VIII. GROUPR

GROUPR produces self-shielded multigroup cross sections, anisotropic group-to-group scattering matrices, and anisotropic photon production matrices for neutrons from ENDF/B-IV, V, or VI evaluated nuclear data. With ENDF-6 format files, incoming and outgoing charged particles can also be handled. Special features are provided for ratio quantities (for example, $\overline{\mu}$, $\overline{\nu}$, or photon yield), inverse velocity, delayed neutron spectra by time group, and anisotropic thermal neutron scattering. Fission is represented as a group-to-group matrix for full generality. Scattering matrices and photon production matrices may be self-shielded if desired.

The Bondarenko narrow-resonance weighting scheme[1] is usually used. Optionally, a weighting flux can be computed for various mixtures of heavy absorbers with light moderators. An accurate pointwise solution of the integral slowing down equation is used. This option is normally called on to account for intermediate resonance effects in the epithermal range.

Neutron data and photon-production data are processed in a parallel manner using the same weight function and quadrature scheme. This helps to assure consistent cross sections for coupled neutron-photon problems. Two-body scattering is computed with a center-of-mass (CM) Gaussian quadrature, which gives accurate results even for small Legendre components of the group-to-group matrix.

User conveniences include free-form input and complete control over which reactions are processed. The neutron group structure, photon group structure, and weight function can each be read in or set to one of the internal options. Output can be printed and/or written to an output "groupwise-ENDF" (GENDF) file for further processing by a formatting module (DTFR, CCCCR, MATXSR), by the covariance module (ERRORR), or by the MCNP continuous-energy Monte Carlo module (ACER).

This chapter describes GROUPR in version 91.91.

A. Multigroup Constants

Multigroup constants are normally used by computer codes that calculate the distributions of neutrons and/or photons in space and energy, and that compute various responses to these distributions, such as criticality, dose to personnel, or activation of materials. These distributions are solutions of the neutral particle transport equation.*

$$
\begin{aligned}
\mu \frac{\partial}{\partial x} \phi(x,\mu,E) \quad &+ \quad \sigma_t(x,E)\,\phi(x,\mu,E) \\
&= \quad \int d\boldsymbol{\Omega}' \int dE'\,\sigma_X(x,E'\!\to\!E,\boldsymbol{\Omega}'\!\to\!\boldsymbol{\Omega})\,\phi(x,\mu',E') \\
&+ \quad Q(x,\mu,E)\,, \qquad (1)
\end{aligned}
$$

where the flux ϕ is allowed to vary with position x, direction $\boldsymbol{\Omega}$ with polar cosine μ, and energy E. Similarly, the macroscopic total cross section σ_t varies with position and energy. The right-hand side of the equation contains the source due to transfers from other directions $\boldsymbol{\Omega}'$ and energies E' (as described by the macroscopic transfer cross section σ_X), and a fixed or external source Q.

The macroscopic cross sections (in units of cm^{-1}) in Eq. (1) can be calculated from microscopic cross sections for the component isotopes or elements (in barns) using

$$
\sigma_t(x,E) = \sum_i \rho_i(x)\,\sigma_t^i(T[x],E)\,, \qquad (2)
$$

where ρ_i is the number density for a constituent (in $\mathrm{barns}^{-1}\mathrm{cm}^{-1}$), which may vary with position, and T is the temperature, which may also vary with position. A similar formula holds for σ_X.

The transfer cross section σ_X (which includes both scattering and fission processes) is normally assumed to depend only on the cosine of the scattering angle, $\mu_0 = \boldsymbol{\Omega}\cdot\boldsymbol{\Omega}'$. This allows σ_X to be expanded using Legendre polynomials

$$
\sigma_X(x,E'\!\to\!E,\boldsymbol{\Omega}'\!\to\!\boldsymbol{\Omega}) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi}\,\sigma_{X\ell}(x,E'\!\to\!E)\,P_\ell(\mu_0)\,. \qquad (3)
$$

Application of the addition theorem and integration over azimuthal angle then gives

$$
\begin{aligned}
\mu \frac{\partial}{\partial x} \phi(x,\mu,E) \quad &+ \quad \sigma_t(x,E)\,\phi(x,\mu,E) \\
&= \quad \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} P_\ell(\mu) \int \sigma_{X\ell}(x,E'\!\to\!E)\,\phi_\ell(x,E')\,dE' \\
&+ \quad Q(x,\mu,E)\,, \qquad (4)
\end{aligned}
$$

where

$$
\phi_\ell(x,E) = \int P_\ell(\mu)\,\phi(x,\mu,E)\,d\mu\,. \qquad (5)
$$

*The following development uses a notation based on Bell and Glasstone[2], where the lower-case sigma is used for both macroscopic and microscopic cross sections, depending on the context. One-dimensional slab geometry is used throughout for simplicity.

The desired responses are then given by

$$R(x) = \int \sigma_r(x,E)\,\phi_0(x,E)\,dE\ , \tag{6}$$

where σ_r is the reaction cross section for the response. The next step is to integrate Eqs. (4) and (6) over a range of energies chosen to lie in group g. The results are

$$\begin{aligned}\mu\frac{\partial}{\partial x}\phi_g(x,\mu) \quad &+ \quad \sum_{\ell=0}^{\infty} P_\ell(\mu)\,\sigma_{t\ell g}(x)\,\phi_{\ell g}(x) \\ &= \quad \sum_{\ell=0}^{\infty}\frac{2\ell+1}{2}P_\ell(\mu)\sum_{g'}\sigma_{X\ell g'\to g}(x)\,\phi_{\ell g'}(x) + Q_g(x,\mu)\ ,\end{aligned} \tag{7}$$

and

$$R(x) = \sum_g \sigma_{rg}(x)\,\phi_{0g}(x)\ , \tag{8}$$

where

$$\phi_{\ell g}(x) = \int_g \phi_\ell(x,E)\,dE\ , \tag{9}$$

$$\sigma_{t\ell g}(x) = \frac{\displaystyle\int_g \sigma_t(x,E)\,\phi_\ell(x,E)\,dE}{\displaystyle\int_g \phi_\ell(x,E)\,dE}\ , \tag{10}$$

$$\sigma_r(x) = \frac{\displaystyle\int_g \sigma_r(x,E)\,\phi_0(x,E)\,dE}{\displaystyle\int_g \phi_0(x,E)\,dE}\ , \tag{11}$$

and

$$\sigma_{X\ell g'\to g} = \frac{\displaystyle\int_g dE\int_{g'} dE'\,\sigma_{X\ell}(x,E'\!\to\! E)\,\phi_\ell(x,E)}{\displaystyle\int_g \phi_\ell(x,E)\,dE}\ . \tag{12}$$

The last three equations provide the fundamental definitions for the multigroup cross sections and the group-to-group matrix. Note that the values of the group constants depend upon the basic energy-dependent cross sections obtained from ENDF/B by way of the RECONR, BROADR, UNRESR, HEATR, and THERMR modules of NJOY, and the shape of ϕ within the group.

B. Group Ordering

Since neutrons normally lose energy in scattering, the scattering source into group g depends on the flux at higher-energy groups g' and the cross section for transferring neutrons from g' to g. For this reason, Eq. (7) is usually solved by sweeping from high energies to low energies. (Any thermal upscatter or fission is handled by iteration.) Data libraries for use with transport codes normally number the groups such that group 1 is the highest-energy group, and all the scattering matrix elements that transfer neutrons into group 1 are given first, followed by those for scattering into group 2, and so on.

However, in ENDF/B the evaluated nuclear data are always given in order of increasing incident energy, and secondary neutron distributions are described by giving emission spectra for given incident energies. Therefore, GROUPR numbers its groups such that group 1 is the lowest-energy group, and it calculates that scattering out of group 1, followed by the scattering out of group 2, and so on.

The "backward" energy-group numbering convention used by GROUPR is a possible source of confusion in interpreting output produced by the various modules of NJOY. All group indices printed by GROUPR or written to the GROUPR output file use the increasing-energy order. The covariance modules and photon interaction module follow the GROUPR ordering convention. Output modules such as DTFR, CCCCR, and MATXSR invert the group order and rearrange the scattering matrices from the GROUPR outscatter organization to the "transport" inscatter form. Any group indices printed by these three output modules will be in the conventional transport decreasing-energy order.

C. Basic ENDF/B Cross Sections

The basic energy-dependent cross sections and energy-angle distributions needed for Eqs. (10), (11), and (12) are obtained from evaluated nuclear data in ENDF/B format[3, 4]. These data are indexed by material (MAT), type of information (MF), and reaction (MT). Materials can be single isotopes, elements, or compounds. Type of information includes energy-dependent cross section (MF=3), angular distributions (MF=4), secondary energy distributions (MF=5), and energy-angle distributions (MF=6). Reactions include the total (MT=1) required for Eq. (10), the partial scattering reactions that must be summed for Eq. (12) [that is, elastic (MT=2), discrete-level inelastic (MT=51–90), (n,2n) (MT=16), etc.], and the many partial reactions that can be used to calculate responses [for example, (n,2n) or (n,α) for activation, gas production, heat production (KERMA), radiation damage (DPA), etc.].

Before using GROUPR, the basic ENDF/B cross sections should have been converted into energy- and temperature-dependent pointwise cross sections in PENDF (pointwise ENDF) format using RECONR and BROADR. For heavy isotopes, un-

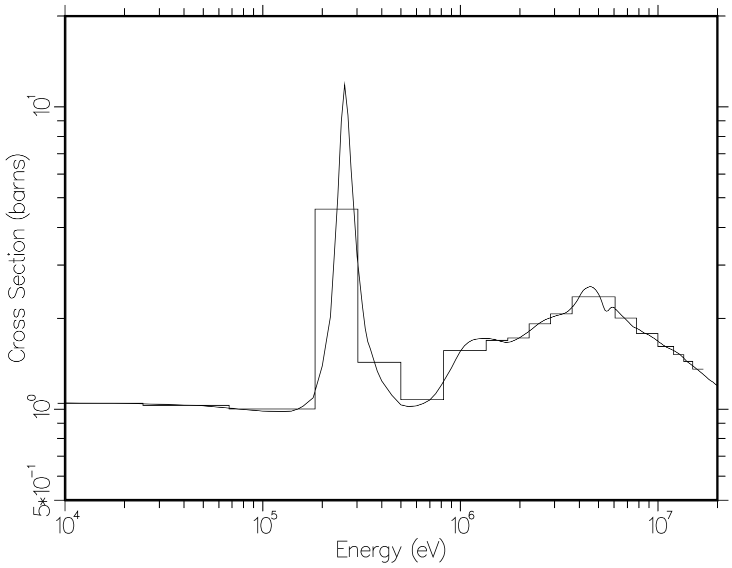

Figure 1: A comparison of the pointwise and multigroup representations for the total cross section of Li-7. The Los Alamos 30-group structure is shown.

resolved self-shielding data should have been added to the PENDF tape* using UNRESR. If needed, heat production cross sections (KERMA), radiation damage production (or DPA), and thermal upscatter data could have also been added to the PENDF tape using HEATR and THERMR. See the chapters on these other modules for more information.

The detailed methods used for evaluating Eqs. (10), (11), and (12) from ENDF and PENDF tapes are given below (see Sections VIII.K, VIII.L, and VIII.N). An example of an ENDF/B pointwise cross section compared with group-averaged cross sections from GROUPR is given in Fig. 1.

D. Weighting Flux

In general, the weighting flux ϕ is not known; it is, after all, the particle distribution being sought in the transport calculation. However, it is often possible to obtain fairly accurate group constants for a particular application if the shape of the flux is reasonably well known over the broad energy ranges of a particular few-group structure (for example, a fission spectrum, thermal Maxwellian, or $1/E$ slowing-down spectrum). Alternatively, one can use many small groups so that mistakes in guessing the shape inside the group are not very important. The key

*The term "tape" is used loosely in this report to refer to any input or output file. Of course, such files would usually be on disk storage in a modern system.

to using the multigroup method effectively is balancing the tradeoffs between the choice of weight function and the number of groups used for each different class of problem being solved.

In many cases of practical interest, the flux ϕ will contain dips corresponding to the absorption resonances of the various materials. In the reaction rate $\sigma(E)\times\phi(E)$, these dips clearly reduce (self-shield) the effect of the corresponding resonance. GROUPR provides two methods to estimate the effect of this self-shielding: the Bondarenko model and the flux calculator.

In the Bondarenko model[1], the narrow resonance (NR) approximation, and the B_N approximation for large systems[2] are invoked to obtain

$$\phi_\ell(E) = \frac{W_\ell(E)}{[\sigma_t(E)]^{\ell+1}} \;, \tag{13}$$

where ϕ_ℓ is the ℓ-th Legendre component of the angular flux, the $W_\ell(E)$ are smooth functions of energy (such as $1/E$+fission), and $\sigma_t(E)$ is the total macroscopic cross section for the material. GROUPR takes all of the W_ℓ to be equal to the single function $C(E)$, where $C(E)$ can be read in or set to one of several internally defined functions. It is further assumed that the important self-shielding effect of the flux can be obtained for isotope i by representing all the other isotopes with a constant "background cross section", σ_0. Therefore,

$$\phi^i_\ell(E) = \frac{C(E)}{[\sigma^i_t(E)+\sigma^i_0]^{\ell+1}} \;, \tag{14}$$

where σ^i_t is the microscopic total cross section for isotope i. The qualitative behavior of Eq. (14) is easy to understand. If σ_0 is larger than the tallest peaks in σ_t, the weighting flux ϕ is approximately proportional to the smooth weighting function $C(E)$. This is called infinite dilution; the cross section in the material of interest has little or no effect on the flux. On the other hand, if σ_0 is small with respect to σ_t, the weighting flux will have large dips at the locations of the peaks in σ_t, and a large self-shielding effect will be expected.

Each component material of a mixture has a different weight function. The macroscopic total cross sections are given by

$$\sigma_{t\ell g} = \sum_i \rho_i\, \sigma^i_{t\ell g}(\sigma^i_0, T) \;, \tag{15}$$

where

$$\sigma^i_{t\ell g}(\sigma_0,T) = \frac{\displaystyle\int_g \frac{\sigma^i_t(E,T)}{[\sigma_0+\sigma^i_t]^{\ell+1}} C(E)\,dE}{\displaystyle\int_g \frac{1}{[\sigma_0+\sigma^i_t]^{\ell+1}} C(E)\,dE} \;. \tag{16}$$

Similar equations are used for σ_R and $\sigma_{X\ell g\to g'}$. On the GROUPR level, σ_0 and T are simply parameters. Subsequent codes, such as 1DX[5] or TRANSX[6], can compute an appropriate value for σ_0, and then interpolate in tables of cross section versus σ_0 and T to get the desired self-shielded group constants.

The appropriate value for σ^i_0 is obvious when a single resonance material is mixed with a moderator material (for example, $^{238}UO_2$), because the admixed materials typically have a constant cross section in the energy range where the heavy isotopes have resonances. For a mixture of resonance materials, the normal procedure is to preserve the average of Eq. (14) in each group by using

$$\sigma^i_{0g} = \frac{1}{\rho_i}\sum_{j\neq i}\rho_j\,\sigma^j_{t0g}(\sigma^j_{0g},T)\;, \tag{17}$$

where the ρ_i are atomic densities or atomic fractions. Eq. (17) is solved by iteration. Interference between resonances in different materials is handled in an average sense only.

In the unresolved energy range (see UNRESR), the explicit dependence of cross section on energy is not known. The integrands are replaced by their expected values

$$\sigma_{x\ell g}(\sigma_0) = \frac{\displaystyle\int_g \left\langle \frac{\sigma_x}{[\sigma_0+\sigma_t]^{\ell+1}} \right\rangle W_\ell\,dE}{\displaystyle\int_g \left\langle \frac{1}{[\sigma_0+\sigma_t]^{\ell+1}} \right\rangle W_\ell\,dE}\;, \tag{18}$$

where the expected values are averages over the distributions of resonance position and width expected in the vicinity of energy E. The UNRESR module produces effective self-shielded point cross sections defined by

$$\langle\sigma_x\rangle_\ell = \frac{\left\langle \dfrac{\sigma_x}{[\sigma_0+\sigma_t]^{\ell+1}} \right\rangle}{\left\langle \dfrac{1}{[\sigma_0+\sigma_t]^{\ell+1}} \right\rangle}\;. \tag{19}$$

Substituting Eq. (19) into Eq. (18) gives an equation of the form of Eqs. (10) and (11), except that σ is replaced by $\langle\sigma\rangle$, and the flux is replaced by an average effective flux. This effective flux can be obtained by manipulating the effective total cross section as follows:

$$\langle\sigma_t\rangle_\ell = \frac{\left\langle \dfrac{\sigma_0+\sigma_t-\sigma_0}{[\sigma_0+\sigma_t]^{\ell+1}} \right\rangle}{\left\langle \dfrac{1}{[\sigma_0+\sigma_t]^{\ell+1}} \right\rangle} = \frac{\left\langle \dfrac{1}{[\sigma_0+\sigma_t]^{\ell}} \right\rangle}{\left\langle \dfrac{1}{[\sigma_0+\sigma_t]^{\ell+1}} \right\rangle} - \sigma_0 \ , \tag{20}$$

from which

$$\left\langle \frac{1}{[\sigma_0+\sigma_t]^{\ell+1}} \right\rangle = \frac{\left\langle \dfrac{1}{[\sigma_0+\sigma_t]^{\ell}} \right\rangle}{\sigma_0+\langle\sigma_t\rangle_k} \ . \tag{21}$$

Eq. (21) defines a recursion relation which can be used to compute the effective flux to any order

$$\left\langle \frac{1}{[\sigma_0+\sigma_t]^{\ell+1}} \right\rangle = \prod_{k=0}^{\ell} \frac{1}{\sigma_0+\langle\sigma_t\rangle_k} \ , \tag{22}$$

This equation reduces to Eq. (14) in the resolved range. It is the formula used in `GENFLX` to compute $\phi_\ell(E)$ for the Bondarenko option.

When heterogeneity effects are important, the background cross section method can be extended as follows. In an infinite system of two regions (fuel and moderator), the neutron balance equations are

$$V_f\sigma_f\phi_f = (1-P_f)V_fS_f + P_mV_mS_m \ , \tag{23}$$

and

$$V_m\sigma_m\phi_m = P_fV_fS_f + (1-P_m)V_mS_m \ , \tag{24}$$

where V_f and V_m are the region volumes, σ_f and σ_m are the corresponding total macroscopic cross sections, S_f and S_m are the sources per unit volume in each region, P_f is the probability that a neutron born in the fuel will suffer its next collision in the moderator, and P_m is the probability that a neutron born in the moderator will suffer its next collision in the fuel. As usual, use is made of the reciprocity theorem,

$$V_f\sigma_fP_f = V_m\sigma_mP_m \ , \tag{25}$$

and the Wigner rational approximation to the fuel escape probability,

$$P_f = \frac{\sigma_e}{\sigma_e+\sigma_f} \ , \tag{26}$$

where σ_e is a slowly varying function of energy called the escape cross section, to obtain an equation for the fuel flux in the form

$$(\sigma_f+\sigma_e)\phi_f = \frac{\sigma_eS_m}{\sigma_m} + S_f \ . \tag{27}$$

In the limit where the resonances are narrow with respect to both fuel and moderator scattering, the source terms S_f and S_m take on their asymptotic forms of σ_p/E and σ_m/E respectively, and this equation becomes equivalent to the Bondarenko model quoted above with

$$\sigma_0^f = \frac{\sigma_e}{\rho_f} \ , \tag{28}$$

and

$$C(E) = \frac{\sigma_e + \sigma_p}{\rho_f E} \ . \tag{29}$$

Note that a large escape cross section (a sample that is small relative to the average distance to collision), corresponds to infinite dilution as discussed above. To illustrate the general case, consider a neutron traveling through a lump of uranium oxide with an energy close to a resonance energy. If the neutron scatters from an oxygen nucleus, it will lose enough energy so that it can not longer react with the uranium resonance. Similarly, if the neutron escapes from the lump, it can no longer react with the uranium resonance. The processes of moderator scattering and escape are equivalent in some way. Comparing Eq. (28) with Eq. (17) gives an "equivalence principle" that says that a lump of particular dimensions and a mixture of particular composition will have the same self-shielded cross sections when the narrow resonance approximation is valid. The effects of material mixing and escape can simply be added to obtain the effective σ_0 for a lump containing admixed moderator material. Therefore, Eq. (17) is extended to read

$$\sigma_{0g}^i = \frac{1}{\rho_i} \left\{ \sigma_e + \sum_{j \neq i} \rho_j \, \sigma_{t0g}^j(\sigma_{0g}^j, T) \right\} \ , \tag{30}$$

where the escape cross section for simple convex objects (such as plates, spheres, or cylinders) is given by $(4V/S)^{-1}$, where V and S are the volume and surface area of the object, respectively. Many codes that use the background cross section method modify the escape cross section as defined above to correct for errors in the Wigner rational approximation ("Bell factor", "Levine factor"), or to correct for the interaction between different lumps in the moderating region ("Dancoff corrections"). These enhancements will not be discussed here.

