O. Operation of this code can be greatly improved by using the most efficient scratch I/O available at your installation.
- IOFILE Opens, closes, creates, and destroys disk files. In Fortran IV this subroutine simply returns.
- DATEIT This subroutine supplies the current date, in format 2A4. In EXPORT mode the program will always supply the date 09/31/79, which is stored in this subroutine.

This use of subroutines for I/O will be maintained in future versions of GROUPIE. Therefore it is recommended that, instead of replacing the calls to these subroutines, you supply equivalent subroutines for your computer. Your version of DROPIT, IBLOCK, IOFILE, and DATEIT will be compatible with all future versions of this code, and this will minimize your maintenance problems. Note that these same routines are also used by LINEAR,⁶ RECENT,⁷ and SIGMAL,⁸ and need only be converted once for use in all codes.

ADDITIONAL GROUP STRUCTURES AND WEIGHTING SPECTRA

If the user wishes to add additional standard group structures or weighting spectra, this can easily be accomplished without greatly increasing the size of the program. The labelled common blocks

/ERNIE/CROSS (4378)

and

/INPAGE/BIGGIE (10020), DUMMY (15)

can be used to store standard group boundaries and weighting spectra. At the point in the program at which the group boundaries and weighting spectrum must be specified, CROSS and BIGGIF have not yet been used (they are used later, during execution). All of CROSS, and all of BIGGIE past BIGGIE (2005), can be used to store these additional data; this amounts to over 12 000 words of core storage. The user must then write subroutines to load the group boundaries and weighting spectra into the appropriate core locations for execution; see subroutines READIN and ORNLGP. The program will use these storage locations later during execution, and will then overwrite any information stored in these locations.

Please contact the author if you would like other group structures built into future versions of this code.

RELATED PROGRAMS

For GROUPIE to calculate Bondarenko self-shielded cross sections and multiband parameters, the evaluated cross sections must be in tabular form, with linear interpolation between tabulated points, and in the ENDF/B format.¹ Several programs are available to convert evaluated data to the required form. The choice of which code to use depends on whether the data are originally in the ENDF/B or the ENDL format. There is also a file-maintenance code to allow the multiband-parameter library to be updated by the insertion of parameters for new or changed evaluations without affecting the multiband parameters for unchanged evaluations.

DATA IN ENDL FORMAT: PROGRAM ENDL2ENDF

The Bondarenko self-shielding factor involves a reciprocal weighting by powers of the total neutron cross section. Since the ENDL library¹⁴ does not explicitly contain a total cross section, program ENDL2ENDF reads data in the ENDL card-image format, reconstructs the total cross section, and outputs the total, elastic, capture, and fission cross sections in the ENDF/B format. Linearization is not required, since neutron-induced cross sections in the ENDL library are already linearly interpolable between tabulated values.

Program ENDL2ENDF is available from the photostore for execution on the CDC-7600 with the command

```
.193026:PROGRAMS [ENDL2ENDF] .
```

The execution line is

```
ENDL2ENDF / 1 1 .
```

The program reads evaluated cross sections in the ENDL card-image format from file ENDLIN, and writes the cross sections in the ENDF/B card-image format in file ENDFOUT.

DATA IN ENDF/B FORMAT: PROGRAMS LINEAR AND RECENT

Data in the ENDF/B format¹ must be linearized using program LINEAR,⁶ and the contribution of any resonance parameters must be added to the tabulated cross sections using RECENT.⁷ For details see Refs. 6 and 7.

TEMPERATURE-DEPENDENT CROSS SECTIONS: PROGRAM SIGMAL

The result of executing either of the above sets of programs will be tabulated cross sections in the ENDF/B format, with linear interpolation between values. All cross sections will correspond to a temperature of 0 K. These data can be used with GROUPIE to obtain 0-K self-shielded cross sections and multiband parameters. Program SIGMAL⁸ can be used to Doppler-broaden the data to give cross sections at any other temperature; for details see Ref. 8. The output from SIGMAL can then be used with GROUPIE to obtain self-shielded cross sections and multiband parameters for the chosen temperature.

MULTIBAND-LIBRARY MAINTENANCE: PROGRAM CROSSUP

GROUPIE can create a binary multiband library for use with any application code. Appendix C describes the format of this library. To simplify maintenance of this library, program CROSSUP is designed to merge two

binary multiband libraries, eliminating duplicate evaluations at the same temperature. CROSSUP can be used to replace the multiband parameters for an evaluation that has been changed, or to insert parameters for a new evaluation, without having to re-create multiband parameters for all other evaluations.

Program CROSSUP is available from the photostore for execution on the CDC-7600, with the command

```
.193026:PROGRAMS[CROSSUP] ,
```

or the CRAY-1, with the command

```
.193026:PROGRAMS:CRAY1 [CROSSUP] .
```

The execution line is

```
CROSSUP/ 1 1 .
```

The program reads the binary multiband files CROSS1 and CROSS2, and combines them to create a binary multiband file CROSS. If parameters for an evaluation having the same ZA and temperature are found in both CROSS1 and CROSS2, the parameters from CROSS1 are written into the new library and the parameters from CROSS2 are ignored. Therefore, to replace the multiband parameters for a given evaluation, the new data should be on CROSS1 and the existing multiband library on CROSS2. After the program has been executed, the new, updated library will be on CROSS.

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APPENDIX A: ENERGY BOUNDARIES OF BUILT-IN GROUP STRUCTURES

The listing below gives the energy boundaries (in eV) for the four standard energy group structures built into GROUPIE. The listings are as follows: (a) boundaries for the 175 TART groups; (b) boundaries for the 171 ORNL groups; (c) boundaries for the 50 ORNL groups; (d) boundaries for the 126 ORNL groups.

