# III. RECONR

The RECONR module is used to reconstruct resonance cross sections from resonance parameters and to reconstruct cross sections from ENDF/B nonlinear interpolation schemes. The output is written as a pointwise-ENDF (PENDF) tape with all cross sections on a unionized energy grid suitable for linear interpolation to within a specified tolerance. Redundant reactions (for example, total or inelastic) are reconstructed to be exactly equal to the sum of their parts at all energies. The resonance parameters are removed from File 2, and the material directory is corrected to reflect all changes. RECONR has the following features:

- Efficient use of dynamic storage allocation and a special stack structure allow large problems to be run on small machines.
- The unionized grid improves the accuracy, usefulness, and ENDF/B compatibility of the output. All summation cross sections are preserved on the union grid.
- A correct directory of the output tape is provided.
- Approximate $\psi\chi$ Doppler broadening may be used in some cases to speed up reconstruction for narrow-resonance materials.
- A resonance-integral criterion is added to the normal linearization criterion in order to reduce the number of points added to the tabulation to represent "unimportant" resonances.
- All ENDF-6 formats are handled except Generalized R-Matrix parameters, energy-dependent scattering radius, and the calculation of angular distributions from resonance parameters.

This manual describes RECONR in versions of NJOY through 91.91.

## A. ENDF/B Cross Section Representations

A typical cross section derived from an ENDF/B evaluation is shown in Fig. 1. The low-energy cross sections are "smooth". They are described in File 3 (see Section II.D for a review of ENDF/B nomenclature) using cross-section values given on an energy grid with a specified law for interpolation between the points. In the resolved resonance range, resonance parameters are given in File 2, and the cross sections for resonance reactions have to be obtained by adding the contributions of all the resonances to "backgrounds" from File 3. At still higher energies comes the unresolved region where explicit resonances are no longer defined. Instead, the cross section is computed from statistical distributions of the resonance parameters given in File 2 and backgrounds from File 3 (or optionally taken directly from

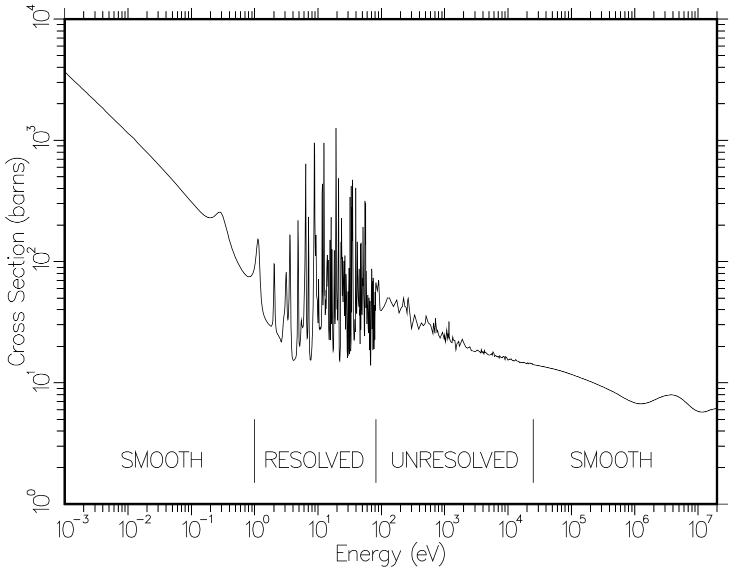


**Figure 1**: A typical cross section reconstructed from an ENDF/B evaluation using RECONR. The smooth, resolved, and unresolved energy regions use different representations of the cross sections. This is the total cross section for $^{235}$U from ENDF/B-V.

File 3 as for smooth cross sections). Finally, at the highest energies, the smooth File 3 representation is used again.

For light and medium-mass isotopes, the unresolved range is usually omitted. For the lightest isotopes, the resolved range is also omitted, the resonance cross sections being given directly in the "smooth" format. In addition, several different resonance representations are allowed (for example, Single-Level Breit-Wigner, Multilevel Breit-Wigner, Reich-Moore, and so on). It is the purpose of RECONR to take all of these separate representations and produce a simple cross section versus energy representation like the one shown in Fig. 1.

## B. Unionization and Linearization Strategy

Several of the cross sections found in ENDF/B evaluations are summation cross sections (for example, total, inelastic, and sometimes (n,2n) or fission), and it is important that each summation cross section be equal to the sum of its parts. However, if the partial cross sections are represented with nonlinear interpolation schemes, the sum cannot be represented by any simple interpolation law. A typical case is the sum of elastic scattering (MT=2 interpolated linearly to represent a constant) and radiative capture (MT=102 interpolated log-log to represent 1/v).

The total cross section cannot be represented accurately by either scheme unless the grid points are very close together. This effect leads to significant balance errors in multigroup transport codes and to splitting problems in continuous-energy Monte Carlo codes.

Furthermore, the use of linear-linear interpolation (that is, $\sigma$ linear in $E$) can be advantageous in several ways. The data can be plotted easily, they can be integrated easily, cross sections can be Doppler-broadened efficiently (see BROADR), and, finally, linear data can be retrieved efficiently in continuous-energy Monte Carlo codes.

Therefore, RECONR puts all cross sections on a single unionized grid suitable for linear interpolation. As described in more detail below, RECONR makes one pass through the ENDF/B material to select the energy grid, and then a second pass to compute cross sections on this grid. Each cross section on the PENDF tape (except for the summation cross sections) is exactly equal to its ENDF/B value. The summation cross sections are then obtained by adding up the partial cross sections at each grid point.

While RECONR is going through the reactions given in the ENDF/B evaluation, it also checks the reaction thresholds against the $Q$ value and atomic weight ratio to the neutron $A$ (AWR in the file) given for the reaction. If the condition

$$\text{threshold} \geq \frac{A+1}{A} Q \tag{1}$$

is not satisfied, the threshold energy is moved up to satisfy the condition (an informative message is printed if the change exceeds 0.1%).

If desired, the unionized grid developed from the ENDF/B file can be supplemented with “user grid points” given in the input data. The code automatically adds 1.E-5 eV, 0.0253 eV, and 20 MeV to the grid if they are not already present.

There are special problems with choosing the energy grid in the unresolved range. In some cases, the unresolved cross section is represented using resonance parameters that are independent of energy. The cross sections are not constant, however, but have a shape determined by the energy variation of neutron wave number, penetrability factors, and so on. RECONR handles this case by choosing a set of energies (about 10 per decade) to be used to calculate the cross sections; the set of energies gives a reasonable approximation to the result intended. For evaluations that use energy-dependent resonance parameters, it is supposed to be sufficient to compute the unresolved cross sections at the given energies and to use interpolation on the cross sections to obtain the appropriate values at other energies. However, some evaluations carried over from earlier versions of ENDF/B were not evaluated using this convention, and cross sections computed using cross-section interpolation are not sufficiently accurate. RECONR detects such cases by looking for large steps between the points of the given energy grid. It then adds additional energy grid points using the same 10-per-decade rule used for energy-independent parameters.

## C. Linearization and Reconstruction Methods

Linearization (`LUNION`) and resonance reconstruction (`RESXS`) both function by inserting new energy grid points between the points of an original grid using an "inverted stack". The general concepts involved are illustrated with a simple example shown in Fig. 2.

The stack is first primed with two starting values. For linearization, they will be two adjacent points on the original union grid. For reconstruction, they will usually be the peaks or half-height energies of resonances. The stack is said to be inverted because the lower energy is at the "top" (`I=2`).