E. Flux Calculator

This narrow-resonance approach is quite useful for practical fast reactor problems. However, for nuclear systems sensitive to energies from 1 to 500 eV, there are many broad- and intermediate-width resonances which cannot be self-shielded with sufficient accuracy using the Bondarenko approach. The GROUPR flux calculator is designed for just such problems.

Consider an infinite homogeneous mixture of two materials and assume isotropic scattering in the center-of-mass system. The integral slowing-down equation becomes

$$\begin{aligned}\sigma(E)\,\phi(E) &= \int_E^{E/\alpha_1} \frac{\sigma_{s1}(E')}{(1-\alpha_1)E'}\,\phi(E')\,dE' \\ &+ \int_E^{E/\alpha_2} \frac{\sigma_{s2}(E')}{(1-\alpha_2)E'}\,\phi(E')\,dE' \ . \end{aligned} \tag{31}$$

Furthermore, assume that material 1 is a pure scatterer with constant cross section and transform to the σ_0 representation. The integral equation becomes

$$\begin{aligned}[\sigma_0+\sigma_{t2}(E)]\,\phi(E) &= \int_E^{E/\alpha_1} \frac{\sigma_0}{(1-\alpha_1)E'}\,\phi(E')\,dE' \\ &+ \int_E^{E/\alpha_2} \frac{\sigma_{s2}(E')}{(1-\alpha_2)E'}\,\phi(E')\,dE' \ . \end{aligned} \tag{32}$$

Finally, assume that the moderator (material 1) is light enough so that all the resonances of material 2 are narrow with respect to scattering from material 1. This allows the first integral to be approximated by its asymptotic form $1/E$. More generally, the integral is assumed to be a smooth function of E given by $C(E)$. In this way, material 1 can represent a mixture of other materials just as in the Bondarenko method. Fission source and thermal upscatter effects can also be lumped in $C(E)$. The integral equation has now been reduced to

$$[\sigma_0+\sigma_t(E)]\,\phi(E) = C(E)\,\sigma_0 + \int_E^{E/\alpha} \frac{\sigma_s(E')}{(1-\alpha)E'}\,\phi(E')\,dE' \ . \tag{33}$$

This is the simplest problem that can be solved using the flux calculator. The results still depend on the single parameter σ_0, and they can be used easily by codes that accept Bondarenko cross sections.

For heterogeneous problems, when the narrow-resonance approximation fails, both S_f and S_m in Eq. (27) will show resonance features. To proceed further with the solution of this equation, it is necessary to eliminate the moderator flux that is implicit in S_m. As a sample case, consider a fuel pin immersed in a large region of water. The fission neutrons appear at high energies, escape from the pin, slow down in the moderator (giving a $1/E$ flux), and are absorbed by the resonances in the pin. In this limit, any dips in the moderator flux caused by resonances in the fuel are small. On the other hand, in a closely packed lattice, the flux in the moderator is very similar to the flux in the fuel, and resonance dips in the moderator flux become very evident. Intermediate cases can be approximated[7] by assuming

$$\phi_m = (1-\beta)\,C(E) + \beta\phi_f \;, \tag{34}$$

where β is a heterogeneity parameter given by

$$\beta = \frac{V_f\sigma_e}{V_m\sigma_m} \;. \tag{35}$$

Note that $\beta \to 0$ gives the isolated rod limit and $\beta \to 1$ gives the close-packed lattice limit. This substitution reduces the calculation of the fuel flux to

$$(\sigma_f + \sigma_e)\,\phi_f = (1-\beta)\,C(E)\,\sigma_e + S_\beta \;, \tag{36}$$

where S_β is the source term corresponding to a homogeneous mixture of the fuel isotopes with the isotopes from the moderator region changed by the factor $\beta\sigma_e/\sigma_m$. If the fuel and moderator each consisted of a single isotope and for isotropic scattering in the center-of-mass system, the integral equation would become

$$\begin{aligned}
[\sigma_0 + \sigma_t(E)]\,\phi_f(E) \;&=\; (1-\beta)\,C(E)\,\sigma_0 \\
&+\; \int_E^{E/\alpha_m} \frac{\beta\sigma_0}{(1-\alpha_m)E'}\,\phi_f(E')\,dE' \\
&+\; \int_E^{E/\alpha_f} \frac{\sigma_{sf}(E')}{(1-\alpha_f)E'}\,\phi_f(E')\,dE' \;,
\end{aligned} \tag{37}$$

where σ_0 is σ_e divided by the fuel density (units are barns/atom), α_m and α_f are the maximum fractional energy change in scattering for the two isotopes, and $\sigma_{sf}(E')$ is the fuel scattering cross section.

This result has a form parallel to that of Eq. (33), but the solution depends on the two parameters β and σ_0. For any given data set, β must be chosen in advance. This might not be difficult if the data are to be used for one particular system, such as pressurized water reactors. The routine also has the capability to include one more moderator integral with a different α value and a constant cross section. The full equation is

$$\begin{aligned}
[\sigma_0 + \sigma_t(E)]\,\phi_f(E) \;&=\; (1-\beta)\,C(E)\,\sigma_0 \\
&+\; \int_E^{E/\alpha_3} \frac{\beta(1-\gamma)(\sigma_0-\sigma_{am}}{(1-\alpha_3)E'}\,\phi_f(E')\,dE' \\
&+\; \int_E^{E/\alpha_2} \frac{\sigma_{am}+\beta\gamma(\sigma_0-\sigma_{am}}{(1-\alpha_2)E'}\,\phi_f(E')\,dE' \\
&+\; \int_E^{E/\alpha_f} \frac{\sigma_{sf}(E')}{(1-\alpha_f)E'}\,\phi_f(E')\,dE' \;,
\end{aligned} \tag{38}$$

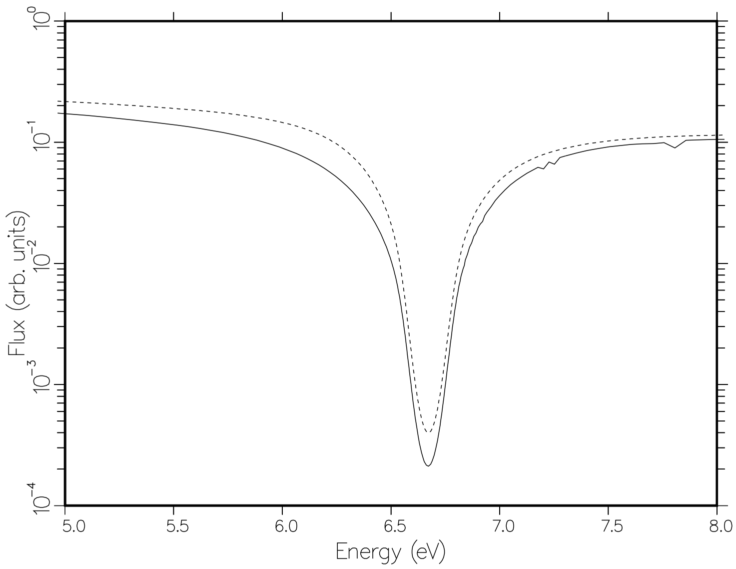

Figure 2: A comparison of the Bondarenko flux model (dashed) with a realistic computed flux (solid) for a ^{238}U oxide pin in water in the region of the 6.7 eV resonance.

where σ_{am} is the cross section of the admixed moderator (with energy loss α_2), and γ is the fraction of the admixed moderator that is mixed with the external moderator (which has energy loss α_3). This allows calculations with H_2O as the moderator and an oxide as the fuel. The flux calculator can thus obtain quite realistic flux shapes for a variety of fuel, admixed moderator, and external moderator combinations. An example comparing the Bondarenko flux with a more realistic computed flux is given in Fig. 2.

In practice, a fuel rod rarely contains only one resonance isotope. As an example, consider a mixture of a few percent of ^{239}Pu with ^{238}U as the major component. There will be a strong dip in the flux associated with the 6.7 eV ^{238}U resonance that will affect the flux in the region of the 7.8 eV ^{239}Pu resonance (the interference effect), and there will also be a dip in the flux corresponding to the 7.8 eV resonance (the self-shielding effect). This additional complication in the flux shape would be expected to change the group constants for ^{239}Pu since both features lie in the same group for typical group structures. However, the effect of the ^{239}Pu on the ^{238}U group constants should be minimal. This argument suggests that the full flux calculation be used for ^{238}U as a single resonance material. The resulting flux would then be used to estimate the flux to be used in averaging the ^{239}Pu cross sections as follows:

$$\phi_{239}(E,\sigma_0) = \frac{\phi_{238}(E,50)}{\sigma_0 + \dfrac{\sigma_{239}(E)}{1+\dfrac{\sigma_{238}(E)}{50}}} \ , \tag{39}$$

where the ^{238}U flux is characteristic of a background of 50 barns/atom, which is representative of many thermal reactor systems. This formula assumes that the effect of ^{239}Pu on the scattering source for the mixture is small, but it retains the absorption effects. The self-shielding of ^{239}Pu is treated in the narrow resonance approximation only. The GROUPR flux calculator includes an option to write out a file containing the calculated flux and cross section needed for this formula (e.g., for ^{238}U) and another option to skip the flux calculation and use the formula above to obtain the weighting flux (e.g., for ^{239}Pu).

The slowing-down integral equation of Eq. (33) or (37) is solved point by point (see subroutine `GENFLX`) using the total and elastic cross sections on the PENDF tape produced by RECONR. In order to keep this task within bounds, the flux is computed from the lower limit of the first group to a specified energy `EHI` or until `NFMAX` values have been computed. The flux at higher energies is continued using the Bondarenko model described above.

F. Fission Source

The fission source was included in the transfer cross section σ_X in the development above. It is usually convenient to separate fission from scattering. Assuming isotropy, the source of fission neutrons into group g is given by

$$S_g = \sum_{g'} \sigma_{fg'\to g}\, \phi_{0g'} \ , \tag{40}$$

where the group-to-group matrix for fission is defined as in Eq. (12), but with ℓ equal to zero. Most existing transport codes do not use this matrix form directly because the upscatter is expensive to handle and a reasonably accurate alternative exists. Except for relatively high neutron energies, the spectrum of fission neutrons is only weakly dependent on initial energy. Therefore, the fission source can be written

$$S_g = \chi_g \sum_{g'} \overline{\nu}_{g'}\, \sigma_{fg'}\, \phi_{0g'} \ , \tag{41}$$

where $\overline{\nu}_g$ is the fission neutron yield, σ_{fg} is the fission cross section, and χ_g is the average fission spectrum (the familiar "chi" vector), which can be defined by

$$\chi_g = \frac{\sum\limits_{g'} \sigma_{fg'\to g}\,\phi_{0g'}}{\sum\limits_{g}\sum\limits_{g'} \sigma_{fg'\to g}\,\phi_{0g'}} \ . \tag{42}$$

The fission neutron yield is given by

$$\overline{\nu}_g = \sum_{g'} \sigma_{fg\to g'} \,/\, \sigma_{fg} \ . \tag{43}$$

Clearly, χ_g as given by Eq. (42) depends on the flux in the system of interest. The dependence is weak except for high incident energies, and a rough guess for ϕ_{0g} usually gives an accurate spectrum. When this is not the case, the problem can be iterated, or the full matrix representation can be used.

It is possible to take advantage of the weak energy dependence of the shape of the fission spectrum at low energies to reduce the time required to process fission and to reduce the size of the fission data on the output file. GROUPR determines a break energy from File 5 such that the fission spectrum is constant below this energy. It only has to make a single calculation of this spectrum χ_g^{LE}. Then it computes a fission neutron production cross section σ_{fPg}^{HE} for groups below the break energy using the normal cross section processing methods. A full matrix $\sigma_{fg'\to g}^{HE}$ is computed for groups above the break point. As an example, consider using the GROUPR 187-group structure and finding that there are 130 constant groups. The 187×187 matrix is reduced to a 57×187 matrix, a 187-element spectrum vector, and a 130-group production vector, for a total reduction in size of 68%. The effective fission matrix is given by

$$\sigma_{fg'\to g} = \sigma_{fg'\to g}^{HE} + \chi_g^{LE}\sigma_{fPg'}^{LE} \ . \tag{44}$$

The fission matrix computed by GROUPR represents the prompt part of fission only. The delayed component of fission is represented by a delayed-neutron yield $\overline{\nu}_g^D$, decay constants for six time groups, λ_i^D, and emission probability spectra for six time groups, χ_{ig}^D. Steady-state fission can be obtained using

$$\overline{\nu}_g^{SS} = \overline{\nu}_g + \overline{\nu}_g^D \ , \tag{45}$$

and

$$\chi_g^{SS} = \frac{\displaystyle\sum_{g'} \sigma_{fg'\to g}\,\phi_{0g'} + \chi_g^D \sum_{g'} \overline{\nu}_{g'}^D\,\sigma_{fg'}\,\phi_{0g'}}{\displaystyle\sum_g \sum_{g'} \sigma_{fg'\to g}\,\phi_{0g'} + \sum_{g'} \overline{\nu}_{g'}^D\,\sigma_{fg'}\,\phi_{0g'}}\ , \tag{46}$$

where

$$\chi_g^D = \sum_i \chi_{ig}^D\ . \tag{47}$$

Note that χ_g^D sums to unity, but the χ for each time group sums to the fraction of the delayed neutron yield that appears in that time group.

In the ENDF/B files, the total fission reaction is represented by MT=18. Important isotopes also give the partial fission reactions (n,f), (n,n′f), (n,2nf), and sometimes (n,3nf) using MT=19, 20, 21, and 38 respectively. The MT=18 representation is adequate for most fission reactor applications, but the partial reactions should be processed for applications with significant flux above 6 MeV. Caution: although the cross section for MT=18 equals the sum of its parts, the group-to-group fission matrix $\sigma_{fg\to g'}$ computed from MT=18 will not, in general, equal the sum of the partial matrices for MT=19, 20, 21, and 38 above the 6-MeV threshold for second-chance fission. The delayed neutron data are given in MT=455. Sample input instructions for processing the various combinations of fission reactions used in ENDF/B will be found in Section VIII.N. GROUPR outputs all the components of fission separately in order to give succeeding modules or codes complete flexibility.

G. Diffusion Cross Sections

The diffusion equation is very commonly used in reactor physics calculations. Starting with Eq. (7), use the Legendre expansion for ϕ_g in the derivative term, and make use of the recursion relation for $\mu P_\ell(\mu)$ and the orthogonality relation for the Legendre polynomials to obtain the transport equation in spherical harmonic form

$$\frac{n+1}{2n+1}\frac{\partial\phi_{n+1,g}}{\partial x} + \frac{n}{2n+1}\frac{\partial\phi_{n-1,g}}{\partial x}\,\sigma_{tng}\,\phi_{ng} = \sum_{g'} \sigma_{sng'\to g}\,\phi_{ng'} + S_{fg} + Q_{ng}\ , \tag{48}$$

where the transfer term has been separated into a scattering term with cross section σ_s, and a fission source term S_f. When this set of equations is truncated at n = N, the result is usually called the "$\mathrm{P_N}$ equations". Now, all terms with $n > 1$ are dropped, and Q is assumed to be isotropic. Thus,

$$\frac{\partial \phi_{1g}}{\partial x} + \sigma_{t0g}\, \phi_{0g} = \sum_{g'} \sigma_{s0g' \to g}\, \phi_{0g'} + S_f + Q_{0g} \ , \tag{49}$$

and

$$\frac{1}{3}\frac{\partial \phi_{0g}}{\partial x} + \sigma_{t1g}\, \phi_{1g} = \sum_{g'} \sigma_{s1g' \to g}\, \phi_{1g'} \ . \tag{50}$$

The second equation can be written in the form of Fick's Law as follows:

$$\phi_{1g} = -D_g \frac{\partial \phi_{0g}}{\partial x} \ , \tag{51}$$

$$D_g = \frac{1}{3} \frac{1}{\sigma_{t1g} - \sum_{g'} \sigma_{s1g' \to g}\, \phi_{1g'} \,/\, \phi_{1g}} \ , \tag{52}$$

where D_g is the diffusion constant. The term in the denominator of the second factor is the transport cross section for diffusion, σ_{trD}. Unfortunately, it depends on a fairly complete knowledge of the neutron current in the system, perhaps from a previous calculation. However, for many problems, σ_{trD} can be simplified by assuming that

$$\sum_{g'} \sigma_{s1g' \to g}\, \phi_{1g'} \approx \sum_{g'} \sigma_{s1g \to g'}\, \phi_{1g} \ , \tag{53}$$

with the result that

$$\sigma_{trD,g} = \sigma_{t1g} - \sum_{g'} \sigma_{s1g \to g'} \ , \tag{54}$$

or

$$\sigma_{trD,g} = \sigma_{t1g} - \overline{\mu}_g\, \sigma_{s0g} \ , \tag{55}$$

where $\overline{\mu}_g$ is the average scattering cosine for neutrons in group g. These forms depend only on the shape of the weighting flux within the group, as usual. Substituting for ϕ_{1g} in Eq. (49) gives

$$\frac{\partial}{\partial x}\left(-D_g \frac{\partial \phi_{0g}}{\partial x}\right) + \sigma_{0tg}\, \phi_{0g} = \sum_{g'} \sigma_{s0g' \to g}\, \phi_{0g'} + S_{fg} + Q_{0g} \ , \tag{56}$$

which is the standard diffusion equation in slab geometry. Neither the diffusion coefficient nor the transport cross section for diffusion is produced directly by GROUPR. However, the components such a $\sigma_{t\ell}$ and $\sigma_{s0g' \to g}$ are made available to subsequent modules.

H. Cross Sections for Transport Theory

The S_N (discrete ordinates) transport codes solve the equation

$$\begin{aligned}\mu\frac{\partial}{\partial x}\phi_g(\mu,x) \quad &+ \quad \sigma_g^{SN}\phi_g(\mu,x) \\ &= \quad \sum_{\ell=0}^{N}\frac{2\ell+1}{2}P_\ell(\mu)\sum_{g'}\sigma_{s\ell g'\to g}^{SN}(x)\,\phi_{\ell g'} \\ &+ \quad S_{fg}+Q_g(\mu,x)\ ,\end{aligned} \tag{57}$$

where once again one-dimensional slab geometry has been used for simplicity.* By comparing Eq. (57) with Eq. (7), it is seen that the S_N equations require the following cross sections:

$$\sigma_{s\ell g'\to g}^{SN}=\sigma_{s\ell g'\to g}, \qquad g'\neq g\ , \tag{58}$$

and

$$\sigma_{s\ell g\to g}^{SN}=\sigma_{s\ell g\to g}-\sigma_{t\ell g}+\sigma_g^{SN}\ , \tag{59}$$

where σ_g^{SN} is not determined and can be chosen to improve the convergence of the S_N calculation. A particular choice of σ_g^{SN} gives rise to a "transport approximation", and various recipes are in use.

Consistent-P approximation:

$$\sigma_g^{SN}=\sigma_{t0g}\ . \tag{60}$$

Inconsistent-P approximation:

$$\sigma_g^{SN}=\sigma_{t,N+1,g}\ . \tag{61}$$

Diagonal transport approximation:

$$\sigma_g^{SN}=\sigma_{t,N+1,g}-\sigma_{s,N+1,g\to g}\ . \tag{62}$$

Bell-Hansen-Sandmeier (BHS) or extended transport approximation:

$$\sigma_g^{SN}=\sigma_{t,N+1,g}-\sum_{g'}\sigma_{s,N+1,g\to g'}\ . \tag{63}$$

*The following development is based on the work of Bell, Hansen, and Sandmeier[8].

Inflow transport approximation:

$$\sigma_g^{SN} = \sigma_{t,N+1,g} - \frac{\sum_{g'} \sigma_{s,N+1,g'\to g}\,\phi_{N+1,g'}}{\phi_{N+1,g}} \ . \tag{64}$$

The first two approximations are most appropriate when the scattering orders above N are small. The inconsistent option removes most of the delta function of forward scattering introduced by the correction for the anisotropy of the total scattering rate, and should normally be more convergent than the consistent option. The diagonal and BHS recipes make an attempt to correct for anisotropy in the scattering matrix and are especially effective for forward-peaked scattering. The BHS form is more often used, but the diagonal option can be substituted when BHS produces negative values. The inflow recipe makes the $N{+}1$ term of the P_N expansion vanish, but it requires a good knowledge of the $N{+}1$ flux moment from some previous calculation. Inflow reduces to BHS for systems in equilibrium by detail balance (i.e., the thermal region). In the absence of self-shielding (that is, $\sigma_0 \to \infty$), the distinction between σ_{t1} and σ_{t0} disappears, and so does the distinction between the inconsistent-P and consistent-P options. Also note that the inflow and BHS versions of σ_g are equivalent to the definitions of $\sigma_{trD,g}$ given in Eqs. (52) and (54), respectively, when $N{=}0$.

These transport-corrected cross sections are not computed directly by GROUPR, but the components needed are written to the GROUPR output file for use by subsequent modules.