(a) 175 (TART)

1.3068E-03	8.1673E+01	3.3453E+05
5.2271E-03	8.4307E+01	3.7765E+05
2.0908E-02	8.8337E+01	4.1230E+05
3.2693E-02	9.1076E+01	5.1230E+05
4.7044E-02	9.3857E+01	6.3247E+05
8.3215E-02	9.6680E+01	7.5270E+05
1.3068E-01	9.8107E+01	8.8337E+05
1.8817E-01	1.0245E+02	1.0245E+06
2.5613E-01	1.0990E+02	1.1761E+06
3.3453E-01	1.1761E+02	1.3381E+06
4.2339E-01	1.2556E+02	1.5106E+06
5.1230E-01	1.3381E+02	1.6936E+06
7.5270E-01	1.4059E+02	1.8870E+06
1.1761E+00	1.5106E+02	2.0908E+06
1.5106E+00	1.6008E+02	2.3051E+06
2.0908E+00	1.6936E+02	2.5299E+06
2.7411E+00	1.7890E+02	2.7411E+06
3.5355E+00	1.8870E+02	3.0108E+06
4.7044E+00	1.9876E+02	3.2669E+06
5.6578E+00	2.0908E+02	3.5355E+06
6.7367E+00	2.2069E+02	3.8105E+06
8.3215E+00	2.7411E+02	4.0688E+06
9.6199E+00	3.8105E+02	4.3960E+06
1.1012E+01	4.7044E+02	4.7044E+06
1.3068E+01	4.9908E+02	4.9908E+06
1.4683E+01	5.6578E+02	5.3525E+06
1.5812E+01	6.0425E+02	5.6578E+06
1.7584E+01	6.3666E+02	6.0425E+06
1.8817E+01	7.1558E+02	6.3666E+06
2.0746E+01	8.3215E+02	6.7367E+06
2.2769E+01	9.1076E+02	7.1558E+06
2.4170E+01	1.0585E+03	7.5270E+06
2.5613E+01	1.3068E+03	7.9096E+06
2.7097E+01	1.5812E+03	8.3215E+06
2.8232E+01	1.8817E+03	8.7867E+06
2.9402E+01	2.0746E+03	9.1076E+06
3.0991E+01	2.2769E+03	9.6648E+06
3.3453E+01	2.4170E+03	1.0120E+07
3.6095E+01	3.3453E+03	1.0585E+07
3.8659E+01	3.7765E+03	1.1012E+07
4.0478E+01	4.2339E+03	1.1547E+07
4.2339E+01	4.7044E+03	1.1993E+07
4.3285E+01	5.1230E+03	1.2499E+07
4.6186E+01	5.6578E+03	1.3068E+07
4.7174E+01	6.0425E+03	1.3542E+07
4.9181E+01	6.3666E+03	1.3863E+07
5.1230E+01	6.7367E+03	1.4134E+07
5.3215E+01	7.1558E+03	1.4407E+07
5.6536E+01	7.5270E+03	1.4683E+07
5.7628E+01	8.3215E+03	1.5186E+07
6.0968E+01	9.1076E+03	1.5744E+07
6.3247E+01	1.0245E+04	1.6334E+07
6.5568E+01	1.0990E+04	1.6923E+07
6.7444E+01	1.1761E+04	1.7523E+07
7.0335E+01	1.2556E+04	1.8134E+07
7.1553E+01	1.3381E+04	1.8755E+07
7.5270E+01	1.4059E+04	2.0000E+07
7.7800E+01	1.4819E+04	
7.9080E+01	1.5106E+04	

(b) 171 (ORNL)

1.0000E-05	3.4307E+04	1.4227E+06
1.0000E-01	4.0868E+04	1.4957E+06
4.1399E-01	4.6309E+04	1.5724E+06
5.3158E-01	5.2475E+04	1.6530E+06
6.8276E-01	5.6562E+04	1.7377E+06
8.7642E-01	6.7379E+04	1.8268E+06
1.1254E+00	7.2060E+04	1.9205E+06
1.4450E+00	7.9503E+04	2.0190E+06
1.8554E+00	8.2500E+04	2.1225E+06
2.3724E+00	8.6517E+04	2.2313E+06
3.0593E+00	9.8057E+04	2.3069E+06
3.9279E+00	1.1109E+05	2.3457E+06
5.0435E+00	1.1679E+05	2.3653E+06
6.4760E+00	1.2277E+05	2.3852E+06
8.3153E+00	1.2907E+05	2.4660E+06
1.0677E+01	1.3569E+05	2.5924E+06
1.3710E+01	1.4264E+05	2.7253E+06
1.7603E+01	1.4966E+05	2.8650E+06
2.2603E+01	1.5764E+05	3.0119E+06
2.9203E+01	1.6573E+05	3.1644E+06
3.7267E+01	1.7422E+05	3.3287E+06
4.7851E+01	1.8316E+05	3.6788E+06
6.1442E+01	1.9255E+05	4.0657E+06
7.8893E+01	2.0242E+05	4.4933E+06
1.0130E+02	2.1280E+05	4.7237E+06
1.3007E+02	2.2371E+05	4.9659E+06
1.6702E+02	2.3518E+05	5.2205E+06
2.1445E+02	2.4724E+05	5.4881E+06
2.7356E+02	2.7324E+05	5.7695E+06
3.5355E+02	2.8725E+05	6.0533E+06
4.5400E+02	2.9452E+05	6.3763E+06
5.8295E+02	2.9720E+05	6.5924E+06
7.4632E+02	2.9550E+05	6.7032E+06
9.6112E+02	3.0197E+05	7.0469E+06
1.2341E+03	3.3373E+05	7.4082E+06
1.5846E+03	3.6883E+05	7.7880E+06
2.0347E+03	3.8774E+05	8.1873E+06
2.2487E+03	4.0762E+05	8.6071E+06
2.4852E+03	4.5049E+05	9.0484E+06
2.1126E+03	4.9787E+05	9.5123E+06
2.7465E+03	5.2340E+05	1.0000E+07
3.0354E+03	5.5023E+05	1.0513E+07
3.3546E+03	5.7844E+05	1.1052E+07
3.7074E+03	6.0810E+05	1.1618E+07
4.3074E+03	6.3928E+05	1.2214E+07
5.3308E+03	6.7206E+05	1.2840E+07
7.1017E+03	7.0554E+05	1.3499E+07
9.1188E+03	7.4274E+05	1.3840E+07
1.1709E+04	7.8082E+05	1.4191E+07
1.5034E+04	8.2085E+05	1.4550E+07
1.9305E+04	8.6294E+05	1.4910E+07
2.1875E+04	9.0718E+05	1.5663E+07
2.3579E+04	9.6164E+05	1.6487E+07
2.4778E+04	1.0000E+06	1.7333E+07
2.6058E+04	1.1648E+06	
2.7000E+04	1.2246E+06	
2.8500E+04	1.2873E+06	
3.1878E+04	1.3534E+06	