This interval or panel is now divided into two parts, and the cross section computed at the intermediate point is compared to the result of linear interpolation between the adjacent points. If the two values do not agree within various criteria, the top of the stack is moved up one notch (`I=3`), and the new value is inserted (`I=2`). The code then repeats the checking process for the new (smaller) interval at the top of the stack. The top of the stack rises until convergence is achieved for the top interval. The top energy and cross section are then saved on a scratch file, the stack index is decremented, and the checks are repeated. This process is continued with the top of the stack rising and falling in response to the complexity of the cross section until the entire panel $\Delta E$ has been converged (`I=1`). The stack is then reprimed with the bounds of the next panel. The process continues until the entire energy range for linearization or reconstruction has been processed.

This stack logic enables a panel to be subdivided into parts as small as $\Delta E/2^n$ where $n$ is the stack size (currently 20), and several different cross sections (elastic, capture, fission) can easily be stored in arrays of this size. By contrast, RESEND used several arrays 500 words long and sometimes ran out of storage while subdividing between resonances.

Intervals are subdivided differently for linearization and resonance reconstruction. In the latter case, the interval is simply divided in half as in RESEND. For linearization, the method developed by D. R. Harris for MINX[1] is used. Analytic formulas are used to choose the optimum intermediate point; this turns out

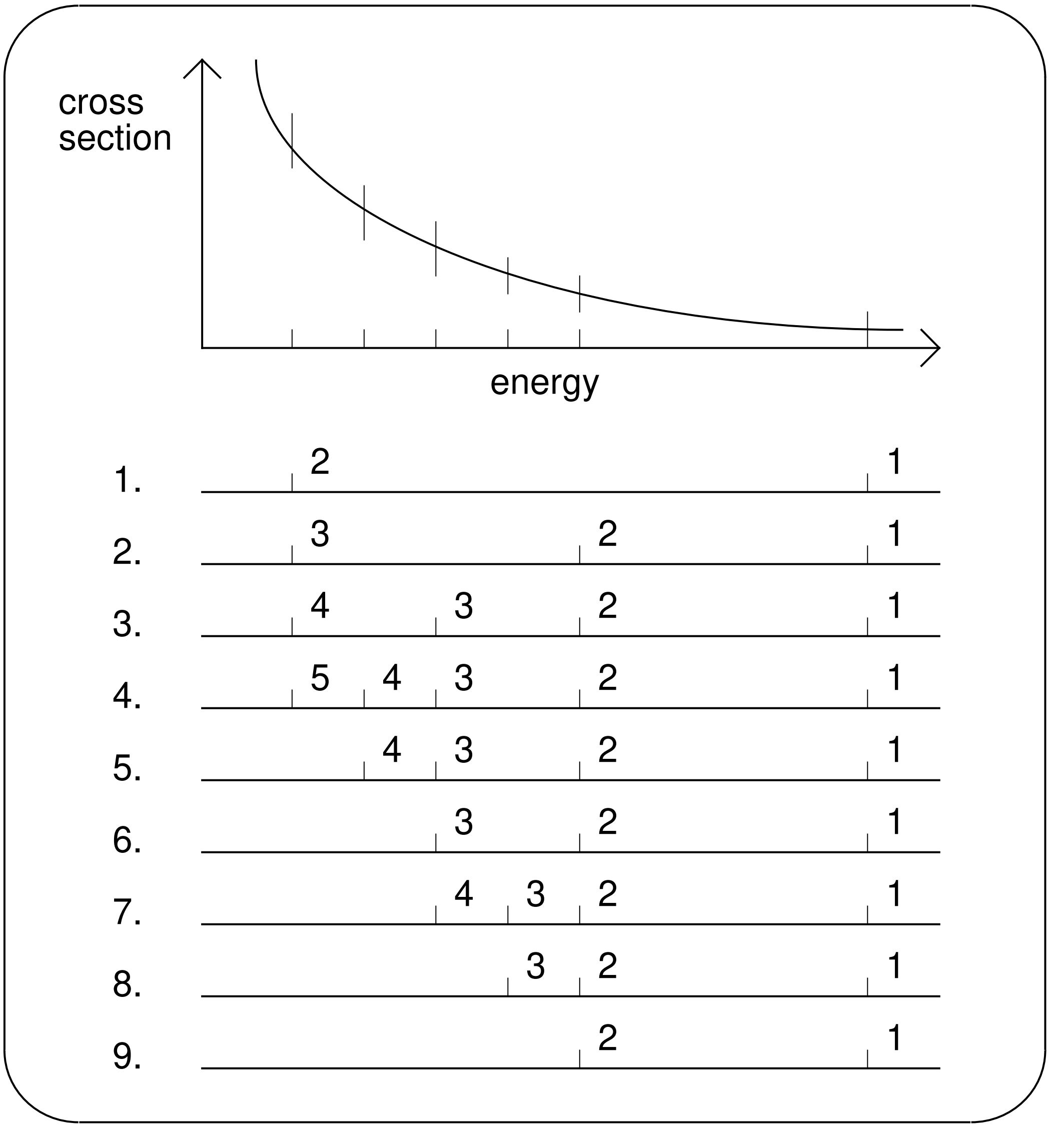


**Figure 2**: Inverted-stack method used in RECONR and several other places in NJOY. Line 1 shows the two initial points (the lower energy is higher in the stack). In line 2, a new point has been calculated at the midpoint, but the result was not converged, and the new point has been inserted in the stack. In line 3, the midpoint of the top panel has been checked again, found to be not converged, and inserted into the stack. The same thing happens in line 4. In line 5, the top panel is found to be converged, and the top point (5) has been written out. The same thing happens in line 6. In line 7, the top panel is tested and found to be not converged. The midpoint is added to the stack. Finally, in line 8, the top panel is found to be converged, and the top point is written out. This leaves two points in the stack (see line 9). Note that the energy points come off the stack in the desired order of increasing energy, and that only one point has to be moved up in the stack as each new result is inserted.

to be the energy where the slope of the actual interpolation function equals the slope of the linear approximation. Formulas are provided for each of the nonlinear ENDF/B interpolation laws: $\sigma$ linear in $\ln(E)$; $\ln(\sigma)$ linear in $E$; and $\ln(\sigma)$ linear in $\ln(E)$.

The convergence criterion used for linearization is that the linearized cross section at the intermediate point is within the fractional tolerance `ERR` (or a small absolute value `ERRLIM`) of the actual cross section specified by the ENDF law. More complicated criteria are used for resonance reconstruction.

There are two basic problems that arise if a simple fractional tolerance test is used to control resonance reconstruction. First, as points are added to the energy grid, adjacent energy values may become so close that they will be rounded to the same number when a formatted output file is produced or when the machine-dependent limit for decimal single-precision accuracy is reached. It clearly makes no sense to continue to add grid points after this limit is reached. Through the use of dynamic format reconstruction, the energy resolution available for formatted NJOY output is 7 significant figures (that is, $\pm 1.234567 \pm n$) rather than the usual 5 or 6 (see Section II.D). On "short-word" machines (32–36 bits per word), the limit set by precision is also about 7 significant figures. On "long-word" machines (typically 60–64 bits per word), binary output files can be used, and NJOY can produce up to 15 significant figures if necessary.

Significant-figure control is implemented as follows: each intermediate energy is truncated to `NDIGIT` significant figures before the corresponding cross sections are computed, and if the resulting number is equal to either of the adjacent values, the interval is declared to be converged. Thus, no identical energies are produced, but an unpredictable loss in accuracy results. The error in the area of this interval is certainly less than $0.5 \times \Delta\sigma \times \Delta E$, so this value is added to an error estimate and a count of panels truncated by the significant figure check is incremented for a later informative diagnostic message.