I. Photon Production and Coupled Sets

Photon transport is treated with an equation similar to Eq. (7), except that the flux, cross sections, and groups are all referred to photon interactions and photon energies instead of to the corresponding neutron quantities. Methods of producing the photon interaction cross sections are described in GAMINR, Chapter IX of this manual. The external photon source Q_g depends on the neutron flux and the photon production cross sections through

$$Q_g(x,\mu) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} P_\ell(\mu) \sum_{g'} \sigma_{\gamma\ell g'\to g}(x)\,\phi_{\ell g'}(x) \ , \tag{65}$$

where $\sigma_{\gamma\ell g'\to g}$ is defined by Eq. (12) with X replaced by γ. The ENDF/B files define σ_γ using a combination of photon production cross sections (MF=13), photon yields (MF=12) with respect to neutron cross sections (MF=3), discrete lines

(MF=12 and 13), and continuous γ distributions (MF=15). Methods for working with these representations will be discussed in more detail below.

The low-energy groups for fission and capture normally have photon emission spectra whose shapes do not change with energy. The same method used for reducing the size of the fission matrix (see Section VIII.F) can be used for these photon production matrices. In mathematical form,

$$\sigma_{\gamma g'\rightarrow g} = \sigma^{HE}_{\gamma g'\rightarrow g} + s^{LE}_{\gamma} g \sigma^{LE}_{\gamma P g'} \ , \tag{66}$$

where $s^{LE}_{\gamma} g$ is the normalized emission spectrum, and $\sigma^{LE}_{\gamma P g}$ is the associated production cross section.

For many practical problems, it is convenient to combine the neutron and photon transport calculations into a single application of Eq. (7) where the photons are treated as additional groups of low-energy neutrons. Since (γ,n) events are not usually very important, the downscattering structure (see Section B) of the transport calculation is preserved for both n$\rightarrow\gamma$ and n$\rightarrow$n events. Cross sections for this application are called "coupled sets". Coupled sets are not produced directly by GROUPR, but the n$\rightarrow$n and n$\rightarrow\gamma$ components are made available to the other modules where they can be combined with $\gamma\rightarrow\gamma$ cross sections from GAMINR. As an example, the MATXSR module can format data for the TRANSX code[6], which can, in turn, prepare coupled sets for use by standard transport codes such as ONEDANT[9]. The normal arrangement of data in a coupled set is shown schematically in Fig. 3.

J. Thermal Data

GROUPR uses the thermal data written onto the PENDF tape by the THERMR module. It does not process ENDF File-7 data directly. Three different representations of thermal scattering are used in ENDF.

For crystalline materials like graphite, coherent elastic (with zero energy change) scattering can take place. The cross section for this process shows well-defined Bragg edges at energies that correspond to the various lattice-plane spacings in the crystalline powder. As shown in THERMR, Chapter VII of this manual, the angular dependence of the coherent elastic cross section can be written as

$$\sigma^{coh}(E,\mu) = \sum_i \frac{b_i}{E}\,\delta(\mu-\mu_i) \ , \tag{67}$$

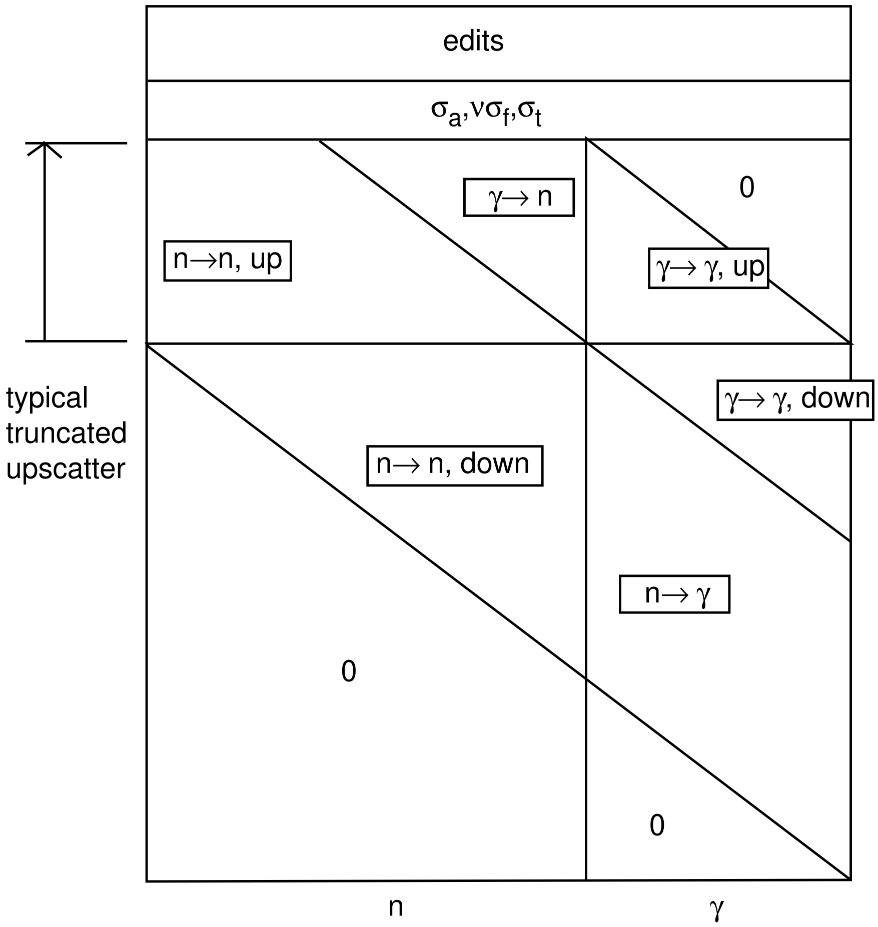

Figure 3: Arrangement of neutron (n) and photon (γ) cross sections in a coupled transport table. The group index increases from left to right, and the position index increases from top to bottom. The $\gamma \rightarrow$n and $\gamma \rightarrow \gamma$ upscatter blocks are normally empty.

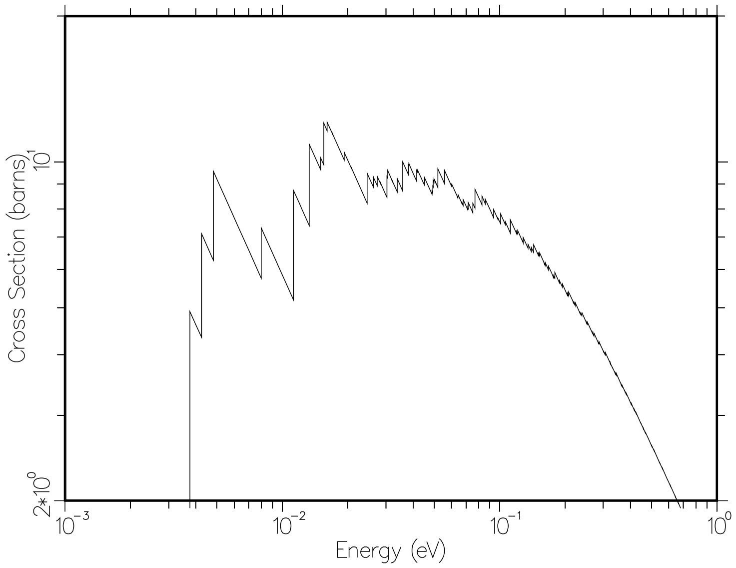

Figure 4: The coherent elastic scattering cross section for BeO showing the Bragg edges. The shape of $\sigma(E)$ between edges is $1/E$. Therefore, the function $E\sigma(E)$ is a stairstep function, where the height of each step depends on the structure factor for scattering from that set of lattice planes [see Eq. (69)].

where

$$\mu_i = 1 - 2\frac{E_i}{E} \; , \tag{68}$$

and where the E_i are the energies of the Bragg edges. THERMR integrates Eq. (67) over all angles, and writes the result to the PENDF tape. Clearly, the b_i can be recovered from

$$E\,\sigma^{coh}(E) = \sum_i{}' \, b_i \; , \tag{69}$$

where the primed sum is over all i such that $E_i < E$. It is only necessary to locate the steps in $E\,\sigma^{coh}(E)$. The size of the step gives b_i, and the E for the step gives E_i. The Legendre cross sections become

$$\sigma_\ell^{coh}(E) = \sum_i{}' \, \frac{b_i}{E} P_\ell(\mu_i) \; , \tag{70}$$

where any terms with $\mu_i < -1$ are omitted from the primed sum. An example of a pointwise cross section for coherent elastic scattering is given in Fig. 4.

For hydrogenous solids like polyethylene and zirconium hydride, the process of incoherent elastic scattering is important. Here the angular cross section is given by

$$\sigma^{iel}(E,\mu) = \frac{\sigma_b}{2}\exp\left[-\frac{2EW}{A}(1-\mu)\right] , \tag{71}$$

(see THERMR, Chapter VIII of this manual). THERMR converts this into an integrated cross section, $\sigma^{iel}(E)$, and a set of N equally probable emission cosines, $\overline{\mu}_i$. These angles are present in File 6 on the PENDF tape. GROUPR can easily determine the Legendre components of the scattering cross section using

$$\sigma_\ell^{iel}(E) = \sigma^{iel}(E)\frac{1}{N}\sum_{i=1}^{N} P_\ell(\mu_i) . \tag{72}$$

The third thermal process is incoherent inelastic scattering. Here the neutron energy can either increase or decrease. The data from THERMR are given as a cross section in File 3 and an energy-angle distribution using a special form of File 6. The distribution is represented by sets of secondary-energy values E' for particular incident energies E. For each $E{\rightarrow}E'$, a scattering probability $f^{inc}(E{\rightarrow}E')$ and a set of equally probable cosines $\mu_i(E{\rightarrow}E')$ are given. The scattering probabilities for each value of E integrate to unity. Although the thermal scattering cross section is a smooth function of incident neutron energy, this is not true for the scattering from E to one particular final energy group g', since the differential cross section tends to peak along the line $E'{=}E$ and at energy-transfer values corresponding to well-defined excitations in the molecule or lattice. If interpolation between adjacent values of E were to be performed along lines of constant E', the excitation peaks and the $E{=}E'$ feature would produce double features in the intermediate spectrum, as shown in Fig. 5. To avoid this problem, while still using a relatively sparse incident energy grid, GROUPR interpolates between E and E' along lines of constant energy transfer. Of course, this breaks down at low values of E', because one of the spectra will go to zero before the other one does. In this range, GROUPR transforms the low-energy parts of the two spectra onto a "unit base," combines them in fractions that depend on E, and scales the result back out to the interpolated value of E' corresponding to E.

K. Generalized Group Integrals

In order to unify many formerly different processing tasks, GROUPR uses the concept of a generalized group integral

$$\sigma_g = \frac{\displaystyle\int_g \mathcal{F}(E)\,\sigma(E)\,\phi(E)\,dE}{\displaystyle\int_g \phi(E)\,dE} , \tag{73}$$

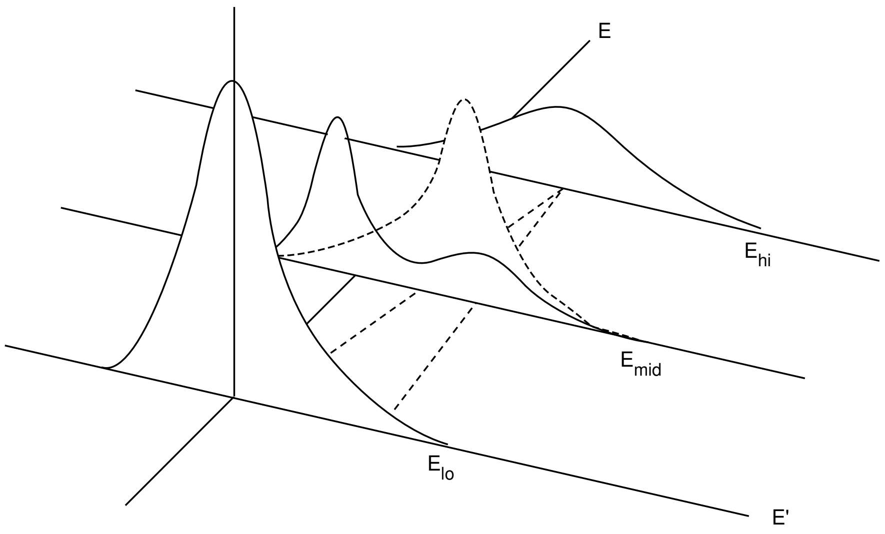

Figure 5: Illustration of thermal interpolation showing the double-humped curve resulting from simple Cartesian interpolation for a discrete excitation (solid) and the more realistic curve obtained by interpolating along lines of constant energy transfer (dashed).

where the integrals are over all initial neutron energies in group g, $\sigma(E)$ is a cross section at E, and $\phi(E)$ is an estimate of the flux at E. The function $\mathcal{F}(E)$ is called the "feed function". It alone changes for different data types. To average a neutron cross section, $\mathcal{F}$ is set to 1. To average a ratio quantity like $\overline{\mu}$ with respect to elastic scattering, $\mathcal{F}$ is set to $\overline{\mu}$. For photon production, $\mathcal{F}$ is the photon yield. For matrices, $\mathcal{F}$ is the ℓ-th Legendre component of the normalized probability of scattering into secondary energy group g' from initial energy E. This definition is clearly independent of whether the secondary particle is a neutron or a photon.

The question of integration grid or quadrature scheme is important for the evaluation of Eq. (73). Each factor in the integrands has its own characteristic features, and it is important to account for them all. First, a grid must be established for each factor. As an example, the grid of $\sigma(E)$ is generated in RECONR such that sigma can be obtained to within a given tolerance by linear interpolation. GROUPR contains a subroutine `GETSIG` which carries out this interpolation at E and also returns the next grid energy in `ENEXT`. Subroutines `GETFLX` and `GETFF` perform similar functions for the flux and feed function. It is now easy to generate a union grid for the three-factor integrand using the following FORTRAN:

```
 ...
CALL GETSIG(E,ENEXT,...)
CALL GETFLX(E,EN,...)
```

```
      IF (EN.LT.ENEXT) ENEXT=EN
      CALL GETFF(E,EN,...)
      IF (EN.LT.ENEXT) ENEXT=EN
       ...
```

On occasion, there will be a discontinuity at `ENEXT` for one of the factors. In order to flag such a case, each "`GET`" routine also sets a discontinuity flag `IDISC`. The grid logic actually used throughout NJOY is as follows:

```
     ...
      CALL GETSIG(E,ENEXT,IDISC,...)
      CALL GETFLX(E,EN,IDIS,...)
      IF (EN.EQ.ENEXT.AND.IDIS.GT.IDISC) IDISC=IDIS
      IF (EN.LT.ENEXT) IDISC=IDIS
      IF (EN.LT.ENEXT) ENEXT=EN
      CALL GETFF(E,EN,IDIS,...)
      IF (EN.EQ.ENEXT.AND.IDIS.GT.IDISC) IDISC=IDIS
      IF (EN.LT.ENEXT) IDISC=IDIS
      IF (EN.LT.ENEXT) ENEXT=EN
      ...
```

This union grid for the integrand in the numerator is used to subdivide the generalized group integral of Eq. (73) into "panels". The main program of GROUPR carries out the integrals with the following logic:

```
      ...
      ELO=EGN(IG)
      EHI=EGN(IG+1)
      ENEXT=EHI
  230 CALL PANEL(ELO,ENEXT,...)
      IF (ENEXT.EQ.EHI) GO TO 240
      ELO=ENEXT
      ENEXT=EHI
      GO TO 230
  240 CONTINUE
      ...
```

A panel is first defined by the energy bounds of group g. Subroutine `PANEL` is called to sum in the contributions from this panel. However, `PANEL` discovers that the integrand has a grid point at `ENEXT` less than `EHI`. It adds in the contributions for the smaller panel `ELO` to `ENEXT` and returns. GROUPR now sees that `ENEXT` is less than `EHI`, so it tries a new panel from the top of the last panel (`ELO=ENEXT`) to `EHI`. This loop continues until a panel with `EHI` as its upper bound is summed in. The integral for this group is then complete.

In this simple way, the algorithm accounts for the user's group structure and for all structure in the integrand. The method used for establishing the RECONR grid makes this integration algorithm equivalent to adaptive integration as used in MINX[10]. It has the great advantage that no "stack" of intermediate results is carried along. This single-pass feature of the quadrature scheme allows many different integrals to be accumulated simultaneously within reasonable storage limits. In this way, GROUPR accumulates cross sections for all values of σ_0 simultaneously. Similarly, group-to-group cross sections are computed for all secondary energy groups and all Legendre orders simultaneously.

Any degree of complexity can be used for the integral over each subpanel. Because $\sigma(E)$ has been linearized, `PANEL` is based on trapezoidal integration. Both $\phi(E)$ and $R(E) = \sigma(E)\times\phi(E)$ are assumed to vary linearly across each panel. In some cases, the feed function is oscillatory over a certain energy range (see Two-Body Scattering, Section VIII.L). It is then convenient to integrate inside the panel using Lobatto quadrature[11] (note the variable `NQ` in `PANEL`). As discussed in more detail later, this method can obtain accurate results for an oscillatory function whose integral is small with respect to its magnitude. This behavior is characteristic of the higher Legendre components of two-body scattering cross sections.

The generalized integration scheme discussed here is also used by the GAMINR and ERRORR modules.

L. Two-Body Scattering

Elastic scattering (ENDF/B MT=2) and discrete inelastic neutron scattering (with MT=51–90) are both examples of two-body kinematics and are treated together by GROUPR. Some other cases that occur for charged particles or in File 6 will be discussed later. The feed function required for the group-to-group matrix calculation may be written

$$\mathcal{F}_{\ell g'}(E) = \int_{g'} dE' \int_{-1}^{+1} d\omega\, f(E\to E',\omega)\, P_\ell(\mu[\omega]) \;, \tag{74}$$

where $f(E\to E',\omega)$ is the probability of scattering from E to E' through a center-of-mass cosine ω and P_ℓ is a Legendre polynomial for laboratory cosine μ. The laboratory cosine corresponding to ω is given by

$$\mu = \frac{1+R\omega}{\sqrt{1+R^2+2R\omega}} \;, \tag{75}$$

and the cosine ω is related to secondary energy E' by

$$\omega = \frac{E'(1+A)^2/A' - E(1+R^2)}{2RE} \;, \tag{76}$$

where A' is the ratio of the emitted particle mass to the incident particle mass (A'=1 for neutron scattering). In Eqs. (75) and (76), R is the effective mass ratio

$$R = \sqrt{\frac{A(A+1-A')}{A'}}\sqrt{1-\frac{(A+1)(-Q)}{AE}} \;, \tag{77}$$

where A is the ratio of target mass to neutron mass, and $-Q$ is the energy level of the excited nucleus (Q=0 for elastic scattering). Integrating Eq. (74) over secondary energy gives

$$\mathcal{F}_{\ell g'}(E) = \int_{\omega_1}^{\omega_2} f(E,\omega)\, P_\ell(\mu[\omega])\, d\omega \;, \tag{78}$$

where ω_1 and ω_2 are evaluated using Eq. (76) for E' equal to the upper and lower bounds of g', respectively.

The scattering probability is given by

$$f(E,\omega) = \sum_{\ell=0}^{L} f_\ell(E)\, P_\ell(\omega) \;, \tag{79}$$

where the Legendre coefficients are either retrieved directly from the ENDF/B File 4 or computed from File 4 tabulated angular distributions (see subroutines `GETFLE` and `GETCO`).

The integration in Eq. (78) is performed (see subroutine `GETDIS`) simultaneously for all Legendre components using Gaussian quadrature.[11] The quadrature order is selected based on the estimated polynomial order of the integrand. A reasonable estimate is given by

$$\mathrm{ND} + \mathrm{NL} + \log(300/A) \;, \tag{80}$$

where ND is the number of Legendre components desired for the feed function, and NL is the number of components required to represent $f(E,\omega)$. The log term approximates the number of additional components required to represent the center-of-mass to lab transformation.

The two-body feed function for higher Legendre orders is a strongly oscillatory function in some energy ranges. An example is shown in Fig. 6. Furthermore, the

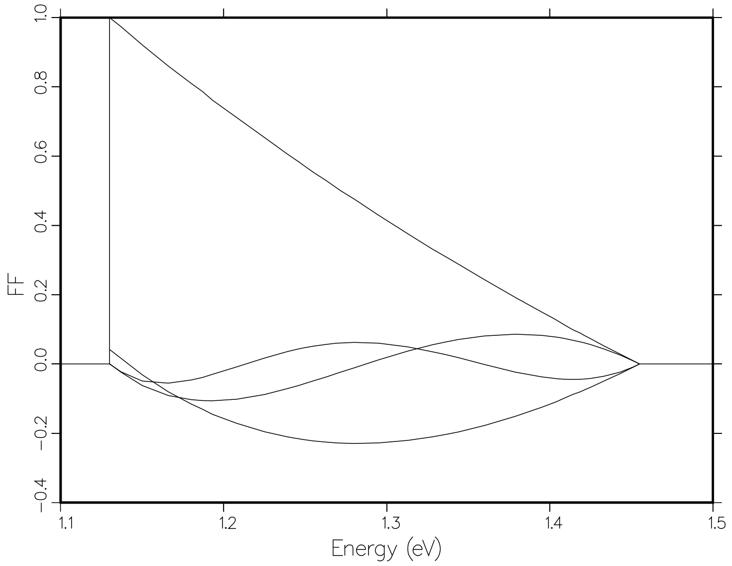

Figure 6: A typical feed function for two-body scattering showing the oscillations that must be treated correctly by the integration over incident energy.

integral of the oscillatory part is often small with respect to the magnitude of the function. Such functions are very difficult to integrate with adaptive techniques, which converge to some fraction of the integral of the absolute value. This is the reason that MINX[10] gives poor answers for small Legendre components of the scattering matrix. Gaussian methods, on the other hand, are capable of integrating such oscillatory functions exactly if they are polynomials. Since a polynomial representation of the feed function is fairly accurate, a Gaussian quadrature scheme was chosen. The scheme used is also well adapted to performing many integrals in parallel. In GROUPR, all Legendre components and all final groups are accumulated simultaneously (see `PANEL`).