(c) 50 (ORNL)

1.0000E-05 7.1020E+03
 6.8256E-01 9.1190E+03
 1.1250E+00 1.1710E+04
 1.5030E+04 1.5030E+04
 1.8550E+00 1.9300E+04
 3.0890E+00 2.4790E+04
 5.0430E+00 2.4790E+04
 8.3150E+00 3.1830E+04
 1.3710E+01 4.0870E+04
 2.2600E+01 5.2480E+04
 3.7270E+01 6.7380E+04
 6.1440E+01 8.6520E+04
 1.0130E+02 1.1110E+05
 1.6700E+02 1.4260E+05
 2.7540E+02 1.8320E+05
 3.5360E+02 2.3520E+05
 4.5400E+02 3.0200E+05
 5.8290E+02 3.8770E+05
 7.4850E+02 4.9790E+05
 9.6110E+02 6.2080E+05
 1.2340E+03 1.3530E+06
 1.5850E+03 2.2310E+06
 2.0350E+03 3.6790E+06
 2.7470E+03 6.0650E+06
 3.3550E+03 1.0000E+07
 4.3070E+03 1.9970E+07
 5.5310E+03

(d) 126 (ORNL)

1.0000E-05 1.1709E+04 2.0242E+05 1.3534E+06
 1.0000E-01 1.5034E+04 2.1260E+05 1.4227E+06
 4.1399E-01 1.9305E+04 2.2371E+05 1.4957E+06
 1.1254E+00 2.1875E+04 2.4724E+05 1.5724E+06
 2.3724E+00 2.3579E+04 2.7324E+05 1.6530E+06
 5.0435E+00 2.4788E+04 2.8725E+05 1.7377E+06
 1.0677E+01 2.6058E+04 2.9452E+05 1.8268E+06
 2.2603E+01 2.7000E+04 2.9720E+05 1.9205E+06
 3.7267E+01 2.8500E+04 2.9850E+05 2.0190E+06
 4.7851E+01 3.1828E+04 3.0197E+05 2.1225E+06
 6.1442E+01 3.4307E+04 3.3373E+05 2.2313E+06
 1.0130E+02 4.0868E+04 3.6883E+05 2.3069E+06
 1.6702E+02 4.6309E+04 4.0762E+05 2.3653E+06
 2.1445E+02 5.2475E+04 4.5049E+05 2.3852E+06
 2.7536E+02 5.6562E+04 4.9787E+05 2.4660E+06
 4.5400E+02 6.7379E+04 5.2340E+05 2.5924E+06
 7.4852E+02 7.2000E+04 5.5023E+05 2.7253E+06
 9.6112E+02 7.9500E+04 5.7844E+05 2.8650E+06
 1.2341E+03 8.2500E+04 6.0810E+05 3.0119E+06
 1.5846E+03 8.6517E+04 6.3928E+05 3.1634E+06
 2.0347E+03 9.8037E+04 6.7206E+05 3.6788E+06
 2.2487E+03 1.1109E+05 7.0551E+05 4.4933E+06
 2.4852E+03 1.1879E+05 7.4274E+05 5.4881E+06
 2.6126E+03 1.2277E+05 7.8082E+05 6.0653E+06
 2.7465E+03 1.2907E+05 8.2085E+05 6.7032E+06
 3.0354E+03 1.3569E+05 8.6294E+05 8.1873E+06
 3.3546E+03 1.4264E+05 9.0718E+05 1.0000E+07
 3.7074E+03 1.4996E+05 9.6164E+05 1.2214E+07
 4.3074E+03 1.5764E+05 1.0026E+06 1.7333E+07
 5.5308E+03 1.6573E+05 1.0505E+06
 7.1017E+03 1.7422E+05 1.1648E+06
 9.1188E+03 1.8316E+05 1.2246E+06
 1.9255E+05 1.2873E+06

APPENDIX B: EXAMPLE OUTPUT LISTINGS

Tables 4, 5, and 6 are examples of Bondarenko self-shielded cross sections (from LSTMG), multiband parameters (from LSTBANDS), and multigroup data in the ENDF/B format (from ENDFOUT). These tables are discussed in detail below.

EXAMPLE LISTING OF SELF-SHIELDING CROSS SECTIONS

Table 4 gives Bondarenko self-shielded cross sections for each energy group and reaction; it gives the unshielded cross section and eleven f-factors (explained below). The column headings have the following meanings:

<u>Heading</u>	<u>Meaning</u>
No.	Group index.
GROUP-MEV	Lower energy limit of group, in MeV (not eV).
REACT	Reaction--total, elastic, capture, or fission.
AVERAGE	The unshielded group-averaged cross section, in barns. The unshielded cross section corresponds to using $\Sigma_0 = \infty$ or $N = 0$.
256	Each column presents an f-factor corresponding to $N = 1$ and different values of Σ_0 . The values of Σ_0 used are multiples of the unshielded <u>total</u> cross section in each group; the multiples used are 256, 64, ..., 1/64, 1/256. For example, in the example listing for group 57, the unshielded total cross section (AVERAGE) is 10.485 barns; therefore the value of Σ_0 used to obtain the f-factor for this group, under the column labeled 64, is $\Sigma_0 = 64 \times 10.485 = 671.04$ barns. In this group, for $\Sigma_0 = 671.04$ barns, the total, elastic, capture, and fission cross sections can be obtained by multiplying the f-factor for each reaction by the unshielded average for each reaction: thus we find
64	
.	
.	
.	
.	
.	
.	
1/64	
1/256	

$$\langle \Sigma_T \rangle = 0.99994 \times 10.485 = 10.484 \text{ b} ,$$

$$\langle \Sigma_{el} \rangle = 0.99994 \times 10.364 = 10.363 \text{ b} ,$$

$$\langle \Sigma_C \rangle = 1.00003 \times 0.12082 = 0.12088 \text{ b} ,$$

$$\langle \Sigma_f \rangle = 0 \text{ (since it is not listed for this group).}$$