The second basic problem alluded to above is that a very large number of resonance grid points arise from straightforward linear reconstruction of the resonance cross section of some isotopes. Many of these points come from narrow, weak, high-energy resonances, which do not need to be treated accurately in many applications. As an example, the capture and fission resonance integrals important for thermal reactors must be computed with a 1/E flux weighting. If the resonance reconstruction tolerance is set high (say 1%) to reduce the cost of processing, the resonance integrals will be computed to only 1% accuracy. However, if the reconstruction tolerance were set to a smaller value, like 0.1%, and if the high-energy resonances (whose importance is reduced by the 1/E weight and the 1/v trend of the capture and fission cross sections) were treated with less accuracy than the low-energy resonances, then it is likely that one could achieve an accuracy much better than 1% with an overall reduction in the number of points (hence computing cost). Since 1/E weighting is not realistic in all applications (for example, in fast reactors), user control of this "thinning" operation must be provided.

Based on these arguments, the following approach was chosen to control the problem of very large files. First, panels are subdivided until the elastic, capture, and fission cross sections are converged to within `ERRMAX`, where `ERRMAX` $\geq$ `ERR`. These two tolerances are normally chosen to form a reasonable band, such as 10% and 0.5%, to ensure that all resonances are treated at least roughly (for example, for plotting). If the resonance integral (1/E weight) in some panel is large, the panel is further subdivided to achieve an accuracy of `ERR` (say 0.5%). However, if the contribution to the resonance integral from any one interval gets small, the interval will be declared converged, and the local value of the cross section will end up with some intermediate accuracy. Once again, the contribution to the error in the resonance integral should be less than $0.5{\times}\Delta\sigma{\times}\Delta E$. This value is added into an accumulating estimate of the error, and a count of panels truncated by the resonance integral check is incremented.

The problem with this test is that RECONR does not know the value of the resonance integral in advance, so the tolerance parameter `ERRINT` is not the actual allowed fractional error in the integral. Instead, it is more like the resonance integral error per grid point (barns/point). Thus, a choice of `ERRINT=ERR/10000` with `ERR`=0.001 would limit the integral error to about 0.001 barn if 10000 points resulted from reconstruction. Since important resonance integrals vary from a few barns to a few hundred barns, this is a reasonable choice. The integral check can be suppressed by setting `ERRINT` very small or `ERRMAX=ERR`.

When resonance reconstruction is complete, RECONR provides a summary of the possible resonance integral error due to significant figure reduction and the integral check over several coarse energy bands. A typical example follows:

```
                  ESTIMATED MAXIMUM ERROR DUE TO
                  RESONANCE INTEGRAL CHECK (ERRMAX, ERRINT)
                  AND SIGNIFICANT FIGURE TRUNCATION (NDIGIT)

     UPPER        ELASTIC     PERCENT ERROR     CAPTURE     PERCENT ERROR
     ENERGY       INTEGRAL   RES-INT SIG-FIG    INTEGRAL   RES-INT SIG-FIG
    1.55E+02
    4.96E+02      7.45E+00     .000    0.000    2.82E-02     .009    0.000
    1.63E+03      5.94E+00     .000    0.000    1.71E-01     .002    0.000
    5.20E+03      4.12E+00     .000    0.000    6.80E-03     .149    0.000
```

```
 1.73E+04     6.49E+00    .000     .000    1.61E-02    .134     .008
 5.62E+04     9.66E+00    .001     .000    1.74E-02    .200     .097
 1.78E+05     4.20E+00    .004     .009    1.19E-02    .216    4.284
 4.00E+05     3.50E+00    .008     .007    5.64E-03    .257    5.265

POINTS ADDED BY RESONANCE RECONSTRUCTION = 12309
POINTS AFFECTED BY RESONANCE INTEGRAL CHECK =   6969
POINTS AFFECTED BY SIGNIFICANT FIGURE REDUCTION =  1262
POINTS REMOVED BY BACKTHINNING =   201
FINAL NUMBER OF RESONANCE POINTS = 12749
```

The last band covers the unresolved range, if present. The parameter NDIGIT and the parameters ERRMAX and ERRINT, taken together, should be considered as adjustment "knobs" that can increase or decrease the errors in their respective columns to get an appropriate balance of accuracy and economy for a particular application.

### D. Resonance Representations

RECONR uses the resonance formulas as implemented in the original RESEND code[2] with four changes: a more efficient calculation of multilevel Breit-Wigner cross sections developed by C. Lubitz of the Knolls Atomic Power Laboratory (General Electric Co.) and coded by P. Rose of the National Nuclear Data Center (NNDC) at Brookhaven National Laboratory, the addition of competitive widths introduced for ENDF/B-V, a $\psi\chi$ Doppler-broadening calculation for single-level Breit-Wigner and Adler-Adler resonance shapes, and a capability to process either the multilevel multichannel R-matrix Reich-Moore parameters or the multilevel single-channel Hybrid R-Function parameters based on the work of M. Bhat and C. Dunford of the NNDC. An expanded discussion of the following formulas can be found in the ENDF/B-V and ENDF-6 format manuals.[3, 4]

**1. Single-Level Breit-Wigner Representation (SLBW)** The subroutine that computes single-level Breit-Wigner cross sections (CSSLBW) uses

$$\begin{aligned}\sigma_n &= \sigma_p \\ &\quad + \sum_\ell \sum_r \sigma_{mr} \Big\{ \Big[ \cos 2\phi_\ell - (1 - \frac{\Gamma_{nr}}{\Gamma_r}) \Big] \, \psi(\theta, x) \\ &\quad + \sin 2\phi_\ell \, \chi(\theta, x) \Big\} \,, \qquad (2)\\ \sigma_f &= \sum_\ell \sum_r \sigma_{mr} \frac{\Gamma_{fr}}{\Gamma_r} \, \psi(\theta, x) \,, \qquad (3)\end{aligned}$$

$$\sigma_\gamma = \sum_\ell \sum_r \sigma_{mr} \frac{\Gamma_{\gamma r}}{\Gamma_r} \psi(\theta, x) \text{ , and} \tag{4}$$

$$\sigma_p = \sum_\ell \frac{4\pi}{k^2}(2\ell+1) \sin^2 \theta_\ell \text{ ,} \tag{5}$$

where $\sigma_n$, $\sigma_f$, $\sigma_\gamma$, and $\sigma_p$ are the neutron (elastic), fission, radiative capture, and potential scattering components of the cross section arising from the given resonances. There can be "background" cross sections in File 3 that must be added to these values to account for competitive reactions such as inelastic scattering or to correct for the inadequacies of the single-level representation with regard to multilevel effects or missed resonances. The sums extend over all the $\ell$ values and all the resolved resonances $r$ with a particular value of $\ell$. Each resonance is characterized by its total, neutron, fission, and capture widths $(\Gamma, \Gamma_n, \Gamma_f, \Gamma_\gamma)$, by its $J$ value (AJ in the file), and by its maximum value (`SMAX`$= \sigma_{mr}/\Gamma_r$ in the code)

$$\sigma_{mr} = \frac{4\pi}{k^2} g_J \frac{\Gamma_{nr}}{\Gamma_r} \text{ ,} \tag{6}$$

where $g_J$ is the spin statistical factor

$$g_J = \frac{2J+1}{4I+2} \text{ ,} \tag{7}$$

and $I$ is the total spin SPI given in File 2, and $k$ is the neutron wave number, which depends on incident energy $E$ and the atomic weight ratio to the neutron for the isotope $A$ (AWRI in the file), as follows:

$$k = (2.196771 \times 10^{-3}) \frac{A}{A+1} \sqrt{E} \text{ .} \tag{8}$$

There are two different characteristic lengths that appear in the ENDF resonance formulas: first, there is the "scattering radius" $\hat{a}$, which is given directly in File 2 as AP; and second, there is the "channel radius" $a$, which is given by