The boundaries of the various regions of the feed function are called "critical points." Between critical points, the feed function is a smooth analytic function of approximately known polynomial order. It is only necessary to add these critical points to the incident energy grid of the feed function (the `ENEXT` variable) and to tell `PANEL` what quadrature order (`NQ`) to use. The critical points are determined in `GETFF` by solving Eq. (76) for the values of E for which $\omega = +1$ and $\omega = -1$ when E' is equal to the various group boundaries. This can be done by writing

$$\frac{E_g}{E} = \frac{1}{(1+A)^2}[R^2 \pm 2R + 1] \; , \tag{81}$$

substituting for E using Eq. (77), and then solving for R. The result is

$$E_{crit} = \frac{\dfrac{(A+1)(-Q)}{A}}{1 - \dfrac{A'F^2}{A(A+1-A')}} \ , \tag{82}$$

where

$$F = \frac{1 \pm \sqrt{D}}{1 + \dfrac{E_F}{(-Q)}} \ , \tag{83}$$

$$D = \left[\frac{A(A+1-A')}{A'} \left(1 + \frac{E_F}{(-Q)} \right) - 1 \right] \frac{E_F}{(-Q)} \ , \tag{84}$$

and

$$E_F = \frac{1+A}{A+1-A'} E_g \ . \tag{85}$$

File 4 can also contain angular distributions for charged-particle emission through discrete levels (see MT=600–648 for protons, MT=650–698 for deuterons, and so on; the elastic case, MT=2, is discussed in the next section). Moreover, File 6 can contain angular distributions for discrete two-body scattering (see Law 3). It can also declare that a particular particle is the recoil particle from a two-body reaction (Law 4), in which case the appropriate angular distribution is obtained from the corresponding Law 3 subsection by complementing the angle. The representation of the angular distribution for these laws is almost identical to that in File 4, and the calculation is done in `GETDIS` using much of the File 4 coding. The effects on the kinematics of the difference in the mass of the emitted and incident particles are handled by the variable A' in the above equations.

M. Charged-Particle Elastic Scattering

Coulomb scattering only occurs in the elastic channel, and this calculation also uses the `GETDIS` subroutine. The problem with Coulomb scattering is that the basic Rutherford formula becomes singular at small angles. In practice, this singularity is removed by the screening effects of the atomic electrons. The forward transport of charged particles in this screening regime is usually handled by continuous-slowing-down theory by using a "stopping power". The new ENDF-6 format allows for three different ways to handle the large-angle scattering regime. First and most general is the nuclear amplitude expansion:

$$\begin{aligned} \sigma &= |\mathrm{nucl} + \mathrm{coul}|^2 \\ &= \sigma_{\mathrm{nucl}} + \sigma_{\mathrm{coul}} + \mathrm{interference} \end{aligned} \tag{86}$$

The Coulomb term is given by the Rutherford formula, a Legendre expansion is defined for the nuclear term, and a complex Legendre expansion is defined for the interference term. This representation cannot be generated directly from experimental data; an R-matrix or phase-shift analysis is necessary.

A method very closely related to experiment ($\sigma_{\rm exp}$) is the nuclear plus interference (NI) formula:

$$\sigma_{\rm NI}(\mu,E) = \sigma_{\rm exp}(\mu,E) - \sigma_{\rm coul}(\mu,E), \tag{87}$$

where the function is only defined for angles with cosines $\mu<\mu_{\rm max}$. The minimum angle is usually taken to be somewhere around 20 degrees (GROUPR uses $\mu_{\rm max}$=0.96). This function is still ill-behaved near the cutoff, and it must be tabulated. The third option is the residual cross section expansion:

$$\sigma_R(\mu,E) = (1-\mu)[\sigma_{\rm exp}(\mu,E) - \sigma_{\rm coul}(\mu,E)]. \tag{88}$$

The $(1-\mu)$ term removes the pole at the origin. The residual is uncertain, but it is usually small enough that the entire curve can be fitted with Legendre polynomials without worrying about what happens at small angles. In practice, both the nuclear amplitude expansion and the nuclear plus interference representation are converted to the residual cross section representation in subroutine `CONVER`. As a result, `GETDIS` only has to cope with the one representation.

N. Continuum Scattering and Fission

In ENDF/B, scattering from many closely-spaced levels or multibody scattering such as (n,2n), (n,n$'\alpha$), and fission is often represented using a separable function of scattering cosine and secondary neutron energy

$$f(E{\to}E',\mu) = F(E,\mu)\,g(E{\to}E')\ , \tag{89}$$

where F is the probability that a neutron will scatter through a laboratory angle with cosine μ irrespective of final energy E'. It is obtained from MF=4. Similarly, g is the probability that a neutron's energy will change from E to E' irrespective of the scattering angle, and it is given in MF=5. Continuum reactions are easily identified by MT numbers of 6–49 and 91. The secondary-energy distributions can be represented in the following ways:

Law	Description
1	Arbitrary tabulated function
5	General evaporation spectrum (Used for delayed neutrons only.)
7	Simple Maxwellian fission spectrum
9	Evaporation spectrum
11	Energy-dependent Watt fission spectrum
12	Energy-dependent spectrum of Madland and Nix

The feed functions for continuum scattering are simply

$$\mathcal{F}_{\ell g'}(E') = \int_{-1}^{+1} P_\ell(\mu)\, f(E,\mu)\, d\mu \int_{g'} g(E,E')\, dE' \; . \tag{90}$$

The first integral is returned by `GETFLE` [FLE for $f_\ell(E)$] as described above, and the second integral is returned by `GETSED` (SED for secondary-energy distribution).

For Law 1, g is given as a tabulated function of E' for various values of E. When $E_1 \le E < E_2$, the term $\int_{g'} g(E,E')\, dE'$ is obtained by interpolating between precomputed values of $\int_{g'} g(E_1,E')\, dE'$ and $\int_{g'} g(E_2,E')\, dE'$ in subroutine `GETSED`. Except in the case of fission, any apparent upscatter produced by the "stairstep" treatment near $E{=}E'$ is added to the in-group scattering term ($g'{=}g$).

For Law 5, $g(x)$ is given versus $x = E'/\theta(E)$ and $\theta(E)$ is given vs. E in File 5. This secondary neutron distribution leads to the following group integral:

$$\int_{g'} g(E,E')\, dE' = \theta(E) \int_{E_1/\theta}^{E_2/\theta} g(x)\, dx \; , \tag{91}$$

with E_1 and E_2 being the lower and upper boundary energies for group g'.

For Law 7, the secondary-energy distribution is given by

$$g(E,E') = \frac{\sqrt{E'}}{I} \exp\left(-\frac{E'}{\theta(E)}\right) \; , \tag{92}$$

where the effective temperature $\theta(E)$ is tabulated in File 5 and the normalization factor is given by

$$I = \theta^{3/2}[\sqrt{\frac{\pi}{4}}\,\mathrm{erf}(x) - x e^{-x}] \; , \tag{93}$$

where

$$x = \frac{E-U}{\theta} \; . \tag{94}$$

Here U is a constant used to define the upper limit of secondary neutron energy $\theta \le E' \le E{-}U$. The desired group integral is given by

$$\int_{g'} g(E,E')\, dE' \quad = \quad \int_{E_1}^{E_2} g(E,E')\, dE'$$

$$= \frac{X_1 - X_2 - Y_1 + Y_2}{\sqrt{\pi/4} - Y - X} \ , \tag{95}$$

where

$$X = \sqrt{x}\, e^{-x} \ , \tag{96}$$

$$Y = \sqrt{\frac{\pi}{4}}\, \mathrm{rerfc}(\sqrt{x}) \ , \tag{97}$$

and where X_1, Y_1, X_2, and Y_2 refer to X and Y evaluated at E_1/θ and E_2/θ. The integral of Eq. (95) is computed in `ANASED` ("`ANA`" for analytic). The function "rerfc" is the reduced complementary error function[11].

For Law 9, the secondary-energy distribution is given by

$$g(E, E') = \frac{E'}{I} \exp\left(-\frac{E'}{\theta(E)}\right) \ , \tag{98}$$

where

$$I = \theta^2[1 - e^{-x}(1 + x)] \ . \tag{99}$$

Here x has the same meaning as above—see Eq. (94). The group integral is

$$\int_{g'} g(E, E')\, dE' = \frac{(1 + x_1)e^{-x_1} - (1 + x_2)e^{-x_2}}{1 - (1 + x)e^{-x}} \ , \tag{100}$$

where x_1 and x_2 refer to E_1/θ and E_2/θ, respectively. This result is also computed in `ANASED`.

For Law 11, the secondary-energy distribution is given by

$$g(E, E') = \frac{e^{-E'/a}}{I} \sinh(\sqrt{bE'}) \ , \tag{101}$$

where

$$I = \frac{1}{2}\sqrt{\frac{\pi a^3 b}{4}}\, e^{x_0}[\mathrm{erf}(\sqrt{x} - \sqrt{x_0}) + \mathrm{erf}(\sqrt{x} + \sqrt{x_0})] - a e^{-x \sinh(abx)} \ . \tag{102}$$

In this case, $a(E)$ and $b(E)$ are given in File 5,

$$x = \frac{E - U}{a} \ , \tag{103}$$

and

$$x_0 = \frac{ab}{4} \ . \tag{104}$$

The group integrals are given by

$$\int_{g'} g(E,E') = \frac{H(x_1,x_2,x_0)}{H(0,x,x_0)} \ , \tag{105}$$

where

$$\begin{aligned} H(x_1,x_2,x_0) &= H_2(\sqrt{x_1}-\sqrt{x_0},\sqrt{x_2}-\sqrt{x_0}) \\ &+ \sqrt{x_0}H_1(\sqrt{x_1}-\sqrt{x_0},\sqrt{x_2}-\sqrt{x_0}) \\ &- H_2(\sqrt{x_1}+\sqrt{x_0},\sqrt{x_2}+\sqrt{x_0}) \\ &+ \sqrt{x_0}H_1(\sqrt{x_1}+\sqrt{x_0},\sqrt{x_2}+\sqrt{x_0}) \ , \end{aligned} \tag{106}$$

and where

$$H_n(a,b) = \frac{1}{\pi}\int_a^b z^n e^{-z^2}\, dz \ . \tag{107}$$

The methods for computing H_n are described in BROADR, Chapter IV of this manual. When $\sqrt{x_2} < .01$, a short-cut calculation can be used for the numerator of Eq. (105)

$$\frac{4\sqrt{x_0}e^{-x_0}}{3\sqrt{\pi/4}}[x_2^{3/2}-x_1^{3/2}] \ . \tag{108}$$

For Law 12, the Madland-Nix option, the secondary-energy distribution is given by

$$g(E,E') = \frac{1}{2}[G(E',E_{fl})+G(E',E_{fh})] \ , \tag{109}$$

where

$$\begin{aligned} &G(E',E_f) \\ &\quad = \frac{1}{3\sqrt{E_f T_m}}\left[u_2^{3/2}E_1(u_2) - u_1^{3/2}E_1(u_1) + \gamma(3/2,u_2) - \gamma(3/2,u_1)\right] \ , \end{aligned} \tag{110}$$

$$u_1 = (\sqrt{E'}-\sqrt{E_f})^2/T_m \ , \text{ and} \tag{111}$$

$$u_2 = (\sqrt{E'}+\sqrt{E_f})^2/T_m \ , \tag{112}$$

and where E_{fl}, E_{fh}, and $T_m(E)$ are given in File 5. The special functions used are the first-order exponential integral, $E_1(x)$, and the incomplete gamma function, $\gamma(n,x)$. The group integrals of this function are very complex[12]. Let

$$\alpha = \sqrt{T_m} \ , \tag{113}$$

$$\beta = \sqrt{E_f} \ , \tag{114}$$

$$A = \frac{(\sqrt{E_1}+\beta)^2}{\alpha^2}\ , \tag{115}$$

$$B = \frac{(\sqrt{E_2}+\beta)^2}{\alpha^2}\ , \tag{116}$$

$$A' = \frac{(\sqrt{E_1}-\beta)^2}{\alpha^2}\ , \text{ and} \tag{117}$$

$$B' = \frac{(\sqrt{E_2}-\beta)^2}{\alpha^2}\ . \tag{118}$$

Then the integral over the range (E_1, E_2) of G is given by one of the following three expression, depending on the region of integration in which E_1 and E_2 lie.

Region I ($E_1 \geq E_f, E_2 > E_f$)

$$\begin{aligned}
&3\sqrt{E_f T_m}\int_{E_1}^{E_2} G(E', E_f)\, dE' \\
&= [\,(\frac{2}{5}\alpha^2 B^{5/2} - \frac{1}{2}\alpha\beta B^2)E_1(B) - (\frac{2}{5}\alpha^2 A^{5/2} - \frac{1}{2}\alpha\beta A^2)E_1(A)\,] \\
&- [\,(\frac{2}{5}\alpha^2 B'^{5/2} + \frac{1}{2}\alpha\beta B'^2)E_1(B') - (\frac{2}{5}\alpha^2 A'^{5/2} + \frac{1}{2}\alpha\beta A'^2)E_1(A')\,] \\
&+ [\,(\alpha^2 B - 2\alpha\beta B^{1/2})\,\gamma(3/2, B) - (\alpha^2 A - 2\alpha\beta A^{1/2})\,\gamma(3/2, A)\,] \\
&- [\,(\alpha^2 B' + 2\alpha\beta B'^{1/2}\,\gamma(3/2, B') - (\alpha^2 A' + 2\alpha\beta A'^{1/2})\,\gamma(3/2, A')\,] \\
&- \frac{3}{5}\alpha^2[\,\gamma(5/2, B) - \gamma(5/2, A) - \gamma(5/2, B') + \gamma(5/2, A')\,] \\
&- \frac{3}{2}\alpha\beta\,[\,\mathrm{e}^{-B}(1+B) - \mathrm{e}^{-A}(1+A) + \mathrm{e}^{-B'}(1+B') - \mathrm{e}^{-A'}(1+A')\,]\ .
\end{aligned} \tag{119}$$

Region II ($E_1 < E_f, E_2 \leq E_f$)

$$\begin{aligned}
&3\sqrt{(E_f T_m)}\int_{E_1}^{E_2} G(E', E_f)\, dE' \\
&= [\,(\frac{2}{5}\alpha^2 B^{5/2} - \frac{1}{2}\alpha\beta B^2)E_1(B) - (\frac{2}{5}\alpha^2 A^{5/2} - \frac{1}{2}\alpha\beta A^2)E_1(A)\,] \\
&- [\,(\frac{2}{5}\alpha^2 B'^2)E_1(B') - (\frac{2}{5}\alpha^2 A'^{5/2} - \frac{1}{2}\alpha\beta A'^2)E_1(A')\,] \\
&+ [\,(\alpha^2 B - 2\alpha\beta B^{1/2})\,\gamma(3/2, B) - (\alpha^2 A - 2\alpha\beta A^{1/2})\,\gamma(3/2, A)\,] \\
&- [(\alpha^2 B' - 2\alpha\beta B'^{1/2}\,\gamma(3,2, B') - (\alpha^2 A' - 2\alpha\beta A'^{1/2})\,\gamma(3/2, A')\,] \\
&- \frac{3}{5}\alpha\beta[\,\gamma(5/2, B) - \gamma(5/2, A) - \gamma(5/2, B') + \gamma(5/2, A')\,] \\
&- \frac{3}{2}\alpha\beta\,[\,\mathrm{e}^{-B}(1+B) - \mathrm{e}^{-A}(1+A) - \mathrm{e}^{-B'}(1+B') + \mathrm{e}^{-A'}(1+A')\,]\ .
\end{aligned} \tag{120}$$

Region III ($E_1 < E_f, E_2 > E_f$)

$$
\begin{aligned}
&3\sqrt{E_f T_m}\int_{E_1}^{E_2} G(E',E_f)\,dE' \\
&= [\,(\frac{2}{5}\alpha^2 B^{5/2} - \frac{1}{2}\alpha\beta B^2)E_1(B) - (\frac{2}{5}\alpha^2 A^{5/2} - \frac{1}{2}\alpha\beta A^2)E_1(A)\,] \\
&- [\,(\frac{2}{5}\alpha^2 B'^{5/2} + \frac{1}{2}\alpha\beta B'^2)E_1(B') - (\frac{2}{5}\alpha^2 A'^{5/2} - \frac{1}{2}\alpha\beta A'^2)E_1(A')\,] \\
&+ [\,(\alpha^2 B - 2\alpha\beta B^{1/2})\,\gamma(3/2,B) - (\alpha^2 A - 2\alpha\beta A^{1/2})\,\gamma(3,2,A)\,] \\
&- [\,(\alpha^2 B' + 2\alpha\beta B'^{1/2})\,\gamma(3/2,B') - (\alpha^2 A' - 2\alpha\beta A'^{1/2})\,\gamma(3/2,A'_)\,] \\
&- \frac{3}{5}\alpha^2[\,\gamma(5/2,B) - \gamma(5/2,A) - \gamma(5/2,B') + \gamma(5/2,A')\,] \\
&- \frac{3}{2}\alpha\beta\,[\,\mathrm{e}^{-B}(1+B) - \mathrm{e}^{-A}(1+A) + \mathrm{e}^{-B'}(1+B') + \mathrm{e}^{-A'}(1+A') - 2\,]\;.
\end{aligned}
\tag{121}
$$

O. File 6 Energy-Angle Distributions

If the File 6 data are expressed as a continuous energy-angle distribution (Law 1) in the laboratory system, it is fairly easy to generate the multigroup transfer matrix. As usual for GROUPR, the task is to calculate the "feed function" (the Legendre moments for transferring to all possible secondary-energy groups starting with incident energy E). The E' integration is controlled by the GETMF6 subroutine, which calls `F6LAB` to generate the integrands. This routine expects data in Law-1 format, where the looping order is E, E', ℓ. The only problems here are handling the new ENDF-6 interpolation laws for two-dimensional tabulations (for example, unit base) and converting tabulated angle functions for $E \to E'$ into Legendre coefficients (which is done with a Gauss-Legendre quadrature of order 8).

If the File 6 data are given in the energy-angle form of Law 7 (where the looping order is E, μ, E'), GROUPR converts it to the Law 1 form using subroutine `LL2LAB`. It does this by stepping through an E' grid that is the union of the E' grids for all the different angles given. At each of these union E' values, it calculates the Legendre coefficients using a Gauss-Legendre quadrature of order 8, and checks back to see if the preceding point is still needed to represent the distribution to the desired degree of accuracy. Now `GETMF6` and `F6LAB` can be used to complete the calculation as above.

If the File 6 data are expressed in the CM system, or if the phase-space option is used, more processing is necessary to convert to the LAB system. This conversion is done for each incident energy E given in the file. The grid for laboratory secondary energy E'_L is obtained by doing an adaptive reconstruction of the emission probability $p_{L\ell}(E,E'_L)$ such that each Legendre order can be expressed as a linear-linear function of E'_L. This part is done in subroutine `CM2LAB`. The values for $p_{L\ell}(E,E'_L)$ are obtained in subroutine `F6CM` by doing an adaptive integration along the contour E'_L=const in the E'_C,μ_C plane using μ_L as the variable of integration:

$$p_{L\ell}(E,E'_L) = \int_{\mu_{\min}}^{+1} p_C(E,E'_C,\mu_C)\,P_\ell(\mu_L)\,J\,d\mu_L\ , \tag{122}$$

where μ is a scattering cosine and L and C denote the laboratory and center-of-mass (CM) systems, respectively. The Jacobian of the transformation is given by

$$J = \sqrt{\frac{E'_L}{E'_C}} = \frac{1}{\sqrt{1+c^2-2c\mu_L}}\ , \tag{123}$$

and the cosine transformation is given by

$$\mu_C = J(\mu_L - c)\ . \tag{124}$$

The constant c is given by

$$c = \sqrt{\frac{A'}{(A+1)^2}}\sqrt{\frac{E}{E'_L}}\ , \tag{125}$$

where A is the ratio of the atomic weight of the target to the atomic weight of the projectile, and A' is the ratio of the atomic weight of the emitted particle to the atomic weight of the projectile. The lower limit of the integral depends on the maximum possible value for the center-of-mass (CM) secondary energy as follows:

$$\mu_{\min} = \frac{1}{2c}\Big(1+c^2-\frac{E'_{C\max}}{E'_L}\Big), \tag{126}$$

where

$$E'_{L\max} = E\Big(\sqrt{\frac{E'_{C\max}}{E}}+\sqrt{\frac{A'}{(A+1)^2}}\Big)^2. \tag{127}$$

An example of the integration contours for this coordinate transformation is given in Fig. 7.