TABLE 4. Results of calculation of Bondarenko self-shielded 0-K neutron cross sections in ^{238}U for 18 of the 175 TART energy groups. The table gives the unshielded total, elastic, and capture cross sections (fission cross sections are all zero), and gives f-factors (explained in the text) from which shielded cross sections can be calculated for 12 values of the background cross section Σ_0 --10 multiples (ranging from 256 to 1/256) of the unshielded total cross section $\langle \Sigma_T(\text{arb}, 0) \rangle$, $\langle \Sigma_T(0, 1) \rangle$, and $\langle \Sigma_T(0, 2) \rangle$.

NO.	GROUP-MEV	REACT	AVERAGE	256	64	16	4	1	1/4	1/16	1/64	1/256	1/TOT	1/TOT**2
55	7.0335-	5	TOTAL	1.5534+	1.00000	0.99999	0.99997	0.99990	0.99974	0.99959	0.99952	0.99950	0.99949	0.99998
			ELAST	1.3936+	1.00000	0.99999	0.99997	0.99990	0.99977	0.99964	0.99957	0.99955	0.99954	0.99909
			CAPT	2.1639+	0.99999	0.99995	0.99980	0.99931	0.99827	0.99724	0.99675	0.99661	0.99657	0.99313
56	7.1553-	5	TOTAL	1.3330+	0.99998	0.99991	0.99965	0.99681	0.99703	0.99524	0.99439	0.99413	0.99406	0.98808
			ELAST	1.3086+	0.99998	0.99992	0.99968	0.99892	0.99728	0.99564	0.99486	0.99462	0.99456	0.98907
			CAPT	2.4426-	0.99987	0.99949	0.99806	0.99342	0.98357	0.97372	0.96908	0.96765	0.96727	0.93467
57	7.5270-	5	TOTAL	1.0485+	0.99999	0.99994	0.99979	0.99927	0.99818	0.99709	0.99657	0.99641	0.99633	0.99635
			ELAST	1.0364+	0.99999	0.99993	0.99989	0.99926	0.99815	0.99703	0.99651	0.99635	0.99630	0.99629
			CAPT	1.2088-	1.00001	1.00003	1.00011	1.00039	1.00100	1.00163	1.00194	1.00204	1.00206	1.00429
58	7.7800-	5	TOTAL	8.8719+	0.00000	0.99998	0.99994	0.99978	0.99945	0.99913	0.99897	0.99893	0.99891	0.99782
			ELAST	8.7037+	0.00000	0.99998	0.99993	0.99976	0.99939	0.99902	0.99885	0.99880	0.99878	0.99756
			CAPT	1.6810+	0.99999	0.99997	0.99981	0.99932	0.99806	0.99682	0.99597	0.99564	0.99564	0.99366
59	7.9080-	5	TOTAL	4.3735+	0.99998	0.99992	0.99968	0.99892	0.99728	0.99564	0.99486	0.99462	0.99456	0.98907
			ELAST	1.2251+	0.99721	0.99828	0.99629	0.90174	0.82435	0.76966	0.74292	0.73332	0.73059	0.72964
			CAPT	3.7484+	0.99861	0.99017	0.86297	0.64258	0.38018	0.21873	0.15517	0.13581	0.13063	0.12887
60	8.1673-	5	TOTAL	1.1632+	1.00000	0.99998	0.99993	0.99976	0.99940	0.99905	0.99888	0.99883	0.99881	0.99763
			ELAST	1.1194+	1.00000	0.99999	0.99997	0.99989	0.99973	0.99957	0.99946	0.99946	0.99946	0.99892
			CAPT	4.3870+	0.99993	0.99972	0.99933	0.99636	0.99097	0.98566	0.98138	0.98242	0.98222	0.98216
61	8.4307-	5	TOTAL	9.6077+	0.99999	0.99994	0.99977	0.99923	0.99808	0.99593	0.99638	0.99622	0.99617	0.99616
			ELAST	9.4934+	0.99998	0.99994	0.99977	0.99923	0.99807	0.99690	0.99636	0.99619	0.99614	0.99613
			CAPT	1.231-	0.99999	0.99997	0.99989	0.99963	0.99915	0.99878	0.99863	0.99859	0.99858	0.99858
62	8.8337-	5	TOTAL	9.9050+	0.99994	0.99987	0.99966	0.99917	0.99834	0.99763	0.99693	0.99631	0.99616	0.99612
			ELAST	8.1143+	0.99999	0.99996	0.99985	0.99950	0.99885	0.99828	0.99802	0.99795	0.99793	0.99792
			CAPT	1.7907+	0.99803	0.99227	0.97117	0.90917	0.80246	0.71887	0.68517	0.67539	0.67284	0.67198
63	9.1076-	5	TOTAL	7.3925+	0.99999	0.99996	0.99985	0.99950	0.99875	0.99801	0.99767	0.99756	0.99753	0.99750
			ELAST	7.0140+	0.99999	0.99998	0.99992	0.99972	0.99930	0.99887	0.99866	0.99860	0.99858	0.99858
			CAPT	3.7864+	0.99999	0.99994	0.99981	0.99954	0.99927	0.99892	0.99867	0.99859	0.99858	0.99858
64	9.3857-	5	TOTAL	5.0074+	0.99999	0.99995	0.99982	0.99940	0.99849	0.99758	0.99716	0.99703	0.99699	0.99698
			ELAST	5.7333+	0.99999	0.99994	0.99979	0.99927	0.99817	0.99707	0.99655	0.99639	0.99635	0.99633
			CAPT	2.7408-	1.00004	1.00016	1.00061	1.00209	1.00525	1.00844	1.00995	1.01042	1.01054	1.01210
65	9.6680-	5	TOTAL	4.6599+	0.99998	0.99992	0.99971	0.99903	0.99758	0.99616	0.99549	0.99539	0.99524	0.99522
			ELAST	4.0687+	0.99997	0.99987	0.99951	0.99833	0.99695	0.99540	0.99425	0.99390	0.99380	0.99373
			CAPT	5.9120-	1.00007	1.00029	1.00112	1.00380	1.00948	1.01516	1.01784	1.01866	1.01888	1.01895
66	9.8107-	5	TOTAL	1.2615+	2.095037	0.83495	0.59632	0.33475	0.16670	0.08651	0.05382	0.04204	0.03833	0.03704
			ELAST	8.6561+	0.99480	0.82854	0.58150	0.31331	0.14417	0.06646	0.03698	0.02730	0.02449	0.02349
			CAPT	3.2588+	0.95468	0.84866	0.62852	0.38153	0.21596	0.13034	0.08064	0.07425	0.06873	0.06665
67	1.0245-	4	TOTAL	0.9999+	2.095037	0.83495	0.59632	0.33475	0.16670	0.08651	0.05382	0.04204	0.03833	0.03704
			ELAST	2.3424+	2.095037	0.83495	0.59632	0.33475	0.16670	0.08651	0.05382	0.04204	0.03833	0.03704
			CAPT	7.7552+	1.095637	0.84877	0.60211	0.31267	0.13865	0.06548	0.03835	0.02936	0.02677	0.02586
68	1.0990-	4	TOTAL	1.3375+	2.095037	0.83495	0.59632	0.33475	0.16670	0.08651	0.05382	0.04204	0.03833	0.03704
			ELAST	4.9996+	0.997208	0.90028	0.71739	0.45851	0.26780	0.17994	0.14829	0.13766	0.13443	0.13326
			CAPT	5.8780+	1.095637	0.84877	0.60211	0.31267	0.13865	0.06548	0.03835	0.02936	0.02677	0.02586
69	1.1761-	4	TOTAL	1.9582+	1.09918	0.99681	0.98849	0.96573	0.93548	0.91415	0.90500	0.90366	0.90306	0.90285
			ELAST	1.8453+	1.09934	0.99744	0.99074	0.97310	0.94739	0.92953	0.92263	0.92065	0.92014	0.91996
			CAPT	1.1285+	0.99653	0.98651	0.95164	0.86251	0.74074	0.66262	0.63394	0.62586	0.62377	0.62307
70	1.2558-	4	TOTAL	1.3581+	0.99999	0.99997	0.99989	0.99963	0.99907	0.99852	0.99826	0.99818	0.99815	0.99812
			ELAST	1.3581+	0.99999	0.99997	0.99989	0.99963	0.99907	0.99852	0.99826	0.99818	0.99815	0.99812
			CAPT	1.4784-	0.99997	0.99988	0.99956	0.99849	0.99617	0.99381	0.99268	0.99233	0.99224	0.99221
71	1.3381-	4	TOTAL	1.5858+	1.09999	0.99997	0.99987	0.99957	0.99893	0.99828	0.99798	0.99788	0.99786	0.99785
			ELAST	1.5044+	1.09999	0.99997	0.99988	0.99960	0.99900	0.99839	0.99811	0.99802	0.99800	0.99799
			CAPT	8.5991+	0.99991	0.99966	0.99870	0.99557	0.98890	0.98421	0.97903	0.97808	0.97782	0.97773
72	1.4059-	4	TOTAL	1.9582+	1.09918	0.99681	0.98849	0.96573	0.93548	0.91415	0.90500	0.90366	0.90306	0.90285
			ELAST	1.1067+	1.09990	0.99961	0.99861	0.99597	0.99173	0.98609	0.98641	0.98589	0.98575	0.98570
			CAPT	2.8775+	0.99156	0.96753	0.88721	0.70241	0.48881	0.37178	0.33246	0.32173	0.31898	0.31806