$$a = 0.123\, A^{1/3} + 0.08 \text{ .} \tag{9}$$

If the File 2 parameter NAPS is equal to one, $a$ is set equal to $\hat{a}$ in calculating penetrabilities and shift factors (see below). The ENDF-6 option to enter an energy-dependent scattering radius is not supported. The neutron width in the equations for the SLBW cross sections is energy dependent due to the penetration factors $P_\ell$; that is,

$$\Gamma_{nr}(E) = \frac{P_\ell(E)\, \Gamma_{nr}}{P_\ell(|E_r|)} \text{ ,} \tag{10}$$

where

$$P_0 = \rho \,, \tag{11}$$

$$P_1 = \frac{\rho^3}{1+\rho^2} \,, \tag{12}$$

$$P_2 = \frac{\rho^5}{9+3\rho^2+\rho^4} \,, \tag{13}$$

$$P_3 = \frac{\rho^7}{225+45\rho^2+6\rho^4+\rho^6} \,, \text{ and} \tag{14}$$

$$P_4 = \frac{\rho^9}{11025+1575\rho^2+135\rho^4+10\rho^6+\rho^8} \,, \tag{15}$$

where $E_r$ is the resonance energy and $\rho{=}ka$ depends on the channel radius or the scattering radius as specified by NAPS. The phase shifts are given by

$$\phi_0 = \hat{\rho} \,, \tag{16}$$

$$\phi_1 = \hat{\rho} - \tan^{-1}\hat{\rho} \,, \tag{17}$$

$$\phi_2 = \hat{\rho} - \tan^{-1}\frac{3\hat{\rho}}{3-\hat{\rho}^2} \,, \tag{18}$$

$$\phi_3 = \hat{\rho} - \tan^{-1}\frac{15\hat{\rho}-\hat{\rho}^2}{15-6\hat{\rho}^2} \,, \text{ and} \tag{19}$$

$$\phi_4 = \hat{\rho} - \tan^{-1}\frac{105\hat{\rho}-10\hat{\rho}^3}{105-45\hat{\rho}^2+\hat{\rho}^4} \,, \tag{20}$$

where $\hat{\rho}{=}k\hat{a}$ depends on the scattering radius. The final components of the cross section are the actual line shape functions $\psi$ and $\chi$. At zero temperature,

$$\psi = \frac{1}{1+x^2} \,, \tag{21}$$

$$\chi = \frac{x}{1+x^2} \,, \tag{22}$$

$$x = \frac{2(E-E'_r)}{\Gamma_r} \,, \tag{23}$$

and

$$E'_r = E_r + \frac{S_\ell(|E_r|) - S_\ell(E)}{2(P_\ell(|E_r|)}\,\Gamma_{nr}(|E_r|) \,, \tag{24}$$

in terms of the shift factors

$$S_0 = 0 \,, \tag{25}$$

$$S_1 = -\frac{1}{1+\rho^2} \,, \tag{26}$$

$$S_2 = -\frac{18+3\rho^2}{9+3\rho^2+\rho^4} \,, \tag{27}$$

$$S_3 = -\frac{675 + 90\rho^2 + 6\rho^4}{225 + 45\rho^2 + 6\rho^4 + \rho^6}\ , \text{ and} \tag{28}$$

$$S_4 = -\frac{44100 + 4725\rho^2 + 270\rho^4 + 10\rho^6}{11025 + 1575\rho^2 + 135\rho^4 + 10\rho^6 + \rho^8}\ . \tag{29}$$

To go to higher temperatures, define

$$\theta = \frac{\Gamma_r}{\sqrt{\dfrac{4kTE}{A}}}\ , \tag{30}$$

where $k$ is the Boltzmann constant and $T$ is the absolute temperature. The line shapes $\psi$ and $\chi$ are now given by

$$\psi = \frac{\sqrt{\pi}}{2}\,\theta\,\mathrm{Re}W(\frac{\theta x}{2},\frac{\theta}{2})\ , \tag{31}$$

and

$$\chi = \frac{\sqrt{\pi}}{2}\,\theta\,\mathrm{Im}W(\frac{\theta x}{2},\frac{\theta}{2})\ , \tag{32}$$

in terms of the complex probability function (see `QUICKW`, `WTAB`, and `W`, which came from the MC$^2$ code[5])

$$W(x,y) = \mathrm{e}^{-z^2}\,\mathrm{erfc}(-iz) = \frac{i}{\pi}\int_{-\infty}^{\infty}\frac{\mathrm{e}^{-t^2}}{z-t}\,dt\ , \tag{33}$$

where $z{=}x{+}iy$. The $\psi\chi$ method is not as accurate as kernel broadening (see BROADR) because the backgrounds (which are sometimes quite complex) are not broadened, and terms important for energies less than about $16kT/A$ are neglected; However, the $\psi\chi$ method is less expensive than BROADR. The current version of RECONR includes Doppler-broadening for the single-level Breit-Wigner and Adler-Adler representations only.

**2. Multilevel Breit-Wigner Representation (MLBW)** The Lubitz-Rose method used for calculating multilevel Breit-Wigner cross sections (`CSMLBW`) is formulated as follows:

$$\sigma_n(E) = \frac{\pi}{k^2}\sum_{\ell}\sum_{s=|I-\frac{1}{2}|}^{I+\frac{1}{2}}\sum_{J=|l-s|}^{l+s} g_J\,|1 - U_{nn}^{\ell sJ}(E)|^2\ , \tag{34}$$

with

$$U_{nn}^{\ell J}(E) = \mathrm{e}^{2i\phi_\ell} - \sum_r \frac{i\Gamma_{nr}}{E_r' - E - i\Gamma_r/2}\ , \tag{35}$$

where the other symbols are the same as those used above. Expanding the complex operations gives

$$\sigma_n(E) = \frac{\pi}{k^2}\sum_\ell \sum_{s=|I-\frac{1}{2}|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} g_J\Big\{\Big(1-\cos 2\phi_\ell - \sum_r \frac{\Gamma_{nr}}{\Gamma_r}\frac{2}{1+x_r^2}\Big)^2 + \Big(\sin 2\phi_\ell + \sum_r \frac{\Gamma_{nr}}{\Gamma_r}\frac{2x_r}{1+x_r^2}\Big)^2\Big\}\ , \qquad (36)$$

where the sums over $r$ are limited to resonances in spin sequence $\ell$ that have the specified value of $s$ and $J$. Unfortunately, the $s$ dependence of $\Gamma$ is not known. The file contains only $\Gamma_J{=}\Gamma_{s_1J}{+}\Gamma_{s_2J}$. It is assumed that the $\Gamma_J$ can be used for one of the two values of $s$, and zero is used for the other. Of course, it is important to include both channel-spin terms in the potential scattering. Therefore, the equation is written in the following form:

$$\sigma_n(E) = \frac{\pi}{k^2}\sum_\ell\Big[\sum_J g_J\Big\{\Big(1-\cos 2\phi_\ell - \sum_r \frac{\Gamma_{nr}}{\Gamma_r}\frac{2}{1+x_r^2}\Big)^2 + \Big(\sin 2\phi_\ell + \sum_r \frac{\Gamma_{nr}}{\Gamma_r}\frac{2x_r}{1+x_r^2}\Big)^2\Big\} + 2D_\ell(1-\cos 2\phi_\ell)\Big]\ , \qquad (37)$$

where the summation over $J$ now runs from

$$||I-\ell|-\frac{1}{2}| \to I+\ell+\frac{1}{2}\ , \qquad (38)$$

and $D_\ell$ gives the additional contribution to the statistical weight resulting from duplicate $J$ values not included in the new $J$ sum; namely,

$$D_\ell = \sum_{s=|I-\frac{1}{2}|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} g_J - \sum_{J=||I-\ell|-\frac{1}{2}|}^{I+\ell+\frac{1}{2}} g_j \qquad (39)$$

$$= (2\ell+1) - \sum_{J=||I-\ell|-\frac{1}{2}|}^{I+\ell+\frac{1}{2}} g_j\ . \qquad (40)$$

A case where this correction would appear is the $\ell{=}1$ term for a spin-1 nuclide. There will be 5 $J$ values: 1/2, 3/2, and 5/2 for channel spin 3/2; and 1/2 and 3/2 for channel spin 1/2. All five contribute to the potential scattering, but the file will only include resonances for the first three.