The CM energy-angle distribution can be given as a set of Legendre coefficients or a tabulated angular distribution for each possible energy transfer $E\to E'$, as a "precompound fraction" $r(E,E')$ for use with the Kalbach-Mann[13] or Kalbach[14] angular distributions, or as parameters for a phase-space distribution. The first

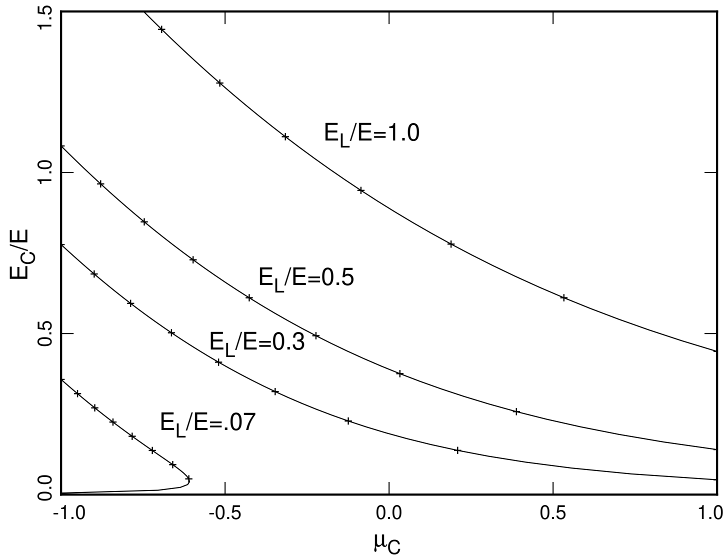

Figure 7: Coordinate mapping between CM and laboratory reference frames for A=2. The parameters E_L and E_C are the secondary energies in the lab and CM frames. The crosses on the curves are at μ_L values of -1.0, -.75, -.50, ..., .75, and 1.0. This figure also illustrates the advantage of integrating over μ_L for the contour in the lower-left corner. The values of E_C and μ_C are single-values functions of μ_L.

three options are processed using `F6DDX`, and the last using `F6PSP`. The Kalbach option leads to a very compact representation. Kalbach and Mann examined a large number of experimental angular distributions for neutrons and charged particles. They noticed that each distribution could be divided into two parts: an equilibrium part symmetric in μ, and a forward-peaked preequilibrium part. The relative amount of the two parts depended on a parameter r, the preequilibrium fraction, that varies from zero for low E' to 1.0 for large E'. The shapes of the two parts of the distributions depended most directly on E'. This representation is very useful for preequilibrium statistical-model codes like GNASH,[15] because they can compute the parameter r, and all the rest of the angular information comes from simple universal functions. More specifically, Kalbach's latest work says that

$$f(\mu) = \frac{a}{2\sinh(a)}\Big[\cosh(a\mu) + r\sinh(a\mu)\Big], \tag{128}$$

where a is a simple function of E, E', and B_b, the separation energy of the emitted particle from the liquid-drop model without pairing and shell terms. The separation energies are computed by function SEPE. This function has a problem for elemental evaluations, because it needs an A value for the calculation, and it is difficult to guess which A value is most characteristic of the element. A short table is included in the function, and an "`ERROR IN SEPE`" will result if the function is called with an element that doesn't appear in the table. Similar routines appear in HEATR and ACER (`SEPH` and `SEP`, respectively). A better long-range solution would be desirable.

The File 6 processing methods in GROUPR apply equally well to neutrons and charged particles. The effects on the kinematics due to the difference in mass between the incident particle and the emitted particle are handled by the variable A' in the above equations.

P. GENDF Output

The group constants produced by GROUPR are normally written to an output file in GENDF (groupwise ENDF) format for use by other modules of NJOY. For example, DTFR can be used to convert a GENDF material to DTF (or "transport") format; CCCCR produces the standard interface files[16] ISOTXS, BRKOXS, and DLAYXS; MATXSR produces a file in MATXS format;[6] and POWR produces libraries of the Electric Power Research Institute (EPRI) codes EPRI-CELL and EPRI-CPM. Other formats can easily be produced by new modules, and some functions such as group collapse, are conveniently performed directly in GENDF format. The GENDF format is also used for GAMINR output, and both ACER and ERRORR use GENDF input for some purposes.

Depending on the sign of `NGOUT2` (see below), the GENDF file will be written in either formatted mode (i.e, BCD, ASCII, EBCDIC, etc.) or in the special NJOY blocked-binary mode. Conversion between these modes can be performed subsequently by the MODER module.

The GENDF material begins with a header record (MF=1, MT=451), but the format of this first section is different from MT=451 on an ENDF or PENDF tape. The section consists of a "CONT" record, containing

`ZA`	Standard 1000*Z+A value
`AWR`	Atomic weight ratio to neutron
`0`	Zero
`NZ`	Number of σ_0 values
`-1`	Identifies a GENDF-type data file
`NTW`	Number of words in title

and a single "LIST" record, containing

`TEMPIN`	Material temperature (Kelvin)
`0.`	Zero
`NGN`	Number of neutron groups
`NGG`	Number of photon groups
`NW`	Number of words in LIST
`0`	Zero
`TITLE`	Title from GROUPR input (`NTW` words)
`SIGZ`	Sigma-zero values (`NZ` words)
`EGN`	Neutron group boundaries, low to high (`NGN+1` words)
`EGG`	Photon group boundaries, low to high (`NGG+1` words).

For photoatomic GENDF files produced by the GAMINR module, the photon group structure is stored in `NGN` and `EGN`, and the number of photon groups is given as `NGG=0`. The word count is seen to be NW=NTW+NZ+NGN+1+NGG+1. The LIST record is followed by a standard ENDF file-end record (FEND). The normal ENDF section-end (SEND) is omitted.

This header is followed by a series of records for reactions. The ENDF ordering requirements are relaxed, and MF and MT values can occur in any order. Each section starts with a "CONT" record.

`ZA`	Standard 1000*Z+A value
`AWR`	Standard atomic weight ratio
`NL`	Number of Legendre components
`NZ`	Number of sigma-zero values
`LRFLAG`	Break-up identifier flag
`NGN`	Number of groups

It is followed by a series of LIST records, one for every incident-energy group with nonzero result,

TEMP	Material temperature (Kelvin)
0.	Zero
NG2	Number of secondary positions
IG2LO	Index to lowest nonzero group
NW	Number of words in LIST
IG	Group index for this record
A(NW)	Data for LIST (NW words),

where `NW=NL*NZ*NG2`. The last LIST record in the sequence is the one with `IG=NGN`. It must be given even if its contents are zero. The last LIST record is followed by a SEND record.

The contents of `A(NW)` change for various types of data. For simple cross section "vectors" (MF=3), NG2 is 2, and A contains the two FORTRAN arrays

```
FLUX(NL,NZ), SIGMA(NL,NZ)
```

in that order. For ratio quantities like fission $\overline{\nu}$, `NG2` is 3, and `A` contains

```
FLUX(NL,NZ), RATIO(NL,NZ), SIGMA(NL,NZ).
```

For transfer matrices (MF=6, 16, 21, etc.), `A` contains

```
FLUX(NL,NZ), MATRIX(NL,NZ,NG2-1).
```

The actual secondary group indices for the last index of `MATRIX` are usually `IG2LO`, `IG2LO+1`, etc., using the GROUPR convention of labeling groups in order of increasing energy. If the low-energy part of the fission matrix (or the fission or capture photon production matrices) uses the special format described in Section F, the spectrum will be found in a LIST record with `IG=0` and the production cross section will be found in a series of records with `IG2LO=0`. The group range for the spectrum ranges from `IG2LO` to `IG2LO+NG2-1`. For `IG2LO=0`, `NG2` will be 2 as for a normal cross section, and the two values will be the flux for group `IG` and the corresponding production cross section.

Finally, for delayed neutron spectra (MF=5), `NL` is used to index the 6 time groups, `NZ` is 1, and there is only one incident energy record (`IG=IGN`). The array `A` contains

```
LAMBDA(NL), CHID(NL,NG2-1),
```

where `LAMBDA` contains the 6 delayed-neutron time constants and `CHID` contains the six spectra.

The GENDF material ends with a material-end (MEND) record, and the GENDF tape ends with a tape-end (TEND) record.

Q. Running GROUPR

The input instructions follow. They are reproduced from the comment cards at the beginning of the 91.0 version of the GROUPR module. Because the code changes from time to time, it is a good idea to check these comment cards in the current version to obtain up-to-date input instructions.

```
*---INPUT SPECIFICATIONS (FREE FORMAT)---------------------------*
*                                                                *
* CARD1                                                          *
*    NENDF   UNIT FOR ENDF/B TAPE                                *
*    NPEND   UNIT FOR PENDF TAPE                                 *
*    NGOUT1  UNIT FOR INPUT GOUT TAPE (DEFAULT=0)                *
*    NGOUT2  UNIT FOR OUTPUT GOUT TAPE (DEFAULT=0)               *
* CARD2                                                          *
*    MATB    MATERIAL TO BE PROCESSED                            *
*            MATB LT 0 IS A FLAG TO ADD MTS TO AND/OR REPLACE    *
*            INDIVIDUAL MTS ON NGOUT1.                           *
*    IGN     NEUTRON GROUP STRUCTURE OPTION                      *
*    IGG     GAMMA GROUP STRUCTURE OPTION                        *
*    IWT     WEIGHT FUNCTION OPTION                              *
*    LORD    LEGENDRE ORDER                                      *
*    NTEMP   NUMBER OF TEMPERATURES                              *
*    NSIGZ   NUMBER OF SIGMA ZEROES                              *
*    IPRINT  LONG PRINT OPTION (0/1=MINIMUM/MAXIMUM)             *
*            (DEFAULT=1)                                         *
* CARD3                                                          *
*    TITLE   RUN LABEL (UP TO 80 CHARACTERS DELIMITED BY *,      *
*            ENDED WITH /)  (DEFAULT=BLANK)                      *
* CARD4                                                          *
*    TEMP    TEMPERATURES IN KELVIN                              *
* CARD5                                                          *
*    SIGZ    SIGMA ZERO VALUES (INCLUDING INFINITY)              *
*                                                                *
*          IF IGN=1, READ NEUTRON GROUP STRUCTURE (6A AND 6B)    *
* CARD6A                                                         *
*    NGN     NUMBER OF GROUPS                                    *
* CARD6B                                                         *
*    EGN     NGN+1 GROUP BREAKS (EV)                             *
*                                                                *
*          IF IGG=1, READ GAMMA GROUP STRUCTURE (7A AND 7B)      *
* CARD7A                                                         *
*    NGG     NUMBER OF GROUPS                                    *
* CARD7B                                                         *
*    EGG     NGG+1 GROUP BREAKS (EV)                             *
*                                                                *
*          WEIGHT FUNCTION OPTIONS (8A,8B,8C,8D)                 *
* CARD8A     FLUX CALCULATOR PARAMETERS (IWT.LT.0 ONLY)          *
*    EHI     BREAK BETWEEN COMPUTED FLUX AND BONDARENKO FLUX     *
*                (MUST BE IN RESOLVED RANGE)                     *
*    SIGPOT  ESTIMATE OF POTENTIAL SCATTERING CROSS SECTION      *
*    NFLMAX  MAXIMUM NUMBER OF COMPUTED FLUX POINTS              *
```

```
*    NINWT   TAPE UNIT FOR NEW FLUX PARAMETERS (DEFAULT=0)       *
*    JSIGZ   INDEX OF REFERENCE SIGMA ZERO IN SIGZ ARRAY         *
*            (DEFAULT=0)                                         *
*    ALPHA2   ALPHA FOR ADMIXED MODERATOR (DEF=0=NONE)           *
*    SAM      ADMIXED MODERATOR XSEC IN BARNS PER ABSORBER       *
*             ATOM (DEF=0=NONE)                                  *
*    BETA     HETEROGENEITY PARAMETER (DEF=0=NONE)               *
*    ALPHA3   ALPHA FOR EXTERNAL MODERATOR (DEF=0=NONE)          *
*    GAMMA    FRACTION OF ADMIXED MODERATOR CROSS SECTION IN     *
*              EXTERNAL MODERATOR CROSS SECTION (DEF=0)          *
* CARD8B     TABULATED (IWT=1 OR -1 ONLY)                        *
*    WGHT    READ WEIGHT FUNCTION AS TAB1 RECORD.                *
*            END WITH A /.                                       *
* CARD8C     ANALYTIC FLUX PARAMETERS (IWT=4 OR -4 ONLY)         *
*    EB      THERMAL BREAK (EV)                                  *
*    TB      THERMAL TEMPERATURE (EV)                            *
*    EC      FISSION BREAK (EV)                                  *
*    TC      FISSION TEMPERATURE (EV)                            *
* CARD8D     INPUT RESONANCE FLUX (IWT=0 ONLY)                   *
*    NINWT   TAPE UNIT FOR FLUX PARAMETERS                       *
*                                                                *
* CARD9                                                          *
*    MFD     FILE TO BE PROCESSED                                *
*    MTD     SECTION TO BE PROCESSED                             *
*    MTNAME  DESCRIPTION OF SECTION TO BE PROCESSED              *
*          REPEAT FOR ALL REACTIONS DESIRED                      *
*          MFD=0/ TERMINATES THIS TEMPERATURE/MATERIAL.          *
* CARD10                                                         *
*    MATD    NEXT MAT NUMBER TO BE PROCESSED                     *
*            MATD=0/ TERMINATES GROUPR RUN.                      *
*                                                                *
*---OPTIONS FOR INPUT VARIABLES----------------------------------*
*                                                                *
*     IGN          MEANING                                       *
*     ---          -------                                       *
*      1           ARBITRARY STRUCTURE (READ IN)                 *
*      2           CSEWG 239-GROUP STRUCTURE                     *
*      3           LANL 30-GROUP STRUCTURE                       *
*      4           ANL 27-GROUP STRUCTURE                        *
*      5           RRD 50-GROUP STRUCTURE                        *
*      6           GAM-I 68-GROUP STRUCTURE                      *
*      7           GAM-II 100-GROUP STRUCTURE                    *
*      8           LASER-THERMOS 35-GROUP STRUCTURE              *
*      9           EPRI-CPM 69-GROUP STRUCTURE                   *
*     10           LANL 187-GROUP STRUCTURE                      *
*     11           LANL 70-GROUP STRUCTURE                       *
*     12           SAND-II 620-GROUP STRUCTURE                   *
*     13           LANL 80-GROUP STRUCTURE                       *
*     14           EURLIB 100-GROUP STRUCTURE                    *
*     15           SAND-IIA 640-GROUP STRUCTURE                  *
*     16           VITAMIN-E 174-GROUP STRUCTURE                 *
*     17           VITAMIN-J 175-GROUP STRUCTURE                 *
*                                                                *
```

```
*     IGG          MEANING                                    *
*     ---          -------                                    *
*      0           NONE                                       *
*      1           ARBITRARY STRUCTURE (READ IN)              *
*      2           CSEWG 94-GROUP STRUCTURE                   *
*      3           LANL 12-GROUP STRUCTURE                    *
*      4           STEINER 21-GROUP GAMMA-RAY STRUCTURE       *
*      5           STRAKER 22-GROUP STRUCTURE                 *
*      6           LANL 48-GROUP STRUCTURE                    *
*      7           LANL 24-GROUP STRUCTURE                    *
*      8           VITAMIN-C 36-GROUP STRUCTURE               *
*      9           VITAMIN-E 38-GROUP STRUCTURE               *
*                                                             *
*     IWT          MEANING                                    *
*     ---          -------                                    *
*      1           READ IN SMOOTH WEIGHT FUNCTION             *
*      2           CONSTANT                                   *
*      3           1/E                                        *
*      4           1/E + FISSION SPECTRUM + THERMAL MAXWELLIAN  *
*      5           EPRI-CELL LWR                              *
*      6           (THERMAL) -- (1/E) -- (FISSION + FUSION)   *
*      7           FAST REACTOR                               *
*      8           THERMAL--1/E--FAST REACTOR--FISSION + FUSION  *
*      9           CLAW WEIGHT FUNCTION                       *
*     10           CLAW WITH T-DEPENDENT THERMAL PART         *
*     11           VITAMIN-E WEIGHT FUNCTION (ORNL-5505)      *
*     -N           COMPUTE FLUX WITH WEIGHT N                 *
*      0           READ IN RESONANCE FLUX FROM NINWT          *
*                                                             *
*     MFD          MEANING                                    *
*     ---          -------                                    *
*      3           CROSS SECTION OR YIELD VECTOR              *
*      5           FISSION CHI BY SHORT-CUT METHOD            *
*      6           NEUTRON-NEUTRON MATRIX (MF4/5)             *
*      8           NEUTRON-NEUTRON MATRIX (MF6)               *
*     12           PHOTON PROD. XSEC (PHOTON YIELDS GIVEN, MF12) *
*     13           PHOTON PROD. XSEC (PHOTON XSECS GIVEN, MF13)  *
*     16           NEUTRON-GAMMA MATRIX (PHOTON YIELDS GIVEN)  *
*     17           NEUTRON-GAMMA MATRIX (PHOTON XSECS GIVEN)   *
*     18           NEUTRON-GAMMA MATRIX (MF6)                 *
*         NOTE: IF NECESSARY, MFD=13 WILL AUTOMATICALLY CHANGE  *
*         TO 12 AND MFD=16 WILL AUTOMATICALLY CHANGE TO 17 OR 18.*
*     21           PROTON PRODUCTION MATRIX (MF6)             *
*     22           DEUTERON PRODUCTION (MF6)                  *
*     23           TRITON PRODUCTION (MF6)                    *
*     24           HE-3 PRODUCTION (MF6)                      *
*     25           ALPHA PRODUCTION (MF6)                     *
*     26           RESIDUAL NUCLEUS (A>4) PRODUCTION (MF6)    *
*     31           PROTON PRODUCTION MATRIX (MF4)             *
*     32           DEUTERON PRODUCTION (MF4)                  *
*     33           TRITON PRODUCTION (MF4)                    *
*     34           HE-3 PRODUCTION (MF4)                      *
*     35           ALPHA PRODUCTION (MF4)                     *
```

```
*     36           RESIDUAL NUCLEUS (A>4) PRODUCTION (MF4)       *
*          NOTE: IF NECESSARY, MFD=21-26 WILL                    *
*          AUTOMATICALLY CHANGE TO 31-36.                        *
*     90+N         RADIOACTIVE NUCLIDE PRODUCTION FROM NTH       *
*                   SUBSECTION FOR MTD IN FILE 9.                *
*    100+N         RADIOACTIVE NUCLIDE PRODUCTION FROM NTH       *
*                   SUBSECTION FOR MTD IN FILE 10.               *
*                                                                *
*     MTD          MEANING                                       *
*     ---          -------                                       *
*     -N           PROCESS ALL MT NUMBERS FROM THE PREVIOUS      *
*                          ENTRY TO N INCLUSIVE                  *
*     221-250      RESERVED FOR THERMAL SCATTERING               *
*     258          AVERAGE LETHARGY                              *
*     259          AVERAGE INVERSE VELOCITY (M/SEC)              *
*                                                                *
*     AUTOMATIC REACTION PROCESSING OPTIONS                      *
*     ------------------------------------                       *
*        3/        DO ALL REACTIONS IN FILE3 ON INPUT PENDF      *
*        6/        DO ALL MATRIX REACTIONS IN ENDF DICTIONARY    *
*       13/        DO ALL PHOTON PRODUCTION CROSS SECTIONS       *
*       16/        DO ALL PHOTON PRODUCTION MATRICES             *
*       21/        DO ALL PROTON PRODUCTION MATRICES             *
*       22/        DO ALL DEUTERON PRODUCTION MATRICES           *
*       23/        DO ALL TRITON PRODUCTION MATRICES             *
*       24/        DO ALL HE-3 PRODUCTION MATRICES               *
*       25/        DO ALL ALPHA PRODUCTION MATRICES              *
*       26/        DO ALL A>4 PRODUCTION MATRICES                *
*                                                                *
******************************************************************
```

In these instructions, CARD1 defines the input and output units for GROUPR. The module requires both ENDF and PENDF input tapes, because the PENDF tapes produced by RECONR, BROADR, etc., do not contain angle (MF=4), energy (MF=5), or photon (MF=12,15) distributions. For materials that do not use resonance parameters to represent part of the cross section, it is possible to use a copy of the ENDF tape in place of the PENDF tape. The normal mode for GROUPR is to use NGOUT1=0; however, sometimes it is convenient to add a new material or reaction to an existing GENDF tape. The old GENDF tape is then mounted on unit NGOUT1, and the revised GENDF tape will be written to NGOUT2.

Card 2 selects the first material to be processed (MATB) and sets up the group structures, weighting option, Legendre order, and self-shielding parameters for all the materials to be processed in this run.