- 1/TOT The totally shielded, flux-weighted f-factor, corresponding to $N = 1$, $\Sigma_0 = 0$.
- 1/TOT**2 The totally shielded, current-weighted f-factor, corresponding to $N = 2$, $\Sigma_0 = 0$.

The combination of AVERAGE, 256, 64, ..., 1/64, 1/256, and 1/TOT describes the self-shielding curve corresponding to $N = 1$ for values of Σ_0 between ∞ (AVERAGE) and 0 (1/TOT).

Since the f-factor for any combination of N and Σ_0 is defined as the ratio of the self-shielded cross section for that combination of N and Σ_0 to the unshielded cross section, the magnitude of the effect of self-shielding can be determined easily. F-factors close to unity indicate little self-shielding; conversely, f-factors that deviate substantially from unity indicate large self-shielding effects.

Microfiche in this format for the entire ENDL library are given in Ref. 5.

EXAMPLE LISTING OF MULTIBAND PARAMETERS

Table 5 gives multiband parameters for ^{238}U . For each group and band, band weights and cross sections are given for total, elastic, capture, and fission. For comparison, this table also contains the group-averaged unshielded cross sections for total, elastic, capture, fission, and remainder. Comparison of the unshielded multigroup cross section to the multiband cross sections can be used to determine the spread of the cross section distribution.

The column REMAINS is obtained by subtracting the elastic, capture, and fission cross sections from the total cross section. Therefore this column should be considered approximate, and should only be used as a rough estimate of where reactions other than elastic, capture, and fission are present.

Listings in this format for the entire ENDL library are given in Ref. 5.

TABLE 5. Multiband parameters (band weights and cross sections) for 0-K neutron cross sections in ^{238}U for 21 of the 175 TART energy groups. Bondarenko self-shielded cross sections, for any value of the background cross section Σ_0 , can be obtained from these parameters with the use of Eq. (19). Unshielded group-averaged cross sections are given for comparison.