The fission and capture cross sections are the same as for the single-level option. The $\psi\chi$ Doppler-broadening cannot be used with this formulation of the MLBW representation.

**3. Adler-Adler Representation (AA)** The multilevel Adler-Adler representation is defined for $\ell$=0 only. It is useful for fissionable materials. The total cross sections are given by

$$\begin{aligned}
\sigma_t(E) &= \frac{4\pi}{k^2}\sin^2\phi_0 \\
&+ \frac{\pi\sqrt{E}}{k^2}\Big\{\sum_r \frac{1}{\nu_r}\Big[(G_r\cos 2\phi_0 + H_r\sin 2\phi_0)\,\psi(\theta,x) \\
&+ (H_r\cos 2\phi_0 - G_r\sin 2\phi_0)\,\chi(\theta,x)\Big] \\
&+ A_1 + \frac{a_2}{E} + \frac{A_3}{E^2} + \frac{A_4}{E^3} + B_1 E + B_2 E^2\Big\}\ , \qquad (41)
\end{aligned}$$

where

$$x = \frac{\mu_r - E}{\nu_r}\ , \qquad (42)$$

and where $\nu_r$ is the resonance half-width (corresponds to $\Gamma/2$ in the Breit-Wigner notation), $\mu_r$ is the resonance energy, $G_r$ is the symmetric total parameter, $H_r$ is the asymmetric total parameter, and the $A_i$ and $B_i$ are coefficients of the total background correction.

The fission and capture cross section both use the form

$$\begin{aligned}
\sigma_x(E) &= \frac{\pi\sqrt{E}}{k^2}\Big\{\sum_r \frac{1}{\nu_r}\left[G_r\psi(\theta,x) + H_r\chi(\theta,x)\right] \\
&+ A_1 + \frac{A_2}{E} + \frac{A_3}{E^2} + \frac{A_4}{E^4} + B_1 E + B_2 E^2\Big\}\ , \qquad (43)
\end{aligned}$$

where the values of $G$, $H$, $A_i$, and $B_i$ appropriate for the desired reaction are used.

Doppler-broadening can be applied as for the SLBW case, except note that $\Gamma_r$ in Eq. (24) must be replaced with $2\nu_r$. Doppler-broadened Adler-Adler cross sections are more accurate than SLBW cross sections because the background is smoother. However, cross sections below about $16kT/A$ will still be inaccurate.

**4. Reich-Moore Representation (RM)** The Reich-Moore representation is a multilevel formulation with two fission channels; hence, it is useful for both structural and fissionable materials. The cross sections are given by

$$\sigma_t = \frac{2\pi}{k^2}\sum_\ell\sum_J g_J\Big\{(1 - \mathrm{Re}\,U^{\ell J}_{nm}) + 2d_{\ell J}[1-\cos(2\phi_\ell)]\Big\}\ , \qquad (44)$$

$$\sigma_n = \frac{\pi}{k^2}\sum_\ell\sum_J g_J\Big\{|1 - U^{\ell J}_{nn}|^2 + 2d_{\ell J}[1-\cos(2\phi_\ell)\Big]\ , \qquad (45)$$

$$\sigma_f = \frac{4\pi}{k^2}\sum_\ell\sum_J g_J \sum_c |\mathcal{I}^{\ell J}_{nc}|^2 \text{ , and} \tag{46}$$

$$\sigma_\gamma = \sigma_t - \sigma_n - \sigma_f \ , \tag{47}$$

where $\mathcal{I}_{nc}$ is an element of the inverse of the complex R-matrix and

$$U^{\ell J}_{nn} = \mathrm{e}^{2i\phi_\ell}\left[2\mathcal{I}_{nn} - 1\right] \ . \tag{48}$$

The elements of the R-matrix are given by

$$R^{\ell J}_{nc} = \delta_{nc} - \frac{i}{2}\sum_r \frac{\Gamma^{1/2}_{nr}\Gamma^{1/2}_{cr}}{E_r - E - \frac{i}{2}\Gamma_{\gamma r}} \ . \tag{49}$$

In these equations, "c" stands for the fission channel, "r" indexes the resonances belonging to spin sequence $(\ell, J)$, and the other symbols have the same meanings as for SLBW or MLBW. Of course, when fission is not present, $\sigma_f$ can be ignored. The R-matrix reduces to an R-function, and the matrix inversion normally required to get $\mathcal{I}_{nn}$ reduces to a simple inversion of a complex number.

As in the MLBW case, the summation over $J$ runs from

$$||I - \ell| - \frac{1}{2}| \rightarrow I + \ell + \frac{1}{2} \ . \tag{50}$$

The term $d_{\ell J}$ in the expressions for the total and elastic cross sections is used to account for the possibility of an additional contribution to the potential scattering cross section from the second channel spin. It is unity if there is a second $J$ value equal to $J$, and zero otherwise. This is just a slightly different approach for making the correction discussed in connection with Eq. (40). Returning to the $I$=1, $\ell$=1 example given above, $d$ will be one for $J$=1/2 and $J$=3/2, and it will be zero for $J$=5/2.

ENDF-6 Reich-Moore evaluations can contain a parameter LAD that indicates that these parameters can be used to compute an angular distribution for elastic scattering if desired (an approximate angular distribution is still given in File 4 for these cases). The current version of RECONR does not compute angular distributions.

**5. Hybrid R-Function Representation (HRF)** The Hybrid R-Function representation, treats elastic scattering as a multilevel cross section using formulas similar to those given above for the Reich-Moore format in the case where fission is absent. The other reactions are treated with formulas similar to those of the SLBW method. The main use for this format is to provide a better representation of competitive reactions than is provided by any of the other formats described above. This treatment can include a background R-function, tabulated charged-particle penetrabilities, and optical model phase shifts. Following the Reich-Moore notation, the elastic cross section is given by

$$\sigma_n = \frac{\pi}{k^2} \sum_{\ell} \sum_{s=|I-\frac{1}{2}|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} g_J |1 - U_{nn}^{\ell sJ}|^2 \ , \tag{51}$$

where the $U$ function is given by the scalar version of Eq. (48):

$$U_{nn}^{\ell sJ} = \mathrm{e}^{2i\phi_\ell} \left[ \frac{2}{R_{nn}^{\ell sJ}} - 1 \right] . \tag{52}$$

The R function itself is given by

$$R_{nn}^{\ell sJ} = 1 - \frac{i}{2} \sum_r \frac{\Gamma_{nr}}{E_r - E - \frac{i}{2}\Gamma_{\gamma r}} - i\, P_{\ell sJ} R_{\ell sJ}^0 \ , \tag{53}$$

where $R_{\ell sJ}^0$ is a (complex) background R function and $P_{\ell sJ}$ is a penetrability factor. The background R function can either be read in or set to zero. The penetrability and shift factors are computed from the scattering radius or channel radius as for SLBW. The phase shifts $\phi_{\ell sJ}$ can be computed from the scattering radius as before, or the (complex) phase shifts can be read in from an optical model calculation.