The names of the available group structures are given in the input instructions, and the energy bounds are tabulated in Appendix A of this report. Of course, it is always possible to read in an arbitrary group structure (see CARD6A through

CARD7B). The energies must be given in increasing order (note that this is opposite from the usual convention). Here is an example of the input cards for the conventional 4-group structure used in many thermal reactor codes:

```
4/ CARD6A
1E-5 .625 5530 .821E6 10E6 / CARD6B  .
```

These cards are read by the standard NJOY free-format input routine (FREE). Fields are delimited by space, and "/" terminates the processing of input on a card. Anything after the slash is a comment.

The available weight function options are listed in the input instructions under IWT, and they are plotted in Appendix B of this report. Just as in the case of group structures, an arbitrary weight function can be read in (see CARD8B). This function is presented to GROUPR as an ENDF/B "TAB1" record. This means that a count of $E, C(E)$ pairs and one or more interpolation schemes are given. For the case of a single interpolation scheme, the input cards would be

```
0. 0. 0 0 1 N N INT
E1 C(E1) E2 C(E2) ... / CARD8B,
```

where N is the count of E, C pairs, and INT specifies the interpolation law to be used for values of E between the grid values E_1, E_2,... according to the following "graph paper" schemes:

INT	Meaning
1	histogram
2	linear-linear
3	linear-log
4	log-linear
5	log-log

For example, I=5 specifies that $\ln C$ is a linear function of $\ln E$ in each panel $E_i \leq E < E_j$. Similarly, I=4 specifies that $\ln C$ is a linear function of E in each panel. As many physical lines as are needed can be used for "CARD8B", as long as the terminating slash is included.

One of the weighting options is a generalized "$1/E$+fission+thermal" function where the thermal temperature, fission temperature, and breakpoint energies (all in eV) are given on CARD8C. The weight function for the Los Alamos LIB-IV cross section library[17] used

```
.10 .025 820.3E3 1.4E6 / CARD8C   .
```

A plot of this function will be found in Appendix B.

The GROUPR flux calculator is selected by a negative sign on `IWT`. The additional `CARD8A` is then read. The calculator option used is determined by the number of parameters given and their values. The parameters `EHI` and `NFLMAX` are used to select the energy range for the flux calculation, and they also determine the cost in time and storage. The actual value for `SIGPOT` is not very critical—a number near 10 barns is typical for fissionable materials.

Nonzero values for `NINWT` and `JSIGZ` will cause the computed flux for a given fissionable isotope (such as ^{238}U) to be written out onto a file. This saved flux can be used as input for a subsequent run for a fissile material (such as ^{239}Pu) with `IWT`=0 to get an approximate correction for resonance-resonance interference. See Eq. (39).

Nonzero values for some of the last five parameters on `CARD8A` select the extended flux calculation of Eq. (37). The simplest such calculation is for an isolated pin containing a heavy absorber with an admixed moderator. For $^{238}UO_2$, the card might be

```
400 10.6 5000 0 0 .7768 7.5 / CARD8A   ,
```

where 7.5 barns is twice the oxygen cross section and α is computed from $[(A-1)/(A+1)]^2$ with $A = 15.858$. A more general case would be a PWR-like lattice of $^{238}UO_2$ fuel rods in water:

```
400 10.6 5000 0 0 .7768 7.5 .40 1.7E-7 .086 / CARD8A   ,
```

where .086 is computed using 3.75 barns for O and 40 barns for the two H atoms bound in water; that is,

$$\gamma = \frac{3.75}{2*20+3.75} = .086\,. \tag{129}$$

A third example would compute the flux for a homogeneous mixture of ^{238}U and hydrogen

```
400 10.6 5000 0 0 0 0 1. 1.7E-7 / CARD8A   .
```

As a final example, consider a homogeneous mixture of uranium and water. This requires `BETA=1` and `SAM=0`. Thus,

```
400 10.6 5000 0 0 .7768 0. 1. 1.7E-7 .086 / CARD8A   .
```

The maximum Legendre expansion order used for scattering matrices is set by LORD. The number of tables produced is LORD+1; that is, ℓ = 0, 1, ... LORD. When more than 1 value of σ_0 is requested, both the ℓ=0 and ℓ=1 components of the total cross section are produced.

Card 3 contains a short descriptive title that is printed on the listing and added to the output GENDF tape. Card 4 gives the NTEMP values of temperature for the run. They must be in ascending order, and if unresolved data are included on the PENDF tape, the temperatures in this list must match the first NTEMP values in MF=2, MT=153 from UNRESR (see STOUNR and GETUNR). Card 5 gives the σ_0 values for the run in descending order, starting with infinity (represented by 10^{10} barns).

This completes the description of the global input parameters for GROUPR. The rest of the input cards request reactions to be processed for the various temperatures and materials desired. Because of the many types of data that it can process, GROUPR does not have a completely automatic mode for choosing reactions to be processed. On the basic level, it asks the user to request each separate cross section or group-to-group matrix using the parameters MFD, MTD, and MTNAME. However, simplified input modes are also available. For example, the one "CARD9" containing

```
3/
```

will process the cross section "vectors" for all of the reaction MT numbers found on the PENDF tape.

For completeness, the full input for MATD, MFD, and MTNAME will be described first. Most readers can skip to the description of automated processing below. The value of MFD depends on the output desired (vector, matrix) and the form of the data on the ENDF evaluation. Simple cross section "vectors" σ_{xg} are requested using MFD=3 and the MTD numbers desired from the list of reactions available in the evaluation (check the directory in MF=1, MT=451 of the ENDF and PENDF tapes for the reactions available). A typical example would be

```
3   1 *TOTAL*/
3   2 *ELASTIC*/
3  16 *(N,2N)*/
3  51 *(N,NPRIME)FIRST*/
3 -66 *(N,NPRIME)NEXT*/
3  91 *(N,NPRIME)CONTINUUM*/
3 102 *RADIATIVE CAPTURE*/  .
```

The combinations of "3 51" followed by "3 −66" means process all the reactions from 51 through 66; that is, (n,n'_1), (n,n'_2), ..., (n,n'_{16}). If self-shielding is requested, the following reactions will be processed using NSIGZ values of background cross section: total (MT=1), elastic (MT=2), fission (MT=18 and 19), radiative capture (MT=102), heat production (MT=301), kinematic KERMA (MT=443), and damage energy production (MT=444). The other File 3 reactions will be computed at $\sigma_0=\infty$ only. This list of reactions can be altered by small changes in INIT if desired.

There are several special options for MTD available when processing cross section vectors:

MTD	Option
259	Average inverse neutron velocity for group in s/m.
258	Average lethargy for group.
251	Average elastic scattering cosine $\overline{\mu}$ computed from File 4.
252	Continuous-slowing-down parameter $\overline{\xi}$ (average logarithmic energy decrement for elastic scattering) computed from File 4.
253	Continuous-slowing-down parameter $\overline{\gamma}$ (the average of the square of the logarithmic energy decrement for elastic scattering, divided by twice the average logarithmic energy decrement for elastic scattering) computed from File 4.
452	$\overline{\nu}$: the average total fission yield computed from MF=1 and MF=3.
455	$\overline{\nu}^D$: the average delayed neutron yield computed from MF=1 and MF=3.
456	$\overline{\nu}^P$: the average prompt fission neutron yield computed from MF=1 and MF=3.

There are also some special options for MFD that can be used when processing cross sections:

MFD	Option
12	Photon production cross section computed from File 12 and File 3.
13	Photon production cross section computed from File 13. Recent versions of GROUPR will automatically shift between 12 and 13, if necessary.
91–99	Isomer production cross sections computed from yields in File 9. MFD=91 is for the first state given in the file (usually the ground state), MFD=92 is for the second state given (usually the first isomeric state), etc.
101–109	Isomer production cross sections as above, except for data given as isomer production cross sections in File 10.

An example of the isomer production capability would be the radiative capture reaction of ENDF/B-V ^{109}Ag(n,γ) from Tape 532:

```
91 102 *(N,G) TO G.S.*/
92 102 *(N,G) TO ISOMER*/  .
```

The next class of reactions usually processed is the group-to-group neutron scattering matrices. The complete list of MTD values is most easily found under File 4 in the MF=1, MT=451 "dictionary" section of the evaluation. An example follows:

```
6   2 *ELASTIC MATRIX*/
6  16 *(N,2N) MATRIX*/
6  51 *(N,NPRIME)FIRST MATRIX*/
6 -66 *(N,NPRIME)NEXT MATRIX*/
6  91 *(N,NPRIME)CONTINUUM MATRIX*/  .
```

Using MFD=6 implies that File 4, or File 4 and File 5, will be used to generate the group-to-group matrix. The elastic matrix will be computed for NSIGZ values of background cross section, but the other reactions will be computed for $\sigma_0=\infty$ only. The list of matrices to be self-shielded can be changed by making small changes to INIT if desired.

The case of fission is more complex. For the minor isotopes, only the total fission reaction is used, and the following input is appropriate for the prompt component:

```
3 18 *FISSION XSEC*/
6 18 *PROMPT FISSION MATRIX*/  .
```

For the important isotopes, partial fission reactions are given. They are really not needed for most fission reactor problems, and the input above is adequate. However, for problems where high-energy neutrons are important, the following input should be used:

```
3 18 *TOTAL FISSION*/
3 19 *(N,F)*/
3 20 *(N,NF)*/
3 21 *(N,2NF)*/
3 38 *(N,3NF)*/
6 19 *(N,F)*/
6 20 *(N,NF)*/
6 21 *(N,2NF)*/
6 38 *(N,3NF)*/  .
```

Note that "6 18" is omitted because it will, in general, be different from the sum of the partial matrices (see Section F). Some materials don't have data for (n,3nf); in these cases, omit the two lines with MTD=38 from the input. The fission matrix is not self-shielded. Since resonance-to-resonance fission-spectrum variations are not described in ENDF/B, it is sufficient to self-shield the cross section and then to use the self-shielding factor for the cross section to self-shield the fission neutron production.

Delayed fission data are available for the important actinide isotopes, and the following input to GROUPR is used to process them:

```
3 455 *DELAYED NUBAR*/
5 455 *DELAYED SPECTRA*/  .
```

The line for MFD=5 automatically requests spectra for all six time groups of delayed neutrons. The six time constants are also extracted from the evaluation. As discussed in Section VIII.F, formatting modules such as DTFR and CCCCR must combine the prompt and delayed fission data written onto the GENDF tape in order to obtain steady-state fission parameters for use in transport codes.

Starting with the ENDF-6 format, neutron production data may also be found in File 6, and `MFD=8` is used to tell the code to use MF6 for this `MTD`. When using full input, the user will have to check the File 1 directory and determine what subsections occur in File 6.

Photon production reactions can be found in the ENDF dictionary under MF=12 and 13. To request a neutron-to-photon matrix, add 4 to this number.* For example,

```
17   3 *NONELASTIC PHOTONS*/
16   4 *INELASTIC PHOTONS*/
16  18 *FISSION PHOTONS*/
16 102 *CAPTURE PHOTONS*/  .
```

Yields (MF=12) are normally used with resonance reactions (MT=18 or MT=102), or for low-lying inelastic levels (MT=51, 52, ...). MT=3 is often used by evaluators as a catch-all reaction at high energies where it is difficult to separate the source reactions in total photon emission measurements. In these cases, photon production cross sections from other reactions like MT=102 are normally set equal to zero at high energies. The general rule for photon emission is that the total production is equal to the sum of all the partial production reactions given in the evaluation. Starting with the ENDF-6 format, photon production may also appear in File 6.

*In recent versions of NJOY, GROUPR will automatically shift between 16 and 17 using data read from the ENDF dictionary by the `CONVER` subroutine. Thus, use of `MFD=17` is no longer necessary.

Use `MFD=18` to process these contributions. Since resonance-to-resonance variations in photon spectra are not given in ENDF/B, GROUPR does not normally self-shield the photon production matrices (although this can be done if desired by making a small change in INIT); instead, it is assumed that only the corresponding cross section needs to be shielded. Subsequent codes can use the cross section self-shielding factor with the infinite-dilution photon production matrix to obtain self-shielded photon production numbers.

This version of GROUPR can also generate group-to-group matrices for charged-particle production from neutron reactions and for all kinds of matrices for incident charged particles. The incident particle is determined by the input tape mounted. The identity of the secondary particle is chosen by using one of the following special `MFD` values:

For distributions given in File 6 (energy-angle):

`MFD`	Meaning
21	proton production
22	deuteron production
23	triton production
24	He-3 production
25	alpha production
26	residual nucleus (A>4) production

For distributions given in File 4 (angle only):

`MFD`	Meaning
31	proton production
32	deuteron production
33	triton production
34	He-3 production
35	alpha production
36	residual nucleus (A>4) production

If necessary, `MFD`=21–26 will automatically change to 31–36.

The user will normally process all reactions of interest at the first temperature (for example, 300 K). At higher temperatures, the threshold reactions should be omitted, because their cross sections do not change significantly with temperature except at the most extreme conditions. This means that only the following reactions should be included for the higher temperatures (if present): total (MT=1), elastic (MT=2), fission (MT=18), radiative capture (MT=102), heating (MT=301), kinematic KERMA (MT=443), damage (MT=444), and any thermal cross sections (MT=221–250). Only the elastic and thermal matrices should be included at the higher temperatures.

Warning: when using the explicit-input option, it is a fatal error to request a reaction that does not appear in the evaluation, cannot be computed from the evaluation, or was not added to the PENDF tape by a previous module. Reactions with thresholds above the upper boundary of the highest energy group will be skipped after printing a message on the output file.

Automated processing of essentially all reactions included in an ENDF/B evaluation is also available. As mentioned above, the single card

```
3/
```

will process all the reactions found in File 3 of the input PENDF tape. However, this list excludes thermal data (MT=221–250) and special options such as MTD=251–253, 258–259, and 452–456. If any of these reactions are needed, they should be given explicitly (see example below). Similarly, the single card

```
6/
```

will process the group-to-group matrices for all reactions appearing in File 4 of the ENDF/B tape, except for MT=103–107 and thermal scattering matrices (MT=221–250). If MT=18 and 19 are both present, only MT=19 will be processed into a fission matrix. For ENDF-6 evaluations, the "6/" option will also process every neutron-producing subsection in File 6. Photon production cross sections are requested using

```
13/
```

and photon-production matrices are requested with the single card

```
16/   .
```

In both cases, all reactions in both File 12 and File 13 will be processed without the need for using MFD=12 or MFD=17. For ENDF-6 libraries, this option will also process all photon-production subsections in File 6. There is no automatic option for delayed neutron data. An example of a processing run for a fissionable isotope with thermal cross sections follows:

```
3/
3 221/ THERMAL XSEC
3 229/ AV.INVERSE VELOCITY
3 455/ DELAYED NUBAR
5 455/ DELAYED SPECTRA
6/
6 221/ THERMAL MATRIX
16/ PHOTON PRODUCTION MATRIX   .
```

An example of charged-particle processing for the incident-neutron part of a coupled n-p-γ library follows:

```
3/ CROSS SECTIONS
6/ NEUTRON PRODUCTION MATRIX
16/ PHOTON PRODUCTION MATRIX
21/ PROTON PRODUCTION MATRIX   .
```

The layout of data in a n-p-γ coupled set is shown in Figure 8.

R. Coding Details

GROUPR begins by reading most of the user's input (see `RUINB`). It then locates the desired material and temperature on the input ENDF, PENDF, and GENDF tapes, and reads in the self-shielded unresolved cross sections (if any) from the PENDF tape using `STOUNR`. If self-shielding was requested, `GENFLX` is used to compute the weighting flux as described in Section VIII.D. The next step is to write the header record for this material on the output GENDF tape.

The code is now ready to begin the loop over reactions for this material and temperature. Either an input card is read to get `MFD`, `MTD`, and reaction name, or the next reaction in an automatic sequence is selected. First, the default Legendre order, secondary group count, and σ_0 count are selected for the reaction in `INIT`, and the retrieval routines are initialized. `GROUPR` then processes the reaction using the `PANEL` logic described in Section J. If a "shortcut" fission spectrum was requested (`MFD=5`), for delayed fission, and for the low-energy "constant" spectra, the spectrum is calculated directly using `GETFF`. As the cross sections for each group are obtained, they are printed out (see `DISPLA`) and written to the GENDF tape. When the last group has been processed, `GROUPR` loops back to read a new input card for a new reaction.

This loop over reactions continues until a terminating "0/" card is read. `GROUPR` then proceeds to the next temperature, if any, and repeats the loop over reactions. After the last temperature has been processed for the first material, an opportunity is provided to change to a new material, keeping all the other input parameters unchanged. A "0/" card at this point causes all the files to be closed, prints out the final messages, and terminates the `GROUPR` run.

Automatic choice of the next reaction to be processed is done in one of two ways. For a simple range of MT numbers, such as the example 51–66 used above, the negative value is stored in the variable `MTDP` in the `GROUPR` subroutine. When `MTDP` is negative, `MTD` is incremented after each reaction until it is greater than the absolute value of `MTDP`. `MTDP` is then reset to one, and the code proceeds to the

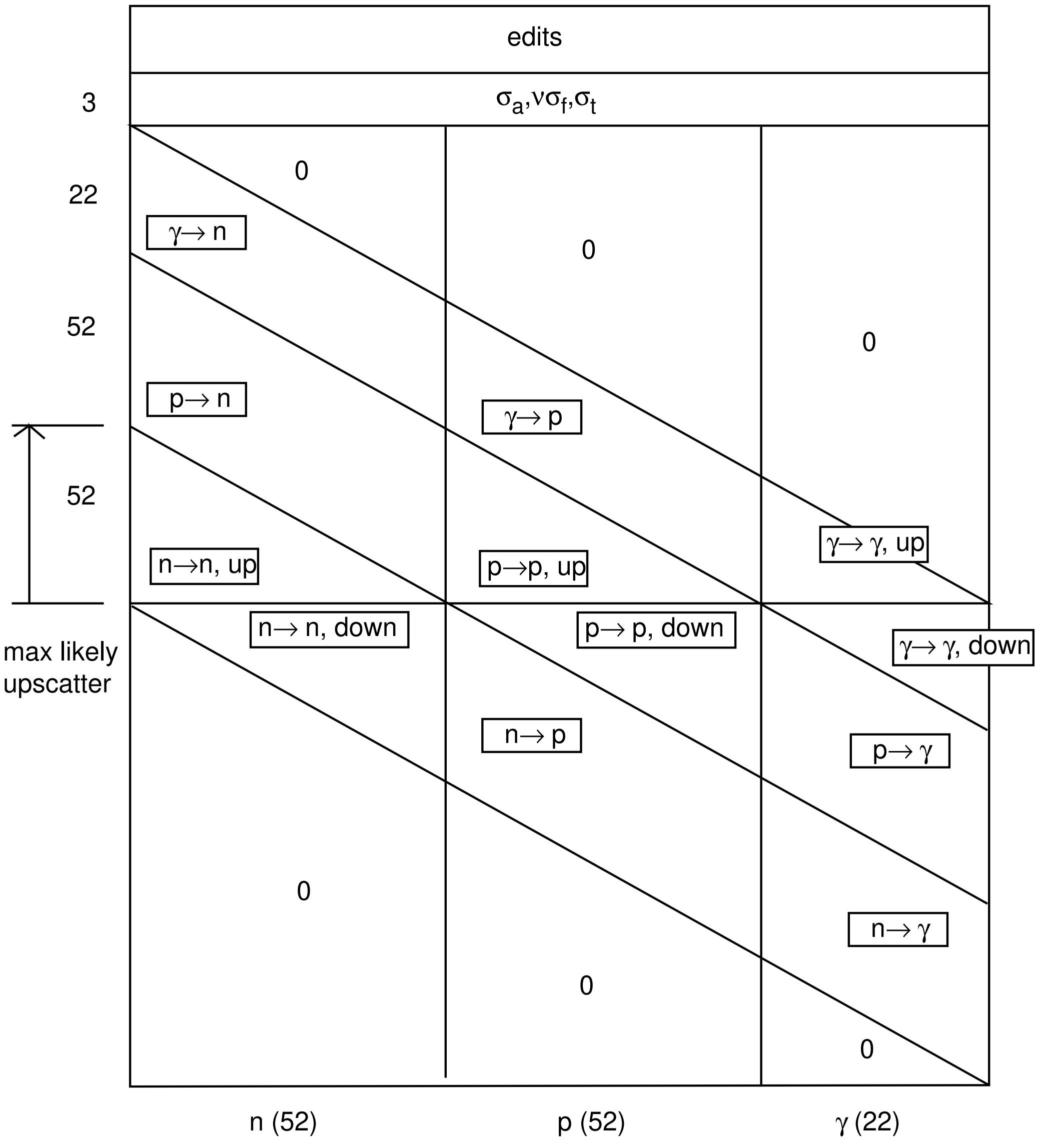

Figure 8: Layout of a coupled table for the simultaneous transport of neutrons, protons, and gamma rays. Normally, only the lower triangle of the "p to n" block would contain values for the upscatter portion of the table (the part above the line in the middle). The "group" index increases from left to right, and the "position" index increases from top to bottom.

next input card. However, MFD=16 will automatically change to 17, if necessary. Similarly, MFD=21, 22, ... will automatically change to MFD=31, 32, ... A more automatic method is triggered by MTD=0. In this case, a subroutine called NEXTR is called to return the next value of MTD to be used, and a subroutine called NAMER is called to generate the reaction name. For MFD=3, NEXTR finds the next reaction in File 3 on the input PENDF tape. MT=251–253 and thermal data (MT=221–250) are excluded. The MT values for the special options (258, 259, etc.) do not appear on the PENDF tape, and they must be requested explicitly if needed. For matrices, GROUPR works with a set of lists loaded into common block /RLIST/ by CONVER. The list MF4 contains all the neutron-scattering MT numbers that appear in the File 4 part of the directory on the ENDF tape, and the list MF6 contains all the MT numbers of sections of File 6 that contain subsections that produce neutrons. Therefore, reading through these two lists returns all the neutron-producing matrix reactions. Similarly, the list MF12 contains all the File 12 entries from the directory, MF13 contains the File 13 entries, and MF18 contains all the MT values for sections in File 6 that contain subsections for photon production. Scanning through these three lists produces all the photon production matrix reactions. Two arrays are used for charged-particle producing reactions; the first index runs through the charged particles in the order p, d, t, ^{3}He, α, recoil. Taking proton production as an example, the list elements MF6P(1,I) contain the MT numbers of sections in File 6 that contain subsections that produce protons. The list elements MF4R(1,I) contain MT numbers from File 4 for two-body reactions that produce protons; namely, MT600–648. NEXTR scans through both of these lists to return indexes to all the reactions that produce protons. The same procedure is used for the other charged particles.