								UNSHIELDED GROUP AVERAGES									
NO.	GROUP-MEV	BAND	WEIGHT	TOTAL	ELASTIC	CAPTURE	FISSION	TOTAL	ELASTIC	CAPTURE	FISSION	REMAINS					
59	7.9080-	5	1	0.59129	9.0961	0	8.3097	0	7.9389	1	0	4 9735	1 1 2251	1 3 7484	1 0	+ 0 0.	+ 0
		2	0	0.23045	3.4163	0	1.1026	1	2.1058	1	0						
		3	0	0.17826	2.0467	2	2.4324	1	1.8043	2	0						
60	8.1673-	5	1	0.57024	1.1282	1	1.1041	1	2.4086	1	0	1 1632	1 1 1194	1 4 3870	1 0	+ 0 0.	+ 0
		2	0	0.42976	1.2097	1	1.1396	1	7.0122	1	0						
		3	0	0.50010	9.0123	0	8.9025	0	1.0973	1	0						
61	8.4307-	5	1	0.52990	9.0123	0	8.0089	1	1.1489	1	0	9 6077	0 9 4954	0 1 1231	1 0	+ 0 0.	+ 0
		2	0	0.82020	8.4997	0	8.0751	0	4.2459	1	0						
		3	0	0.17980	1.6316	1	8.2933	0	8.0228	0	0						
62	8.8337-	5	1	0.55119	7.0588	0	6.8319	0	2.2682	1	0	7 3925	0 7 0140	0 3.7849	1 0	+ 0 0.	+ 0
		2	0	0.44881	7.8024	0	7.2376	0	5.6475	1	0						
		3	0	0.47764	5.6631	0	5.3340	0	3.2916	1	0						
63	9.1076-	5	1	0.52236	6.3222	0	6.0985	0	2.2372	1	0	6 0074	0 5 7333	0 2 7408	1 0	+ 0 0.	+ 0
		2	0	0.58263	4.3840	0	3.6541	0	7.2997	1	0						
		3	0	0.41737	5.0450	0	4.6475	0	3.9749	1	0						
64	9.3857-	5	1	0.76485	3.6168	0	1.3957	0	2.2241	0	0	1 2615	2 8 6561	1 3 9588	1 0	+ 0 0.	+ 0
		2	0	0.17382	7.4062	1	4.1019	1	3.2825	1	0						
		3	0	0.06133	1.8019	3	1.2777	3	5.5473	2	0						
67	1.0245-	4	1	0.61029	1.8376	1	1.7631	1	5.5542	1	0	3 0999	2 2 3424	2 7 5752	1 0	+ 0 0.	+ 0
		2	0	0.27318	5.8834	1	5.2789	1	5.9600	0	0						
		3	0	0.06026	5.8634	2	4.5834	2	1.2881	2	0						
68	1.0990-	4	1	0.95627	4.3967	3	3.2222	3	1.1733	3	0	1 3375	2 7 4996	1 5 8755	1 0	+ 0 0.	+ 0
		2	0	0.79842	9.9309	0	8.6997	0	1.2363	0	0						
		3	0	0.11520	1.1583	2	6.9407	1	6.0992	1	0						
69	1.1761-	4	3	0.86638	1.3021	3	6.9523	2	6.0729	2	0	1 9582	1 1 8453	1 1 1285	0 0	+ 0 0.	+ 0
		1	0	0.87223	1.6297	1	1.5903	3	9.9399	1	0						
		2	0	0.17777	4.2006	3	3.5863	1	6.1427	0	0						
70	1.2558-	4	1	0.59111	1.3017	1	1.2895	1	1.2204	1	0	1 3581	1 1 3433	1 1 4784	1 0	+ 0 0.	+ 0
		2	0	0.48089	1.4189	1	1.4014	1	1.7569	1	0						
		3	0	0.47063	1.1017	1	1.0977	4	0.0014	2	0						
71	1.3381-	4	2	0.52937	1.2090	1	1.1972	1	1.1799	1	0	1 1585	1 1 1504	1 8 1291	2 0	+ 0 0.	+ 0
		1	0	0.90478	1.0992	1	1.0846	1	1.4614	1	0						
		2	0	0.09522	4.1991	1	1.3159	1	2.8832	1	0						
72	1.4059-	4	1	0.74960	8.8233	0	6.7688	0	5.4485	2	0	9 4061	0 9 1120	0 2 9410	1 0	+ 0 0.	+ 0
		2	0	0.25040	1.1151	1	1.0139	1	1.0114	0	0						
		3	0	0.80130	8.0785	0	7.9560	0	1.3030	1	0						
74	1.6008-	4	1	0.12419	2.0947	1	1.1735	1	9.0736	0	0	1 8305	1 9 5538	0 8 9515	0 0	+ 0 0.	+ 0
		3	0	0.07450	1.2658	2	2.3103	1	1.0362	2	0						
		1	0	0.45621	6.0713	0	5.9881	0	8.3251	2	0						
75	1.6936-	4	2	0.54379	8.2139	0	7.8965	0	3.1743	1	0	7 2364	0 7.0258	0 2.1060	1 0	+ 0 0.	+ 0
		1	0	0.47989	2.0318	0	1.1569	0	8.7224	1	0						
		2	0	0.46138	5.7598	0	4.7664	0	1.0008	0	0						
76	1.7890-	4	3	0.58773	7.1654	1	5.4428	1	1.7190	1	0	3 6982	2 3.2567	2 4 4149	1 0	+ 0 0.	+ 0
		1	0	0.65143	2.5233	1	2.4626	1	6.1063	1	0						
		2	0	0.25081	1.8228	2	1.6430	2	1.7944	1	0						
77	1.8870-	4	3	0.9776	3.1471	3	2.7457	3	4.0149	2	0	1.0774	2 7 7496	1 3 0245	1 0	+ 0 0.	+ 0
		1	0	0.77681	1.0251	1	9.2833	0	9.7434	1	0						
		2	0	0.13759	6.0096	1	4.7159	1	1.2730	1	0						
78	1.9876-	4	3	0.8561	1.0690	3	7.4524	2	3.2400	2	0	2.7712	1 2 1093	1 6 6189	0 0	+ 0 0.	+ 0
		1	0	0.72348	1.1383	1	1.1159	1	2.3229	1	0						
		2	0	0.24704	2.6048	1	2.3733	1	2.2628	0	0						
79	2.0908-	4	3	0.02948	4.4236	2	2.4275	2	1.9984	2	0						

EXAMPLE LISTING OF UNSHIELDED GROUP-AVERAGED
CROSS SECTIONS IN THE ENDF/B FORMAT

To maintain compatibility with all other TCP programs (see Operation at Other Installations), the unshielded group averages are output in linearly interpolable form rather than as histograms. In this form, they can be read by DOWNER²⁷ to perform group collapse, by EVALPLOT to obtain plots, by MIXER²⁸ to treat composite mixtures, and by VIRGIN¹² to perform uncollided, or virgin flux calculations.