Note that resonance parameters are given explicitly for all three quantum numbers $\ell$, $s$, and $J$. No correction to the potential scattering cross section from repeated $J$ values is needed.

Elastic angular distributions can also be computed from HRF parameters if the LAD parameter is set; however, RECONR does not yet support the calculation of angular distributions. Infinitely dilute cross sections in the unresolved-energy range are computed in `CSUNR1` or `CSUNR2` using average resonance parameters and probability distributions from File 2. With the approximations used, these cross sections are not temperature dependent; therefore, the results are a good match to resolved resonance data generated using `TEMPR`>0. The formulas used are based on the single-level approximation with interference.

$$\sigma_n(E) \quad = \quad \sigma_p + \frac{2\pi^2}{k^2} \sum_{\ell,J} \frac{g_J}{\overline{D}} [\overline{\Gamma}_n^2 R_n - 2\overline{\Gamma}_n \sin^2 \phi_\ell] \ , \tag{54}$$

$$\sigma_x(E) = \frac{2\pi^2}{k^2} \sum_{\ell,J} \frac{g_J}{\overline{D}} \overline{\Gamma}_n \overline{\Gamma}_x R_x \text{ , and} \tag{55}$$

$$\sigma_p = \frac{4\pi}{k^2} \sum_{\ell} (2\ell+1) \sin^2 \phi_\ell \text{ ,} \tag{56}$$

where $x$ stands for either fission or capture, $\overline{\Gamma}_i$ and $\overline{D}$ are the appropriate average widths and spacing for the $\ell$,$J$ spin sequence, and $R_i$ is the fluctuation integral for the reaction and sequence (see `GNRL`). These integrals are simply the averages taken over the chi-square distributions specified in the file; for example,

$$\begin{aligned} \overline{\Gamma}_n \overline{\Gamma}_f R_i &= \left\langle \frac{\Gamma_n \Gamma_f}{\Gamma} \right\rangle \\ &= \int dx_n P_\mu(x_n) \int dx_f P_\nu(x_f) \int dx_c P_\lambda(x_c) && (57) \\ &\times \frac{\Gamma_n(x_n)\,\Gamma_f(x_f)}{\Gamma_n(x_n) + \Gamma_f(x_f) + \Gamma_\gamma + \Gamma_c(x_c)} \text{ ,} && (58) \end{aligned}$$

where $P_\mu(x)$ is the chi-square distribution for $\mu$ degrees of freedom. The integrals are evaluated with the quadrature scheme developed by R. Hwang for the $MC^2$-2 code[6] giving

$$R_f = \sum_i W_i^\mu \sum_j W_j^\nu \sum_k W_k^\lambda \frac{Q_i^\mu \, Q_j^\nu}{\overline{\Gamma}_n Q_i^\mu + \overline{\Gamma}_f Q_j^\nu + \Gamma_\gamma + \overline{\Gamma}_c Q_k^\lambda} \text{ .} \tag{59}$$

The $W_i^\mu$ and $Q_i^\mu$ are the appropriate quadrature weights and values for $\mu$ degrees of freedom, and $\Gamma_\gamma$ is assumed to be constant (many degrees of freedom). The competitive width $\overline{\Gamma}_c$ is assumed to affect the fluctuations, but a corresponding cross section is not computed. The entire competitive cross section is supposed to be in the File 3 total cross section as a smooth background.

It should be noted that the reduced average neutron width (AMUN) is given in the file, and

$$\overline{\Gamma}_n = \Gamma_n^0 \sqrt{E}\, V_\ell(E) \text{ ,} \tag{60}$$

where the penetrabilities for the unresolved region are defined as

$$V_0 = 1 \text{ ,} \tag{61}$$

$$V_1 = \frac{\rho^2}{1+\rho^2} \text{ , and} \tag{62}$$

$$V_2 = \frac{\rho^4}{\rho + 3\rho^2 + \rho^4} \text{ .} \tag{63}$$

Other parameters are defined as for SLBW.

Unresolved parameters can be given as independent of energy, with only fission widths dependent on energy, or as fully energy dependent. The first two options are processed in CSUNR1, and the last one is processed in CSUNR2.

## E. Code Description

The flow of this module is controlled by the RECONR routine. The first step is to read cards 1, 2, and 3 of the user's input. The TAPEID record of the input tape (NENDF) is read and printed, then the new TAPEID record is written to the output tape (NPEND). RECONR is now ready to enter the loop over the desired materials.

For each material, STORAG is used to allocate space for the energy nodes and for scratch storage (ENODE, SCR), and RUIN is called to read cards 4 through 7 of the user's input. Subroutine RUIN automatically adds the ENDF energy limits of 1E-5 eV and 20 MeV and the thermal energy 0.0253 eV to any energy grid points entered by the user. If the reconstruction temperature (TEMPR) is greater than zero, a table of $\psi$ and $\chi$ functions is generated (the W table; see WTAB and QUICKW). The FINDF utility subroutine is then used to find the first card of File 1 (MF=1,MT=451) for the desired material.

File 1 on the input ENDF tape is examined to obtain certain constants and flags and to analyze the directory (ANLYZD). Subroutine ANLYZD determines which reactions should be considered "redundant"; that is, the reactions that are sums of other reactions and will be included on the output PENDF tape. The total cross section (MT=1 for neutrons, MT=501 for photons) will always be included; the nonelastic cross section (MT=3) will be included if it is needed for photon production (that is, MF=12, MT=3 is found); the inelastic cross section (MT=4) will be included if sections with MT in the range 51–91 occur in the file, and the total fission reaction (MT=18) will be called redundant if the partial fission representation (MT=19, 20, 21, 38) is found. Space for the new material directory is then reserved (MFS, MTS, NCS). Section identification and card counts will be entered into these arrays as they are determined.

The next step is to read File 2, which contains resolved and unresolved resonance parameters (if any). The array RES is assigned to contain the File 2 data and RDFIL2 is called to read them. While the resonance parameters are being stored, RECONR adds each resonance energy to its list of energy nodes (ENODE). In the unresolved energy range, RECONR uses the energies of tabulated parameters or fission widths if available. If the evaluation uses energy-independent parameters, or if the energy steps between the nodes are too large, RDFIL2 creates additional node energies at a density of approximately 10 points per decade. Note that regions where the unresolved representation for an element overlaps the resolved or smooth ranges are found and marked by negative energy values. The energy nodes are sorted into order and duplications are removed. When control is returned to RECONR, any unused space in the RES array is released to be made available for other uses.

If unresolved data is present, subroutine GENUNR is called to compute the infinitely-dilute unresolved average cross sections on the unresolved energy grid using CSUNR1 or CSUNR2. Any backgrounds on File 3 are included, except in regions of resolved-unresolved or unresolved-smooth overlap. The computed cross sections are arranged in the order required by the special section with MF=2 and MT=152, which is written onto the PENDF tape by RECOUT. Using the normal ENDF style, this format is defined by the following:

```
[MAT,2,152/ZA,AWR,LSSF,0,0,INTUNR]HEAD
[MAT,2,152/0.,0.,5,1,NW,NUNR/
           E1,STOT1,SELAS1,SFIS1,SCAP1,STRN1,
           E2,STOT2,SELAS2,SFIS2,SCAP2,STRN2,
           ...
           ENUNR,STOTNUNR,....]LIST
```

where NW=6+6*NUNR. The definitions of the energy and cross section entries are fairly obvious, except STRN stands for the current-weighted total cross section. This format is specialized to "infinite dilution." The more general form used for self-shielded effective cross sections will be described in the UNRESR and GROUPR chapters of this manual.