Subroutine NAMER generates name strings with up to 15 Hollerith words with 4 characters each (60 characters). The names depend on the "ZA" of the projectile and the MT number for the reaction. The parameter MFD is used to choose between the suffixes "cross section" and "matrix". Some examples of the names produced follow:

Name	Name	Name
(N,TOTAL)	(N,HEAT)	(P,P02)
(N,ELASTIC)	(N,P02)	(P,N00)
(N,2N)	(P,ELASTIC)	(G,TOTAL)
(N,N01)	(P,2N)	(G,PAIR)

Subroutines MFCHK and MFCHK2 are used with the full input for reaction selection in GROUPR to check whether MFD=17 is needed when MFD=16 was requested, or whether one of the charged-particle File 4 values MFD=31-36 is needed when MFD=21-26 were requested. The lists in common block /RLIST/ are used, just as for NEXTR.

Subroutine GENGPN generates the group bounds in /GROUPN/ for the neutron group structure from input cards, from data statements, or by calculation. Some of the data statements use energies in eV and some use lethargy. GENGPG generates the photon group structure in /GROUPG/ from input cards or data statements; in this case, all bounds are in eV.

Subroutine GENWTF sets up the weight function option requested with IWT by reading the input cards into /WEIGHTS/, transferring numbers from data statements to /WEIGHTS/, or simply reporting the analytic weight option requested. GETWTF returns the values of the weight function at energy E by calculation or by interpolation in the table established by GENWTF. The current version returns the same value for all Legendre orders. Choosing ENEXT is difficult for GETWTF because the functions have not been explicitly linearized. It is important to generate extra grid points in energy regions where the weight function may vary faster than the cross section (for example, in the fusion peak).

Subroutine GENFLX computes the self-shielded weighting flux using either the Bondarenko model or the flux calculator, and it writes the result on a scratch tape using the LOADA routine from the NJOY level. When fluxes are needed for the generalized group integrals, they are read from this scratch file using FINDA (see GETFLX). GENFLX starts by checking for the weighting option. If the Bondarenko model was selected, it initializes GETY1 and GETWTF to read the total cross section from the PENDF tape and the smooth weighting function $C(E)$ set up by GENWTF. It then steps through the union grid of $\sigma_t(E)$ and $C(E)$ computing the flux vs. σ_0 and Legendre order by means of Eq. (14). In the unresolved energy range, GETUNR is used to retrieve the unresolved cross sections as a function of σ_0, and Eq. (22) is used to compute the weighting flux. In both cases, the data at each energy are stored as the 1+(LORD+1)*NSIGZ components

```
E, PHI(IL,IZ) ,
```

where IL runs from 1 to LORD+1 and IZ runs from 1 to NSIGZ.

If the flux calculator option was requested, GENFLX sets up the parameters for the calculation and requests needed storage space. Next, the cross section retrieval routines GETY1 and GETY2 are set up to return total and elastic cross sections from the PENDF tape. A lower energy limit (ELO) is chosen, and the cross sections are read into storage until a maximum energy EHI or a maximum number of points NEMAX is reached.

The slowing-down equation, either Eq. (33) or Eq. (37), is then solved from the break energy down to ELO. The scattering source from energies above the break is based on the NR approximation. When the calculation is finished, fluxes from 10^{-5} eV to ELO are written to the scratch file using LOADA in the same format used for the Bondarenko option. From ELO to the energy break point, fluxes are transferred from memory to the LOADA file. Finally, above the break point, fluxes are computed and saved using the Bondarenko model.

Subroutine INIT is used to set up the number of σ_0 values, secondary energy groups, and Legendre components for each combination of MFD and MTD. If MFD=6, a special copy of File 6 is made for use in GETAED. The list of reactions to be self-shielded can be changed if desired. The number of secondary groups NG helps determine the storage required for the accumulating group integrals (see dynamic storage array ANS with pointer IANS in GROUPR). For simple cross section vectors, NG=2. The NZ*NL flux components are stored first, followed by the NZ*NL cross section components. When all the panels for one group have been processed, dividing position 2 by position 1 gives the group-averaged cross section. For ratio quantities like $\overline{\nu}$ and $\overline{\mu}$ (MTD=251–253, 452, 455, 456), NG is 3. Once again, the flux components are stored first, followed by the NL*NZ components of RATIO*SIGMA, followed by the components of the cross section. This arrangement allows for the calculation of group-averaged values of RATIO*SIGMA, RATIO, or cross section by dividing position 2 by 1, position 2 by 3, or position 3 by 1, respectively. For matrices, NG is set to one more than the number of secondary groups (NGN or NGG). The NL*NZ flux components are stored first, followed by the NL*NZ integrals for each secondary-energy group in turn.

Subroutine PANEL performs the generalized group integrals using the logic described in Section J. For most calls to PANEL, the lower point of each "panel" was computed as the upper point of the previous panel. Therefore, PANEL is careful to save these previous values. However, if the bottom of the panel is just above a discontinuity, new values of cross section and flux are retrieved. Once the values at the lower boundary of the panel are in place, new values for the top of the panel are retrieved (see FLUX, SIG). If the top of the panel is at a discontinuity in σ or at a group boundary, the energy used is just below the nominal top of the panel. "Just below" and "just above" are determined by RNDOFF and DELTA. For maximum accuracy, these numbers should be chosen such that RNDOFF>1, DELTA<1, and RNDOFF*DELTA<1 for the precision of the machine being used.

For simple average cross sections, the integrals of $\sigma\times\phi$ and ϕ are computed for the panel using trapezoids. This is justified by the linearization of σ; the value of $\sigma\times\phi$ at the midpoint is too uncertain to justify a more complex treatment. For two-body scattering, the feed function is far from linear over the panel. In fact, it can show oscillations as described in Section L. The integral of the triple product $\mathcal{F}\times\sigma\times\phi$ is obtained by Lobatto quadrature of order 6 or 10 using the quadrature points and weights given in the data statements (see QP6, QW6, QP10, QW10). The cross section and reaction rate are determined at each quadrature point by interpolation, and the feed function is obtained by GETFF. For many reactions, FF will be nonzero for only a certain range of secondary groups. IG1 is the index to the first nonzero result, and NG1 is the number of nonzero values of FF in the range. PANEL maintains the two corresponding values IGLO and NG to specify the nonzero range of values in array ANS. Finally, the flux and cross section at the top of the panel are transferred to FLST and SLST, and control is returned to the panel loop in GROUPR.

Subroutine DISPLA is used to print cross sections and group-to-group matrices on the output listing (NSYSO). Small values are removed for efficiency. Note that different formats are used in different circumstances. Infinitely dilute data are printed without σ_0 labels. Isotropic matrices are printed with several final groups on each line. Delayed neutron spectra are printed using the Legendre order variable for time groups and with the time constants given on a heading line.

Subroutine GETFLX returns NL by NZ components of the weighting flux. If NSIGZ is 1, the flux is computed using GETWTF, and all Legendre orders are taken to be equal. When self-shielding has been requested, the flux components are obtained by interpolating between adjacent values retrieved with FINDA from the scratch tape written by GENFLX. The grid energies found on the scratch tape are used to get ENEXT. The flux is taken to be continuous, so IDIS is always set to zero.

Subroutine GETYLD returns the yield needed by GETFF for fission (MT=452, 455, or 456 from File 1) or radionuclide production yields from File 9 (MFD=91–99). This routine also retrieves the delayed neutron time constants when MTD=455. Tabulated yields are obtained by interpolation using the utility routine TERPA. Polynomial data are expanded by direct computation in this subroutine.

Subroutine GETSIG returns NL*NZ components of the cross section using point data from the PENDF tape and self-shielded unresolved data, if present, from GETUNR. The routine starts by adjusting MF and MT for the special options (MTD=258–259, MFD=91–99, etc.) and locating the desired section on the PENDF tape. GETSIG is then called for each desired energy value E in increasing order.

For MTD=258 or 259, the appropriate velocity or lethargy is computed from E and returned. In the more general cases, GETY1 is used to retrieve the pointwise cross section from the PENDF tape, and GETUNR is called to replace this value with self-shielded unresolved cross sections if necessary.

The unresolved cross sections are handled using STOUNR and GETUNR. STOUNR locates the desired material and temperature in MF=2, MT=152 of the PENDF tape, and then it copies the data into the dynamic storage array with pointer IUNR. The σ_0 grid on the PENDF tape does not have to agree with the list requested for GROUPR, but a diagnostic message will be printed if they are different. However, the NTEMP values of temperature requested by GROUPR must agree with the first NTEMP temperatures on the PENDF tape, or a fatal error will result. GETUNR checks whether E is in the unresolved energy range and whether MT is one of the resonance reactions. If so, it locates the desired interpolation range in the UNR array in dynamic storage, and interpolates for the self-shielded cross sections. If this is an energy range where resolved and unresolved ranges overlap, the resolved part is added to the background σ_0 before interpolation. The subroutine TERPU is used for interpolating in the unresolved cross section tables. MT=261 is used to select the ℓ=1 component of the total cross section. Note that GETSIG also uses this ℓ=1 value for $\ell=2,3,\ldots$.

Subroutine GETFF returns the feed function FF using different portions of the coding for different options. The first section is used for cross sections and ratio quantities. The same yield YLD is returned for every ℓ-component in FF.

The second section of GETFF is for neutron continuum transfer matrices. The yield is either determined from MT [for example, YLD=2 for MT=16, the (n,2n) reaction], or it is obtained using GETYLD for fission. Next, the angular distribution is obtained using GETFLE [see F in Eq. (89)], and the secondary energy distribution is obtained using GETSED [see g in Eq. (89)]. Finally, the product of the three factors is loaded in FF. Note that the range of groups returned extends from IGLO=1 to the highest nonzero result, for a total of NG groups. Since FF for these reactions is a smooth function of incident energy, NQ is set to zero, and no additional quadrature points will be used in PANEL.

The third section of GETFF is for gamma production matrices. The photon yields are obtained using GETGYL. In general, there are NYL different yields, each one corresponding to a different discrete gamma ray, or to the continuum. The angular distributions for these gamma rays are obtained using GETGFL (most ENDF/B photons are given as isotropic). The energy distribution for the continuum (if any) is obtained by GETSED. Now, the code loops through the photon group structure placing each discrete photon in the appropriate group and adding in the continuum part. During this loop, the range of nonzero values (IGLO, IGHI) is determined. Finally, the nonzero values are packed into FF, and IGLO and NG are returned to describe the distribution. Once again, NQ=0 is used.

The fourth section of GETFF handles two-body scattering, either elastic or discrete-level inelastic, and both neutrons and charged particles. First, subroutine PARTS is called to set up the particle type, A' value, and the scattering law for reactions that use File 4. Then GETDIS is called to finish the processing.

The fifth section handles thermal-neutron scattering. The bulk of the work is done by GETAED, which is discussed below. GETFF takes the output of GETAED and packs it into the final result, FF.

The last two sections of GETFF are used to process energy-angle distributions from ENDF-6 format sections of File 6. The subroutine simply calls GETMF6.

Subroutine PARTS is used to set up particles for reactions that use File 4. Different branches are used for ENDF-6 and earlier ENDF versions because the MT numbers used for charged-particle discrete levels have been changed. For example, proton levels use MT=600–649 in ENDF-6 libraries, but MT=700–719 in earlier libraries. If MFD=3, no action is taken. For other MFD values, the routine determines ZAP, APRIME, and LAW. The result depends on whether File 4 or File 6 data are to be used.

Subroutine GETMF6 is used to compute the feed function for reactions represented in File 6. As is common with NJOY subroutines, it is called with ED=0 to initialize the subroutine. The first step is to locate the desired section of File 6 on the input ENDF tape. It then sets the parameter ZAD (for ZA desired) based on the input value MFD and searches through the section for the desired subsection. If this subsection has LAW=4, it defines a recoil particle; the code backs up to the first subsection in the section, which is assumed to be the subsection describing the emitted particle. The subroutine has now arrived at statement number 140, where it decides whether to branch to special coding for two-body reactions (statement number 500) or phase-space reactions (statement number 150). All the other options have a TAB2 record at this point that defines the incident energy grid. For LAW=1, the data for the first incident energy are read in and converted to the lab frame by CM2LAB. Similarly, for LAW=7, the data are read in and converted to a LAW=1 format by LL2LAB.

For a normal entry, GETMF6 interpolates for the particle yield for the current particle. For all of the laws except 2–5 (discrete two-body laws), it then checks to see whether the energy `ED` is in the current panel (or if this is the first time in the first panel). If not, it moves the high data to the low position and reads in new high data. Of course, it also converts the new high data to the correct form with `CM2LAB` or `LL2LAB`. Once `ED` is in the current panel, the code reaches statement number 300, which sets up the loop over secondary energy by initializing `F6LAB`. This loop uses a grid that consists of the `EPNEXT` values returned by `F6LAB` and the group bounds `EG(I)`. The actual integral over E'_L inside each group uses trapezoidal integration. The last step for laws 1, 6, and 7 is to add in the contributions to the feed function from discrete energies in File 6. For the discrete two-body laws (2–5), the routine goes through statement number 500, which simply calls `GETDIS`. For all laws, the last step is to check the normalization of the feed function. If the error is large, a message is printed out. In any case, the results are adjusted to preserve exact normalization.

Subroutine `CM2LAB` is used to convert a CM distribution starting at `INOW` in `CNOW` into a lab distribution, which will be stored starting at `JNOW`. The purpose of this routine is to generate a good grid for the lab secondary energy E'_L by adaptive reconstruction. The reconstruction stack is first primed with $p_{L\ell}(E,0)$ as computed by `F6CM` and $p_{L\ell}(E,E'_{\rm next})$ (also from `F6CM`), where the value $E'_{\rm next}$ is the value `EPNEXT` returned by the first call to `F6CM`. This panel is then divided in half, and the value returned by `F6CM` is compared with the linear interpolate. If they agree within 1% (see `TOL`), this panel is converged. Otherwise, it is subdivided further. When convergence has been achieved for this panel, a new panel is chosen, and it is subdivided to convergence. When the entire range for E'_L has been processed, the final parameters are loaded into the new File 6 record for $p_{L\ell}(E,E'_L)$ (which starts at `JNOW` in `CNOW`), and the routine returns to `GETMF6`.

Subroutine `F6CM` is used to compute the Legendre coefficients of the double-differential scattering function $p_\ell(E\rightarrow E')$ in the lab system from data given in File 6 in the CM frame. The memory area `CNOW` contains the data for one particular incident energy E, and the routine must be called first with `EP=0` for each new value of E. Thereafter, values of `EP` can be requested in any order. This is required by the adaptive scheme used to generate the lab E' grid in `CM2LAB`. The conversion uses Eqs. (122)–(127). On a normal entry with $E'_L{>}0$, the code computes the lower limit of the integral $\mu_{\rm min}$. It then sets up an adaptive integration over a panel starting at $\mu{=}1$. The value for E'_C is computed using

$$E'_C = (1 + c^2 - 2c\mu_L)E'_L \ , \tag{130}$$

which is based on Eq. (123), and either `F6DDX` or `F6PSP` is called to compute

$p_C(E, E'_C, \mu_C)$ and EPNEXT. The lower limit of the integration panel is then computed by setting E'_C equal to EPNEXT and solving for the CM cosine using

$$\mu_C = \frac{\mu_L - c}{\sqrt{1 + c^2 - 2c\mu_L}} \ . \tag{131}$$

Of course, the larger between this result and $\mu_{\min}$ is used as the lower bound of the panel. Therefore, the adaptive integration operates on a nice continuous function. It continues subdividing the μ_C grid in this panel until convergence is achieved within 0.5% for all Legendre orders (see TOL/.005/). The lower bound of this panel becomes the upper bound of a new panel, and a new lower bound is selected as above. The integration is carried out over successive panels until $\mu_{\min}$ is reached. When the routine reaches statement number 310, the calculation of the continuum part of $p_{L\ell}$ is finished for these values of E and E'_L. It checks for possible contributions from delta functions. Warning: this section of the code is not finished. Next, the routine scans through the computed coefficients and zeros out any small ones that may just be noise. Finally, it chooses a value for EPNEXT and returns.

Function F6DDX is used to compute the double-differential scattering function $f(E \rightarrow E', \omega)$, where secondary energy E' and scattering cosine ω are in the CM system. On entry, CNOW contains the File 6 data for a particular value of E, and F6DDX must be called once with EP=0 for each new value of E. Thereafter, EP values can be requested in any order (this is required by the adaptive scheme used to convert to the lab system in F6CM). For a normal entry with EP>0, the code searches for the panel in the data that contain the requested value of E'. If LANG=1 for this subsection of File 6, the data are already given as Legendre coefficients, and the code simply interpolates for the desired results. If LANG=2, the data use the Kalbach-Mann scheme for representing the energy-angle distribution. This routine includes both the original Kalbach-Mann representation[13] and the newer Kalbach representation.[14] It has been set to use the latter by the statement DATA K86/1/. The code interpolates for the model parameters at E' and computes the desired answer with the model's formulas. The ENDF-6 format also allows CM distributions given as values tabulated versus scattering cosine (see LANG=11–15). This capability is not included in F6DDX; a fatal error message is issued if this option is encountered. Note that there is a "stub" at statement number 200 to take special action at low energies. It is currently disabled by the statement EFIRST=0., but it may be used sometime in the future to account for the fact that the low-energy dependence of the scattering function must vary as $f(E') = c\sqrt{E'}$.

Subroutine `SEPE` computes the neutron separation energy for the target `IZAT` using the liquid-drop model without pairing and shell terms. This quantity is required for the Kalbach-systematics approach to calculating the energy-angle distributions for particle emission with File 6. The formula used describes the reaction $a + B \rightarrow C + d$:

$$
\begin{aligned}
E_{sep} \;=\;& 15.68(A_C - A_B) \\
-\;& 28.07\left(\frac{(N_C - Z_C)^2}{A_C} - \frac{(N_B - Z_B)^2}{A_B}\right) \\
-\;& 18.56(A_C^{2/3} - A_B^{2/3}) \\
+\;& 33.22\left(\frac{(N_C - Z_C)^2}{A_C^{4/3}} - \frac{(N_B - Z_B)^2}{A_B^{4/3}}\right) \\
-\;& 0.717\left(\frac{Z_C^2}{A_C^{1/3}} - \frac{Z_B^2}{A_B^{1/3}}\right) \\
+\;& 1.211\left(\frac{Z_C^2}{A_C} - \frac{Z_B^2}{A_B}\right) \\
-\;& 0.0\;,
\end{aligned}
\tag{132}
$$

where A stands for atomic weight, Z for charge number, and N for neutron number. Note that, even for reactions like (n,2n), C is the residual nucleus resulting from the removal of one particle d; it is not necessarily the real physical residual nucleus for the reaction. If the target `IZAT` is an element, E_{sep} has to be computed for some dominant isotope in the element. Dominant isotopes are assigned in this subroutine for some materials that often appear as elements in ENDF/B evaluations; if the particular target required does not appear, a fatal error message is issued. The user will have to add a line to the subroutine for the material and reassemble the code.