In linearly interpolable form, each group is represented by two energy-cross section pairs, one pair at each of the lower and upper energy limits of the group. At both energy points, the cross section is equal to the unshielded group average. For threshold reactions, an additional point is inserted at the lowest group energy at which the reaction is non-zero. The cross section at this point is set equal to zero.

For example, Table 6 illustrates the ²³⁸U total cross section in the TART 175-group structure. Between 0.0013068 and 0.0052271 eV, the unshielded total cross section is 15.296 barns. Similarly, between 0.0052271 and 0.020908 eV, the unshielded total cross section is 11.6886 barns.

TABLE 6. Unshielded, group-averaged neutron cross sections for ^{238}U as output by GROUPIE in the ENDF/B format. Entries in the main body of the table are (energy, cross section) pairs; the energies are TART 175-group boundaries (in eV); the cross sections (in barns) hold between successive energies.

9	22380+	4	2.36005+	0	0	0	0	0	08015	3	1	1			
0	+	0	0	+	0	0	0	1	3508015	3	1	2			
	350			2					8015	3	1	3			
1	30680-	3	1.52960+	1	5.22710-	3	1.52960+	1	5.22710-	3	1.16886+	18015	3	1	4
2	09080-	2	1.16886+	1	2.09080-	2	1.06125+	1	3.26690-	2	1.06125+	18015	3	1	5
3	26690-	2	1.01392+	1	4.70440-	2	1.01392+	1	4.70440-	2	9.67737+	08015	3	1	6
8	32150-	2	9.67737+	0	8.32150-	2	9.30096+	0	1.30680-	1	9.30096+	08015	3	1	7
1	30680-	1	9.05725+	0	1.88170-	1	9.05725+	0	1.88170-	1	8.88707+	08015	3	1	8
2	56130-	1	8.88707+	0	2.56130-	1	8.76820+	0	3.34530-	1	8.76820+	08015	3	1	9
3	34530-	1	8.67317+	0	4.23390-	1	8.67317+	0	4.23390-	1	8.59811+	08015	3	1	10
5	12300-	1	8.59811+	0	5.12300-	1	8.50355+	0	7.52700-	1	8.50355+	08015	3	1	11
7	52700-	1	8.40357+	0	1.17610+	0	8.40357+	0	1.17610+	0	8.31990+	08015	3	1	12
1	51060+	0	8.31990+	0	1.51060+	0	8.25249+	0	2.09080-	0	8.25249+	08015	3	1	13
2	09080+	0	8.27077+	0	2.74110+	0	8.27077+	0	2.74110+	0	8.30182+	08015	3	1	14
3	53530+	0	8.30182+	0	3.53530+	0	8.47035+	0	4.70440+	0	8.47035+	08015	3	1	15
4	70440+	0	9.44771+	0	5.65780+	0	9.44771+	0	5.65780+	0	7.35556+	28015	3	1	16
7	36760+	0	7.35556+	2	6.73670+	0	8.93210+	0	8.93210+	0	8.93210+	18015	3	1	17
8	32150+	0	1.12732+	1	9.61990+	0	1.12732+	1	9.61990+	0	1.06071+	18015	3	1	18
1	51060+	1	06071+	1	1.10120+	1	9.21062+	0	1.30680+	1	9.21062+	08015	3	1	19
1	30680+	1	8.30498+	0	1.46830+	1	8.30498+	0	1.46830+	1	7.70958+	08015	3	1	20
1	58120+	1	7.70958+	0	1.58120+	1	7.25588+	0	1.75840+	1	7.25588+	08015	3	1	21
1	75840+	1	6.85155+	0	1.86170+	1	6.85155+	0	1.86170+	1	5.49242+	18015	3	1	22
2	07460+	1	5.49242+	1	2.07460+	1	7.94886+	2	2.27690+	1	7.94886+	28015	3	1	23
2	27690+	1	4.00222+	1	2.41700+	1	4.00222+	1	2.41700+	1	2.0926+	18015	3	1	24
2	56130+	1	2.0926+	1	2.56130+	1	1.06876+	1	2.70970+	1	1.06876+	18015	3	1	25
2	70970+	1	9.36238+	0	2.86230+	1	9.36238+	0	2.86230+	1	8.45919+	08015	3	1	26
2	94020+	1	8.45919+	0	2.94020+	1	7.55816+	0	3.09910+	1	7.55816+	08015	3	1	27
3	09910+	1	6.00943+	0	3.34530+	1	6.00943+	0	3.34530+	1	0.1995+	18015	3	1	28
3	60090+	1	0.1995+	1	3.60090+	1	1.27857+	3	3.86590+	1	1.27857+	38015	3	1	29
3	86590+	1	2.56269+	1	4.04780+	1	2.56269+	1	4.04780+	1	7.3975+	18015	3	1	30
4	23390+	1	1.73975+	1	4.23390+	1	1.62600+	1	4.32850+	1	1.62600+	18015	3	1	31
4	32850+	1	1.52969+	1	4.61860+	1	1.52969+	1	4.61860+	1	1.42124+	18015	3	1	32
4	71740+	1	1.42124+	1	4.71740+	1	35	3	4.91810+	1	35113+	80	3	1	33
4	91810+	1	1.25808+	1	5.12300+	1	1.25808+	1	5.12300+	1	1.15545+	18015	3	1	34
5	33210+	1	1.15545+	1	5.33210+	1	1.03678+	1	5.65360+	1	1.03678+	18015	3	1	35
5	65360+	1	9.39730+	0	5.76280+	1	9.39730+	0	5.76280+	1	8.43832+	08015	3	1	36
6	09680+	1	8.43832+	0	6.09680+	1	6.83569+	0	6.32470+	1	6.83569+	08015	3	1	37
6	32470+	1	2.53972+	1	6.55680+	1	2.53972+	1	6.55680+	1	1.29073+	38015	3	1	38
6	67440+	1	2.9073+	3	6.67440+	1	2.36562+	1	7.03350+	2	2.36562+	18015	3	1	39
7	73350+	1	5.5343+	1	7.5530+	1	5.5343+	1	7.5530+	1	3.3299+	18015	3	1	40
7	52700+	1	1.33299+	1	7.52700+	1	1.04846+	1	7.78000+	1	1.04846+	18015	3	1	41
7	78000+	1	8.87187+	0	7.90800+	1	8.87187+	0	7.90800+	1	4.97354+	18015	3	1	42
8	16730+	1	4.97354+	0	8.16730+	1	1.16323+	1	8.43070+	1	1.16323+	18015	3	1	43
8	43070+	1	9.60774+	0	8.83370+	1	9.60774+	0	8.83370+	1	9.90502+	08015	3	1	44
9	10760+	1	9.30502+	0	9.10760+	1	7.39249+	0	9.38570+	1	7.39249+	08015	3	1	45
9	38570+	1	6.00741+	0	9.66800+	1	6.00741+	0	9.66800+	1	4.65991+	08015	3	1	46
9	81070+	1	4.65991+	0	9.81070+	1	1.26150+	2	1.02450+	2	1.26150+	28015	3	1	47
1	02450+	2	3.09990+	2	1.09990+	2	3.09990+	2	1.09990+	2	3.3752+	28015	3	1	48
1	17610+	2	1.33752+	2	1.17610+	2	1.95819+	1	1.25580+	2	1.95819+	18015	3	1	49
1	25580+	2	1.35810+	1	1.33810+	2	1.35810+	1	1.33810+	2	1.15851+	18015	3	1	50
1	40590+	2	1.15851+	1	1.40590+	1	1.39441+	1	1.51060+	2	1.39441+	18015	3	1	51
1	51060+	2	1.40611+	0	1.60080+	1	9.49611+	0	1.60380+	2	1.85053+	18015	3	1	52
1	69360+	2	1.85053+	1	1.69360+	2	7.23644+	0	1.78900+	2	7.23644+	08015	3	1	53
1	78900+	2	7.84069+	0	1.88700+	2	7.84069+	0	1.88700+	2	3.69822+	28015	3	1	54
1	98760+	2	3.69822+	2	1.98760+	1	1.07741+	2	2.09080+	2	1.07741+	28015	3	1	55
2	09080+	2	2.77117+	1	2.74110+	2	2.77117+	1	2.74110+	2	1.74810+	18015	3	1	56
2	26690+	1	1.74810+	1	3.26690+	2	2.95882+	3	3.81050+	2	2.95882+	18015	3	1	57
3	81050+	2	1.74810+	1	4.70440+	1	1.87356+	1	4.70440+	2	1.76085+	18015	3	1	58
4	99080+	2	1.6085+	1	1.99080+	1	2.28630+	1	5.65780+	2	2.28630+	18015	3	1	59
5	65780+	2	3.35260+	1	6.04250+	2	3.35260+	1	6.04250+	2	1.91045+	18015	3	1	60