The subroutine LUNION is used to linearize and unionize the ENDF data. Space is reserved for two buffers to be used by LOADA/FINDA and for the linearization stack (X and Y). The length of the stack (NDIM) determines the smallest possible subdivision of each panel (energy points as close as $2^{-\mathtt{NDIM}}$ times the panel width can be generated). Since the number of energies in the union grid may soon exceed the capacity of any reasonable memory array, the existing list of energy nodes is copied to binary scratch storage (the LOADA/FINDA). This storage system consists of the buffers BOLD and BNEW and the scratch units IOLD and INEW. The energy grid points will "ping-pong" back and forth between units 14 and 15 as the union grid is built up. Subroutine LUNION now starts with MT=2 and checks each reaction in sequence to determine whether the current grid (on IOLD) is sufficient to represent the reaction to within the desired tolerance using linear interpolation. If not, RECONR uses ISLIN1 to select the optimum points to be added to the new grid (on INEW). The units INEW and IOLD are swapped, and the next MT is processed. When all nonredundant reactions have been examined, the list of energies in LOADA/FINDA storage is the desired linearized and unionized grid. The storage used is released.

This grid is used as the starting point for resonance reconstruction in RESXS. Subroutine RESXS first reserves space for the LOADA/FINDA buffers BUFR and BUFG, the linearization stack (X and Y), and the partial cross sections (SIG). The length of the stack (NDIM) determines the smallest possible subdivision of a panel between two nodes (energy points as close a $2^{-\mathtt{NDIM}}$ times the panel width can be generated). Subroutine RESXS then examines the grid on NGRID (IOLD from LUNION) panel by panel. Grid points are added and cross sections computed until the convergence criteria discussed in Section C are satisfied. The cross sections are copied to NOUT using LOADA, and RESXS continues to the next panel. This procedure is continued until all panels are converged. The result is a tape (NOUT) containing the energy grid in the resonance region and the total, elastic, fission, and capture cross sections at each energy point.

Unionization is obtained automatically in the resonance region since the three partials are computed simultaneously in SIGMA. This routine calls CSNORP if there are no resonance parameters, CSSLBW for single-level Breit-Wigner parameters, CSMLBW for multilevel Breit-Wigner parameters, CSAA for multilevel Adler-Adler parameters, CSRMAT for Reich-Moore parameters, CSHYB for Hybrid R-Function parameters, and SIGUNR for unresolved resonance parameters. This last routine retrieves the cross sections from the table prepared by GENUNR. A special feature of RECONR is the ability to reconstruct the cross sections at TEMPR by $\psi\chi$ broadening if single-level Breit-Wigner (SLBW) or Adler-Adler (AA) parameters are given. The Doppler-broadened resonance shapes are obtained using QUICKW (see description in UNRESR) in CSSLBW or CSAA and the linearization procedure proceeds as before.

The resonance cross sections on NGRID are merged with the ENDF cross sections in EMERGE. First, the background grid from LUNION is merged with the resonance grid from RESXS and written onto the LOADA/FINDA file, which will accumulate the total cross section and any other redundant reactions required (IOLD/INEW). A loop is then set up over all nonredundant reactions. For each grid point, the ENDF background cross section is obtained by interpolation. If this grid point has a resonance contribution on NRES, it is added. The resulting net cross section at this point is added into the appropriate redundant cross sections on IOLD/INEW and also saved on NGRID. When all the energies for this reaction have been processed, the cross sections on NGRID are converted into a TAB1 record and written on NSCR. This loop is continued until all reactions have been processed. When EMERGE is finished, NSCR contains cross sections for all the nonredundant reactions, and IOLD contains the redundant summation reactions.

Control now passes to RECOUT, which writes the new File 1 comments and dictionary. It also writes a default version of the section with MF=2 and MT=151 that gives no resonance parameters. The upper limit of the resolved energy range, ERESH, is added to the "C2" field of the third card so that BROADR knows not to broaden into the unresolved energy range. For materials with unresolved data, a specially formatted section (MF=2, MT=152) is written containing the infinitely-dilute unresolved cross sections. This section can be used by BROADR and GROUPR to correct for resolved-unresolved overlap effects, if necessary. Subroutine RECOUT then steps through the reactions on NSCR and IOLD. Redundant reactions are converted to TAB1 records and inserted in the correct order. Nonredundant reactions are simply copied. Finally, a MEND record is added and control is returned to RECONR.

Now RECONR either directs that this process be repeated for another isotope or writes a TEND record and terminates. The result is a new tape in ENDF format containing the desired pointwise cross sections. Note that only Files 1, 2, 3, 10, and 13 are included for neutron tapes. Only Files 1 and 23 are included for photon tapes.

## F. Input Instructions

The input instructions for each module are given in the code as comment cards at the beginning of the source code for each module. The RECONR instructions are reproduced here for the convenience of the reader.

```
*---INPUT SPECIFICATIONS (FREE FORMAT)---------------------------*
*                                                                *
* CARD 1                                                         *
*    NENDF    UNIT FOR ENDF/B TAPE                               *
*    NPEND    UNIT FOR PENDF TAPE                                *
* CARD 2                                                         *
*    LABEL    66 CHARACTER LABEL FOR NEW PENDF TAPE              *
```

```
*             DELIMITED WITH *, ENDED WITH /.                     *
* CARD 3                                                          *
*    MAT      MATERIAL TO BE RECONSTRUCTED                        *
*    NCARDS   NUMBER OF CARDS OF DESCRIPTIVE DATA FOR NEW MF1     *
*             (DEFAULT=0.)                                        *
*    NGRID    NUMBER OF USER ENERGY GRID POINTS TO BE ADDED.      *
*             (DEFAULT=0.)                                        *
* CARD 4                                                          *
*    ERR      FRACTIONAL RECONSTRUCTION TOLERANCE USED WHEN       *
*             RESONANCE-INTEGRAL ERROR CRITERION (SEE ERRINT)     *
*             IS NOT SATISFIED.                                   *
*    TEMPR    RECONSTRUCTION TEMPERATURE (DEG KELVIN)             *
*             (DEFAULT=0.)                                        *
*    NDIGIT   NO. SIGNIFICANT DIGITS (DEFAULT=7)                  *
*    ERRMAX   FRACTIONAL RECONSTRUCTION TOLERANCE USED WHEN       *
*             RESONANCE-INTEGRAL ERROR CRITERION IS SATISFIED     *
*             (ERRMAX.GE.ERR, DEFAULT=20.*ERR)                    *
*    ERRINT   MAXIMUM RESONANCE-INTEGRAL ERROR (IN BARNS)         *
*             PER GRID POINT (DEFAULT=ERR/10000)                  *
*             (NOTE: THE MAX CROSS SECTION DIFFERENCE FOR         *
*              LINEARIZATION, ERRLIM, AND FOR RECONSTRUCTION,     *
*              ERRMIN, ARE ALSO TIED TO ERRINT.  TO GET MAXIMUM   *
*              ACCURACY, SET ERRINT TO A VERY SMALL NUMBER.       *
*              FOR ECONOMICAL PRODUCTION, USE THE DEFAULTS.)      *
* CARD 5                                                          *
*    CARDS    NCARDS OF DESCRIPTIVE COMMENTS FOR MT451            *
*             EACH CARD DELIMITED WITH *, ENDED WITH /.           *
* CARD 6                                                          *
*    ENODE    USERS ENERGY GRID POINTS                            *
*       CARDS 3, 4, 5, 6 MUST BE INPUT FOR EACH MATERIAL DESIRED *
*       MAT=0/ TERMINATES EXECUTION OF RECONR.                    *
*                                                                 *
*******************************************************************
```