Subroutine `LL2LAB` is used to change an energy-angle distribution in File 6 from Law-7 format to Law-1 format using the laboratory Legendre representation. Law 7 represents the double-differential scattering distribution $f(E \rightarrow E', \mu)$ by giving a series of tables of $f(E \rightarrow E')$ for series of μ values. On entry, the entire Law-7 section is stored in `C` starting at `INOW`. The code loops through a set of E' values chosen to be the union of all the E' grids for all the different μ values. For each point on this union grid, the code interpolates for all the corresponding $f(\mu)$ values, and it uses them to compute `NL` Legendre coefficients $f_\ell(E')$. After completing the calculation for a new value of E', it checks the normalization of the result, and then it checks back to see whether the previous value is still needed to represent the curves $f_\ell(E')$ within a tolerance of 0.5% (see `DATA TOL/.005/`). The results are written in `C` starting at `JNOW`. They have the Law-1 Legendre form, namely, sets of values E', $f_0(E')$, $f_1(E')$, $\ldots$, $f_{\mathrm{NL}-1}(E')$, given for a series of E' values starting with zero.

Subroutine F6LAB is used to return the Legendre coefficients of the double-differential scattering function $f_\ell(E \rightarrow E')$ for particular values of E and E' in the lab system (see E and EP) from a part of File 6 in Law-1 format. Since Law-7 sections have been converted to Law-1 format using LL2LAB, and since CM sections in Law-1 format have been converted to the lab frame using CM2LAB, the only two roles left for this subroutine are interpolation to the desired values of E and E' and preparation of Legendre coefficients for sections that use the File-6 variant with LAW=1 and LANG=11–15 (laboratory distributions tabulated) vs. μ. Only the continuum portion of the distribution is processed here; any delta functions given in File 6 must be handled separately. The routine is initialized by calling it with EP=0. The data for the two incident energy values that bracket E are already present in CLO and CHI. At this point, the routine extracts various parameters from the C array and prepares the variables used to control interpolation. These variables are complicated, because this routine handles three different interpolation schemes: "cartesian", "unit base", and "corresponding point" (see the ENDF-6 manual[4] for more details). For a normal entry, the code searches the data in CLO and CHI for the intervals containing E'. If LANG=1, it performs a two-dimensional interpolation for the NL coefficients at E and E'. For LANG>1, it computes the Legendre coefficients from the tabulations in File 6, and then it does the two-dimensional interpolation. Finally, it computes EPNEXT and returns.

Subroutine GETDIS is used to compute the feed function for elastic or discrete inelastic scattering of neutrons or charged particles using either File 4 or File 6 data. First, the angular distribution is retrieved with GETFLE, and an appropriate quadrature order is selected using Eq. (80). Then, a group loop from low energy to high energy is used to compute the ω_1 and ω_2 limits of Eq. (78), and the range (ω_1, ω_2) is subdivided using the appropriate Gauss-Legendre quadrature points (see QP4, QP8, QP12, and QP20). The function $f(E, \omega)$ is computed at each of these quadrature points using Eq. (79) and the angular distribution previously returned by GETFLE. The laboratory cosine at the quadrature point, $\mu[\omega]$, is computed using Eq. (75). Finally, the integrand of Eq. (78) is multiplied by the appropriate quadrature weight (QW4, QW8, QW12, or QW20) and added into the accumulating integral. This process is continued until $\omega_2 = 1$. The nonzero values of FF and the parameters IGLO and NG are then complete for this value of E.

The next step is to determine ENEXT based on the next critical point as given by Eqs. (82)–(85). Special cases are used for elastic scattering to avoid numerical problems. Note that the discontinuity flag `IDISC` is set for critical points. The `NQ` variable is also set to force `PANEL` to subdivide the initial-energy integration.

Subroutine `GETFLE` retrieves or computes the Legendre coefficients for the angular distribution of a reaction at incident energy E. When called with `E=0`, `GETFLE` requests storage for the raw data, reads in the File 4 information for the first two incident energies on the file, and then uses `GETCO` to retrieve the corresponding coefficients. On subsequent entries with `E>0`, `GETFLE` simply interpolates for the desired coefficients. When `E` exceeds the upper energy in storage, the values for the upper energy are moved to the lower positions, and new upper values are read and converted to coefficients. An isotropic distribution is returned if `E` is outside the range of the angular data from File 4.

Subroutine `GETAED` retrieves angle-energy data for thermal scattering reactions. For coherent elastic scattering, the routine reads through the cross section on the PENDF tape using `GETY1` and locates the Bragg edges. On each subsequent call to `GETAED`, the Legendre components of the cross section are computed using Eq. (70). For incoherent elastic scattering, the routine is first initialized by reading in the raw data for the first energy. On subsequent entries, a test is made to see whether E is in the range `ELO` to `EHI`. If not, the high data are moved to the low positions, and new high data are read. The Legendre components are then computed using Eq. (72). For incoherent inelastic scattering, `GETAED` is initialized by reading in the raw data for the first two incident energies. On subsequent entries, the subroutine checks to see whether `E` is between `ELO` and `EHI`. If not, the data for `EHI` are moved to the low positions, and new raw data are read from File 6 and binned. Once the correct data are in place, the desired energy-angle distribution is computed by using a combination of interpolation along lines of constant energy transfer and unit-base interpolation.

Subroutine `GETGFL` returns the Legendre coefficients for the angular distributions for all discrete and continuum photons for a reaction simultaneously. When called with `ED`=0, the routine reads File 14 into scratch storage and finds the starting location for the subsection describing each photon. On subsequent entries with `ED>0`, `GETGFL` sets up a loop over the `NG` photons on this section of File 14. For each photon, it searches for the energy panel that contains `ED`, uses `GETCO` to retrieve or compute the Legendre coefficients at the upper and lower File 14 energies, and interpolates for the desired coefficients at `ED` using `TERP1`. Since most ENDF/B photons are represented as isotropic, a special short-cut calculation is provided for that case. Isotropic results are also returned if `ED` is outside the range of the data in File 14.

Subroutine GETCO is used by both GETFLE and GETGFL to retrieve or compute Legendre coefficients from data in File 4 or File 14 format. The user can request output in either the the lab or CM system, and the raw data can be either Legendre coefficients or tabulated probability versus emission cosine. However, if the raw data are in the laboratory system, CM coefficients cannot be produced. If the raw data are already in the form of coefficients in the desired system, GETCO simply checks for the maximum Legendre order needed using a tolerance of TOLER=1E-6 and returns the coefficients in FL and the order in NL. If coordinate conversion is required, or if the raw data are tabulated, GETCO sets up the integral over cosine using Gauss-Legendre quadrature of order 20 (see QP and QW). The scattering probability for the quadrature point is computed from the coefficients or obtained by interpolating in the tabulation. The Legendre polynomials in the desired reference system are then computed. If the raw data are in the CM system (ω) and the result is to be in the lab system (μ), the desired polynomials are $P_\ell(\mu[\omega])$; otherwise, the quadrature angle is used directly to compute the polynomials. Once the coefficients have been computed, they are checked using TOLER to determine the maximum order required, NL, and the final results are returned in FL.

Subroutine GETGYL is used to retrieve the yields for all photons emitted in a specified reaction simultaneously. The raw data are obtained from the ENDF/B tape as either yields (MF=12) or production cross section (MF=13). In the latter case, GETGYL actually returns the fraction of the total yield assigned to each photon. The cross section returned by GETSIG is the total photon production cross section from MF=13 on the PENDF tape, which makes the resulting integral correct. Using the normal GROUPR procedure, GETGYL is initialized by calling it with ED=0. The entire File 12 or File 13 is read into scratch storage, and the starting location for each subsection is determined. On subsequent entries (ED>0), the routine loops over the NYL photons found, and uses TERPA to compute the yield at ED. If this is a primary photon, a discontinuity is set up at the energy where the photon will change groups. For MF=12, the calculation is finished. For MF=13, the numbers calculated above are converted to fractions of the total yield by dividing by the total production subsection from File 13. This routine does not handle ENDF/B transition probability arrays directly, because they will have been converted to File 12 yields by CONVER.

Subroutine CONVER converts ENDF/B evaluations to a standard form. If transition probability arrays were used in File 12, they are converted to yields and written back into File 12. If a section with MF=1 and MT=456 is missing from the evaluation, a copy of MT=452 is added to the tape as MT=456. In addition, a second copy of the modified tape is made on unit NSCR. While CONVER is reading through the tape, lists of the reactions in File 4, File 12, and File 13 are written to /RLIST/ for use by the automatic reaction selection logic in NEXTR. For ENDF-6 evaluations containing File 6, the routine scans through File 6 looking for sections that produce neutrons, photons, or charged particles. The MT numbers for these sections are stored into MF6, MF18, and MF6P. The routine also checks for sections of File 4 containing charged-particle angular distributions and records their MT numbers in MF4R. Finally, if the section MF6/MT2 contains charged-particle elastic scattering information given using the nuclear-plus-interference format, it is converted into the residual-cross-section format for GETDIS.

Subroutine GETSED returns the secondary-energy distribution for neutrons or continuum photons for all groups simultaneously. Both tabulated and analytic functions are handled. GETSED is initialized for a particular reaction by calling it with ED=0. First, scratch storage is allocated, and all the subsections are read in. Analytic subsections are left in their raw form, but tabulated subsections are averaged over outgoing energy groups for each of the given incident energies. The array LOC contains pointers for each subsection. On subsequent entries (ED>0), GETSED loops over the subsections for this reaction. It first retrieves the fractional probability for the subsection using TERPA. If an analytic law is specified, ANASED is used to compute the group integral for each secondary-energy group. Each integral is multiplied by the fractional probability for the law and accumulated into SED. For tabulated data, the routine simply interpolates between the two values for the group integrals using TERP1, and accumulates them into SED. Note that various restrictions on the ordering of subsections and prohibition of multiple tabulated subsections needed for earlier versions of GROUPR are no longer required. Upscatter is not allowed in secondary-energy distributions except for fission or photon production. If found, it is put into the "in-group" ($g'=g$).

Subroutine ANASED is used to calculate the integral from E1 to E2 for one of the analytic laws [see Eqs. (92)–(121)]. The routine starts with statement functions for the reduced complementary error function, rerfc(x). The parameters are then retrieved from the raw data, and the code branches to the appropriate block of coding. The resulting integral is returned in G.

Subroutine HNAB is used to compute the special functions required for analytic law 11, the energy-dependent Watt spectrum. The method used is described in the BROADR chapter of this manual.

S. Error Messages

The fatal error messages and warning message from GROUPR are listed below, along with recommended actions to recover from the problem.

`ERROR IN GROUPR***UNABLE TO FIND MAT=---, T=---.`

Check for input error or wrong PENDF tape mounted.

`ERROR IN GROUPR***STORAGE EXCEEDED.`

Main container array is not big enough. See the variables `IAMAX=25000` in `GROUPR` and `A(25000)` in `/GSTORE/`.

`ERROR IN GROUPR***PHOTONS NOT ALLOWED WITH IGG=0.`

In order to produce photon data, a photon group structure must be requested. Check the input on card 2.

`ERROR IN GROUPR***ILLEGAL MFD.`

Check input `MFD`; legal values are 3, 5, 6, 8, 16, 17, 18, 21–26, 31–36, 91–99, 101–109.

`MESSAGE FROM GROUPR---AUTO FINDS NO REACTIONS FOR MF=--.`

An automatic reaction selection card of the form "MFD" was given in the input, but the ENDF and PENDF tapes do not contain any sections that would produce the desired cross sections or matrices.

`ERROR IN RUINB***NTEMP=0 NOT ALLOWED.`

There must be at least one temperature requested.

`ERROR IN RUINB***TOO MANY TEMPERATURES.`

The maximum number of temperatures is 10. See the variables `NTMAX` and `TEMP(10)` in `/TEMPR/`.

`ERROR IN RUINB***NSIGZ=0 NOT ALLOWED.`

There must be at least one background cross section. The first input value is automatically changed to 1E10.

`ERROR IN RUINB***TOO MANY SIGMA ZEROES.`

The maximum number of sigma-zero values is 10. See `NZMAX` and `SIGZ(10)` in `/SIGZER/`.

`ERROR IN GENGPN***TOO MANY GROUPS.`

The maximum number of neutron group boundaries is 641. See `NGMAX` and `EG(641)` in `/GROUPN/`.

`ERROR IN GENGPN***READ-IN GROUP STRUCTURE IS OUT OF ORDER.`

Group structures must be given in ascending energy order.

`ERROR IN GENGPN***ILLEGAL GROUP STRUCTURE.`

Check input; current legal values are 1 through 17.

ERROR IN GENGPG***TOO MANY GROUPS.

The maximum number of photon group boundaries is 150. See the variables NGMAX and EGG(150) in /GROUPG/.

ERROR IN GENGPG***ILLEGAL GROUP STRUCTURE.

Check input; current legal values are 1 through 9.

ERROR IN GENWTF***ILLEGAL WEIGHT FUNCTION REQUESTED.

Check input; current legal values are -11 through $+11$.

ERROR IN GENFLX***TOTAL NOT DEFINED OVER ENERGY RANGE.

A complete total cross section is needed for self-shielding. This means that "dosimetry" and "activation" tapes, which normally give only a few key reactions, must be processed using NSIGZ=1 (infinite dilution).

ERROR IN GETFWT***E OUTSIDE RANGE OF DATA IN NINWT.

A premature end-of-file was found on the input flux tape when using the IWT=0 option. Check to be sure the tape was the output from a legal flux calculator run.

ERROR IN GETFWT***REQUESTED E IS OUT OF ORDER.

The cause could be an improper input tape. Check as above.

ERROR IN GETFWT***TEMPERATURE NOT ON NINWT.

The IWT=0 calculation must be consistent with the previous flux calculator run. Check to see if the correct tape was mounted.

ERROR IN PANEL***ELO.GT.EHI.

This indicates some error in the energy grid for PANEL. It usually occurs if RNDOFF and DELTA are incorrect for your machine. Make sure that RNDOFF>1, that DELTA<1, and that the product RNDOFF*DELTA< 1 when evaluated on your machine (for example, 1.00000001 is <u>not</u> greater than unity on a 32-bit machine).

ERROR IN GETYLD***ILLEGAL LND.

The maximum number of time groups is 6. See NDN and DNTC(6) in /DELAYN/.

ERROR IN GETSIG***ILLEGAL MT.

Check input for MTD. Legal values are 1–150, 201–250, 251–253, 258–259, 300–450, 452, 455, and 456.

MESSAGE FROM STOUNR---NO UNRESOLVED SIGMA ZERO DATA....

This message probably means that UNRESR was never run for this material. Infinitely dilute values will be used.

MESSAGE FROM STOUNR---SIGMA ZERO GRIDS DO NOT MATCH....

The unresolved calculations will probably work best if the σ_0 grid in GROUPR matches the one in UNRESR. However, this is not necessary. GETUNR will interpolate to get values on the GROUPR grid from the UNRESR grid. A message is issued in case this isn't what the user really intended.

`ERROR IN STOUNR***STORAGE EXCEEDED.`

There is not enough storage for unresolved cross section data on PENDF tape. This means that there is no more room in the main container array. See `IAMAX=25000` and `A(25000)` in `/GSTORE/`.

`ERROR IN STOUNR***CANNOT FIND TEMP=---`

The list of temperatures requested for the GROUPR run must agree with the first `NTEMP` temperatures on the PENDF tape. Check your BROADR and UNRESR runs.

`ERROR IN GETFF***OPTION NOT AVAILABLE FOR THIS MT.`

The `GETFF` routine branches to different blocks of coding for different combinations of `MFD` and `MTD`, but if no appropriate branch is found for the current values, this error message is issued. It probably indicates an error in the evaluation.

`ERROR IN GETMF6***DESIRED PARTICLE NOT FOUND.`

The outgoing particle for a group-to-group matrix is implied by the value of `MFD` (for example, protons for `MFD=21`). This message means that the section of File 6 requested with `MFD` and `MTD` does not contain a subsection that produces that particle. Check the user input. This message should not occur with automatic reaction selection.

`ERROR IN GETMF6***ILLEGAL LAW.`

The value of the `LAW` parameter is greater than 7. This implies an error in the evaluation.

`ERROR IN GETMF6***STORAGE EXCEEDED.`

Since the block of storage called `SC` was reserved with `NC=-1`, the only recourse is to increase the size of the main container array. See `A(25000)` and `IAMAX=25000` in `GROUPR`.

`MESSAGE FROM GETMF6---BAD GRIDS FOR CORRESPONDING POINT ....`

Corresponding-point interpolation won't work correctly unless the two grids above and below the point of interest have the same number of points. This message means that there is an error in the evaluation.

`ERROR IN CM2LAB***STORAGE EXCEEDED.`

Once again, the only recourse is to increase the size of the main container array. See `A(25000)` and `IAMAX=25000` in `GROUPR`.

`ERROR IN F6DDX***ILLEGAL LANG.`

The value of `LANG` for tabulated angular distributions must be in the range 11–15.

`ERROR IN F6DDX***TABULATED ANGULAR DISTRIBUTION NOT CODED.`

This option needs to be implemented in a future version.

`ERROR IN SEPE***DOMINANT ISOTOPE NOT KNOWN.`

The calculation of the neutron separation energy needed for the Kalbach model for particle energy-angle distributions needs a guess for the dominant isotope in an element. It will have to be added to the code. The same problem will occur with the parallel routines in HEATR and ACER.

`ERROR IN LL2LAB***STORAGE EXCEEDED.`

The size of the main container array will have to be increased. See `A(25000)` and `IAMAX=25000` in `GROUPR`.

`ERROR IN F6LAB***ILLEGAL LANG.`

The value of `LANG` must be in the range 11–15 for tabulated angular distributions.

`ERROR IN GETDIS***ILLEGAL NQP GT 20.`

The highest quadrature order available is currently 20. See data statements for `QP` and `QW`.

`ERROR IN GETFLE***DESIRED ENERGY ABOVE HIGHEST ENERGY GIVEN.`

Should not occur for well-constructed ENDF files. Check the evaluation to be sure File 3 and File 4 are consistent.

`MESSAGE FROM GETFLE---LAB DISTRIBUTION CHANGED TO CM.`

Angular distributions for two-body reactions are supposed to be given in the CM frame by ENDF conventions. Some old evaluations for heavy materials violate this rule; changing to the CM frame has little effect on the answers.

`ERROR IN GETAED***NOT CODED FOR ENDF-FORMATTED FILE 6.`

This subroutine uses a special form of File 6 that is not consistent with the one described in ENDF–102.[3, 4]

`ERROR IN GETAED***STORAGE EXCEEDED.`

This message also indicates that the main container array is too small. See `IAMAX=25000` in `GROUPR` and `A(25000)` in `/GSTORE/`.

`MESSAGE FROM BINA---DISCRIMINANT=---//SET TO ABS...`

The subroutine is having trouble finding the boundaries of equal-probability bins for the thermal interpolation method. If this negative value is small, the message can be ignored.

`ERROR IN GETGFL***DESIRED ENERGY AT HIGHEST GIVEN ENERGY.`

This problem should not occur in a well-constructed ENDF file. Check Files 3, 12, 13, and 14 for consistency.

`ERROR IN GETCO***LIMITED TO 21 LEGENDRE COEFFICIENTS.`

This limit is consistent with ENDF/B procedures. See `NLMAX/21/` and `P(21)`. If `NLMAX` is increased, it might also be advisable to increase the quadrature order (currently 20).

`ERROR IN GETCO***LAB TO CM CONVERSION NOT CODED.`

The need for this type of conversion rarely occurs on the current ENDF evaluations, because CM is consistently used for two-body reactions, and the laboratory frame is consistently used for continuum reactions. There are a few exceptions for the heavy isotopes, where CM and lab are essentially equivalent, but they were errors when the files were generated.

`ERROR IN GETGYL***LO=2 NOT CODED.`

This message should not occur, because any transition probability arrays on the ENDF tape should have been converted to yields by `CONVER`.

`ERROR IN GETGYL***TOO MANY GAMMAS.`

The current limit is 100 photons. See `NYLMAX/100/` and `LOCA(100)`.

`ERROR IN GETGYL***STORAGE EXCEEDED.`

Main container array is too small. See the variables `IAMAX` in `GROUPR` and `A(25000)` in `/GSTORE/`.

`MESSAGE FROM CONVER---CANNOT DO COMPLETE PARTICLE PRODUCTION...`

With the advent of the ENDF-6 format, it will be possible to make evaluations that fully describe all the products of a nuclear reaction. Some carry-over evaluations from earlier ENDF/B versions also have this capability, but many do not. This message is intended to goad evaluators to improve things!

`MESSAGE FROM CONVER---GAMMA PRODUCTION PATCH MADE FOR ...`

This patch is used to correct the old ENDF/B-III evaluations for MAT=1149 and MAT=1150 (chlorine and potassium).

`ERROR IN GETSED***TOO MANY SUBSECTIONS.`

The current limit is 20. See `NKMAX/20/` and `LOC(20)`.

`ERROR IN GETSED***INSUFFICIENT STORAGE FOR RAW ENDF DATA.`

The space allocated for raw File 5 or File 15 data is determined by `MAXRAW/1200/`. It can be increased at will, if there is enough room in the main container array.

`MESSAGE FROM GETSED---UPSCATTER CORRECTION....`

This reaction should not have upscatter. The error is placed into the in-group element.

`ERROR IN ANASED***ILLEGAL LF.`

Legal values are 5, 7, 9, 11, and 12.

`ERROR IN F6PSP***3, 4, OR 5 PARTICLES ONLY.`

Phase-space formulas for 3, 4, or 5 particles are provided in this routine. Check for an error in the evaluation.

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