APPENDIX C: MULTIBAND LIBRARY FORMAT

The binary multiband library is written and read using three-argument BUFFER IN and BUFFER OUT statements. The library contains a random-access directory to allow the multiband parameters for any given evaluation to be retrieved directly using random access. The same group structure must be used for all evaluations. The binary file contains the following:

- (a) A six-word pointer-counter set with addresses:
- 0* Number of words in library description (usually 24A4).
 - 1 Starting address of library description.
 - 2 Number of energy boundaries (number of groups plus one).
 - 3 Starting address of energy boundaries.
 - 4 Number of ZA values and temperatures in random-access directory.
 - 5 Starting address of random-access directory.
- (b) The library description--currently 24 words in A4 format. This information is used to identify the contents of the library, e.g.,

3 BAND LIBRARY DERIVED FROM ENDL LIBRARY - 790915

- (c) The energy boundaries in ascending energy order, in eV.
- (d) Random-access directory--three words for each ZA and temperature. The contents of the words are as follows:
- word 1 Starting address of multiband parameters (24 bits).
 Number of words per band (6 bits).
 Number of bands per group (6 bits).
 ZA (18 bits).
 - word 2 Floating-point kelvin temperature.
 - word 3 Date multiband parameters were created (A8) in the form
 mm/dd/yy; e.g., July 4, 1976 is 07/04/76.
- The entries in the random-access directory are in ascending order of ZA and temperature.

* diskfile address

(e) Multiband parameters for each ZA and temperature--there are (number of groups) $\times$ (number of bands per group) $\times$ (number of words per band) words for each ZA and temperature. For example, a 175-group, 2-band, 5-word-per-band array uses 1750 words. All numbers are in floating point. For checking, the three words from the random-access directory for each ZA and temperature are written immediately preceding the multiband parameters for each ZA and temperature. The words for each band are in the order

- 1 band weight (a fraction, 0.0 to 1.0),
- 2 band total cross section in barns,
- 3 band elastic cross section in barns,
- 4 band capture cross section in barns (optional), and
- 5 band fission cross section in barns (optional).

For each band, three to five words are given. If five words are given, there are cross sections for all four reactions. If four words are given, there is no fission cross section. If three words are given, there is no capture or fission cross section.

Data for all bands of the lowest-energy group are given first, then data for all bands of the next lowest-energy group, and so on up to the highest-energy group. Within each group, bands are arranged in order of increasing total cross section.

The binary file layout just described is illustrated in the following diagram:

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