A sample input for processing two isotopes from ENDF/B-IV Tape 407 follows (the line numbers are for reference only and are not part of the input):

```
 1.  0
 2.  4
 3.  RECONR
 4.  20 -21
 5.  *PENDF TAPE FOR U-235 AND PU239 FROM T407*/
 6.  1261 2/
 7.  .005/
 8.  *92-U-235 FROM T407*/
 9.  *PROCESSED WITH NJOY*/
10.  1264 2/
11.  .005/
12.  *94-PU-239 FROM T407*/
13.  *PROCESSED WITH NJOY*/
14.  0/
```

Card 4 tells RECONR that the input ENDF tape (Tape 407) will be on unit 20, and that the output PENDF tape will be on unit 21. Because of the minus sign, the PENDF tape will be in NJOY blocked-binary mode. The first MAT number (1261 for U-235) is given on Card 6, and the second one (1264 for Pu-239) is on card 10. In both cases, the reconstruction tolerance is 0.5% and the default integral thinning parameters are taken. Note the "0/" in line 14 that terminates the RECONR portion of the run. The resulting PENDF tape will contain the desired TAPEID card, followed by U235, a MEND card, PU-239, a MEND card, and a TEND card.

## G. Error Messages

`ERROR IN RECONR***ILLEGAL NSUB FOR RECONR`

RECONR only processes sublibraries that contain cross section data. Check whether the right input ENDF input tape was mounted.

`ERROR IN RUINA***ILLEGAL NDIGIT`

Value must be between 1 and 15 on a long-word machine, or between 1 and 7 on a short-word machine.

`ERROR IN ANLYZD***TOO MANY REDUNDANT REACTIONS`

Increase the size of `MTR(10)` in `/RECON/` and increase `MTMAX=10` in `RECONR`.

`ERROR IN RDFILE2***STORAGE IN ENODE EXCEEDED`

Too many energy nodes including the user's nodes and the energies from MF=2. Increase `NODMAX` in `RECONR`.

`ERROR IN RDFIL2***STORAGE IN A EXCEEDED`

Too much resonance data. The main container array is too small. Increase `/RSTORE/` and `JX` in `RECONR` or decrease buffer sizes `NBUFG`, `NBUFR`, or `NBUF`.

`ERROR IN RDFIL2***STORAGE IN EUNR EXCEEDED.`

The limit `MAXUNR=200` has been exceeded.

`ERROR IN RDFIL2***MLBW FICTITIOUS J VALUES NOT ALLOWED.`

This reflects an error in the evaluation.

`ERROR IN RDFIL2***ENERGY-DEPENDENT SCATTERING RADIUS NOT CODED.`

This option is not coded, nor is it allowed in ENDF/B-VI. Other national files may have different procedures.

`MESSAGE FROM RDFIL2***CALCULATION OF ANGULAR DISTRIBUTION NOT...`

This option is not yet available in RECONR.

`ERROR IN RDFIL2***HYBRID COMPETING REACTIONS NOT YET ADDED`

This option is not yet available in RECONR.

```
ERROR IN LUNION***ILL BEHAVED THRESHOLD
```

The routine is having trouble adjusting the threshold to agree with the Q value. Check the points near the threshold for this evaluation.

```
ERROR IN LUNION***EXCEEDED STACK
```

Increase length of linearization stack `NDIM` (currently 20).

```
ERROR IN ISLIN1***X1=--- GE X2=---
```

The interpolation interval is bad.

```
ERROR IN ISLIN1***XM=--- LE X1=---
```

```
ERROR IN ISLIN1***XM=--- GE X2=---
```

Desired point is outside the interpolation range.

```
ERROR IN RESXS***STACK EXCEEDED
```

Increase length of reconstruction stack `NDIM` (currently 20).

```
ERROR IN SIGMA***GENERAL R-MATRIX NOT INSTALLED.
```

This option is not yet available in RECONR.

```
ERROR IN SIGMA***ILLEGAL OPTION.
```

There is a problem with the ENDF tape.

```
ERROR IN CSMLBW***NOT CODED FOR TEMPERATURE GT 0 DEG K
```

The $\psi\chi$ Doppler-broadening option is only coded for single-level Breit-Wigner and Adler-Adler resonance parameters. Use `TEMPR`=0. only.

```
ERROR IN CSRMAT***NOT CODED FOR TEMPERATURE GT 0 DEG K
```

The $\psi\chi$ Doppler-broadening option is only coded for single-level Breit-Wigner and Adler-Adler resonance parameters. Use `TEMPR`=0. only.

```
ERROR IN CSHYBR***DOPPLER BROADENING NOT PROVIDED FOR HYBRID
```

The $\psi\chi$ Doppler-broadening option is only coded for single-level Breit-Wigner and Adler-Adler resonance parameters. Use `TEMPR`=0. only.

```
ERROR IN CSAA***BAD LI VALUE
```

There is an error in the evaluation format.

```
MESSAGE FROM EMERGE---NEGATIVE ELASTIC CROSS SECTIONS FOUND
```

Negative elastic cross sections can occur for SLBW evaluations.

```
ERROR IN RECOUT***FOR MF --- MT ---
```

Indexing and pair count for this section do not make sense.

## H. Input-Output Units

The following logical units are used:

| | |
|---|---|
| 10 | `NSCR1` in `RECONR`, `NOUT` in `LUNION`, and `NIN` in `EMERGE`. Contains copy of nonredundant sections from original ENDF tape. |
| 11 | `NSCR2` in `RECONR`; `NGRID` in `LUNION`, `RESXS`, and `EMERGE`. Contains union grid for ENDF tape (not counting resonances). |
| 12 | `NSCR3` in `RECONR`, `NOUT` in `RESXS`, and `NRES` in `EMERGE`. Contains resonance grid and cross sections. |
| 13 | `NSCR4` in `RECONR` is used for two separate purposes. In `RESXS` it is a binary scratch file `NSCR` used for the unthinned resonance data. In `EMERGE` and `RECOUT`, it is `NMERGE` and contains the nonredundant reactions on the union grid. |
| 14/15 | `IOLD/INEW` in `LUNION`. Are used locally only to accumulate union grid for ENDF cross sections. Destroy after use. |
| 14/15 | `IOLD/INEW` in `EMERGE`. Are used locally only to accumulate summation cross sections on union grid. |
| 20-99 | User's choice for NENDF and NPEND to link RECONR with other NJOY modules. |
| 5,6,7 | See the NJOY chapter for a description of the I/O units. |

Note that 11, 12, 14, and 15 are always binary. Unit 10 has the same mode as NENDF. Unit 13 is binary when used in RESXS, and it has the same mode as NPEND elsewhere. NPEND can have a different mode than NENDF.

## I. Storage Allocation

Storage allocation in RECONR is sensitive to (1) the amount of resonance parameter data, (2) the size of the resonance reconstruction stack, (3) the use of $\psi\chi$ broadening, and (4) the sizes of the `LOADA/FINDA` buffers. Other storage requirements are minor.

Buffer sizes can be reduced or increased at will. The result is a storage/speed tradeoff with no change in capability or accuracy. See `NBUFG=2000`, `NBUFR=2000`, and `NBUF=2000` in `RECONR`.

The $\psi\chi$ broadening option requires 7688 words of additional storage. Therefore, the container array in `/RSTORE/` can be reduced significantly if $\psi\chi$ is not required. No code changes are needed—just avoid `TEMPR` greater than zero.

Resonance reconstruction in `RESXS` uses 5×`NDIM` words. The parameter `NDIM` determines the smallest subdivision of a panel that can be obtained. Using `NDIM=20` allows points to be generated with spacing as small as one-millionth of the panel size ($2^{20}$).

## J. References


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**CONTENTS**