4 BROADR

BROADR module generates Doppler-broadened cross sections in PENDF format starting from piecewise linear cross sections in PENDF format. The input cross sections can be from RECONR or from a previous BROADR run. The code is based on SIGMA1[27] by D. E. Cullen. The method is often called "kernel broadening" because it uses a detailed integration of the integral equation defining the effective cross section. It is a fully accurate method, treating all resonance and non-resonance cross sections including multilevel effects. BROADR has the following features:

- An alternate calculation is used for low energies and high temperatures that corrects a numerical problem of the original SIGMA1. (This problem has been corrected in another way in later versions of SIGMA1.)
- Dynamic storage allocation is used, which allows the code to be run on large or small machines with full use of whatever storage is made available.
- Reactions are broadened in parallel on a union grid, with the top of the resolved resonance range being the typical upper limit for Doppler broadening.
- The union grid is constructed adaptively to give a linearized representation of the broadened cross section with tolerances consistent with those used in RECONR. Energy points may be added to or removed from the input grid as required for the best possible representation. Precision up to 9 significant figures is allowed for energies.
- The summation cross sections such as total, nonelastic, and sometimes fission or (n,2n) are reconstructed to equal the sum of their parts.
- Standard thermal cross sections, integrals, and ratios are computed when the temperature is 293.6K (0.0253 eV).
- The file directory (actually an index to the reactions present) is updated.

This chapter describes the BROADR module in NJOY2016.0.

4.1 Doppler-Broadening Theory

The effective cross section for a material at temperature T is defined to be that cross section that gives the same reaction rate for stationary target nuclei as the real cross section gives for moving nuclei. Therefore,

$$\rho v \overline{\sigma}(v,T) = \int d\mathbf{v}' \rho \, |\mathbf{v} - \mathbf{v}'| \, \sigma(|\mathbf{v} - \mathbf{v}'|) \, P(\mathbf{v}', T) \ , \tag{82}$$

where $\mathbf{v}$ is the velocity of the incident particles, $\mathbf{v}'$ is the velocity of the target, ρ is the density of target nuclei, σ is the cross section for stationary nuclei, and $P(\mathbf{v}', T)$ is the distribution of target velocities in the laboratory system. For many cases of interest, the target motion is isotropic and the distribution of velocities can be described by the Maxwell-Boltzmann function

$$P(\mathbf{v}', T)\, d\mathbf{v}' = \frac{\alpha^{3/2}}{\pi^{3/2}} \exp(-\alpha v'^2)\, d\mathbf{v}' \ , \tag{83}$$

where $\alpha = M/(2kT)$, k is Boltzmann's constant, and M is the target mass.

Eq. 82 can be partially integrated in terms of the relative speed $V = |\mathbf{v} - \mathbf{v}'|$ to give the standard form of the Doppler-broadened cross section:

$$\overline{\sigma}(v) = \frac{\alpha^{1/2}}{\phi^{1/2}\, v^2} \int_0^\infty dV\, \sigma(V)\, V^2 \left\{ \mathrm{e}^{-\alpha(V-v)^2} - \mathrm{e}^{-\alpha(V+v)^2} \right\} . \tag{84}$$

It is instructive to break this up into two parts:

$$\overline{\sigma}(v) = \sigma^*(v) - \sigma^*(-v) \ , \tag{85}$$

where

$$\sigma^*(v) = \frac{\alpha^{1/2}}{\pi^{1/2} v^2} \int_0^\infty dV\, \sigma(V)\, V^2\, \mathrm{e}^{-\alpha(V-v)^2} \ . \tag{86}$$

The exponential function in Eq. (86) limits the significant part of the integral to the range

$$v - \frac{4}{\sqrt{\alpha}} < V < v + \frac{4}{\sqrt{\alpha}}.$$

For $\sigma^*(-v)$, the integral depends only on velocities satisfying

$$0 \le V < \frac{4}{\sqrt{\alpha}}.$$

These results can be converted to energy units using

$$E_m = \frac{1}{2} m \left(\frac{4}{\sqrt{\alpha}}\right)^2 = \frac{16kT}{A}.$$

Some examples are given in Table 1. Doppler-broadening effects will be important below this energy and for any features such as resonances, thresholds, or artificial discontinuities in evaluations that are not slowly varying with respect to $2\sqrt{E_m E}$. As an example, for ^{235}U at 100 eV, Doppler effects are important for features smaller than about 0.8 eV.

Table 1: Energy Parameter for Effective Doppler-Broadening

Target	Temperature	Energy Parameter (E_m)
^{2}H	300K	0.2 eV
^{235}U	300K	0.0017 eV
^{235}U	1.0 keV	69 eV

The numerical evaluation of Eq. (86) developed for SIGMA1 assumes that the cross section can be represented by a piecewise linear function of energy to acceptable accuracy. This is just the form of the NJOY PENDF files (see RECONR). Defining the reduced variables $y = \sqrt{\alpha x}$ and $x = \sqrt{\alpha V}$, the cross section becomes

$$\sigma(x) = \sigma_i + s_i(x^2 - x_i^2) \ , \tag{87}$$

with slope $s_i = (\sigma_{i+1} - \sigma_i)/(x_{i+1}^2 - x_i^2)$. Eq. (86) can now be written as

$$\sigma^*(y) = \frac{1}{\pi^{1/2} y^2} \sum_{i=0}^{N} \int_{x_i}^{x_{i+1}} \sigma(x)\, x^2 \mathrm{e}^{-(x-y)^2} dx = \sum_i \left\{ A_i \left[\sigma_i - s_i x_i^2\right] + B_i s_i \right\} \ , \tag{88}$$

where

$$\begin{aligned} x_0 &= 0 \ , \\ x_{N+1} &= \infty \ , \\ A_i &= \frac{1}{y^2} H_2 + \frac{2}{y} H_1 + H_0 \ , \text{ and} \\ B_i &= \frac{1}{y^2} H_4 + \frac{4}{y} H_3 + 6H_2 + 4yH_1 + y^2 H_0 \ , \end{aligned}$$

and where H_n is shorthand for $H_n(x_i - y, x_{i+1} - y)$. The extrapolations to zero and infinity assume a constant cross section ($s_0 = s_N = 0$). The H functions are the incomplete probability integrals defined by

$$H_n(a,b) = \frac{1}{\sqrt{\pi}} \int_a^b z^n \, \mathrm{e}^{-z^2} \, dz \ . \tag{89}$$

These functions can be computed in two ways. First,

$$H_n(a,b) = F_n(a) - F_n(b) \ , \tag{90}$$

where

$$F_n(a) = \frac{1}{\sqrt{\pi}} \int_a^\infty z^n \, \mathrm{e}^{-z^2} \, dz \ . \tag{91}$$

These functions satisfy a recursion relation that can be used to obtain

$$F_0(a) = \frac{1}{2}\mathrm{erfc}(a) \ , \tag{92}$$

$$F_1(a) = \frac{1}{2\sqrt{\pi}} \exp(-a^2) \ , \text{ and} \tag{93}$$

$$F_n(a) = \frac{n-1}{2} F_{n-2}(a) + a^{n-1} F_1(a) \ , \tag{94}$$

where $\mathrm{erfc}(a)$ denotes the complementary error function

$$\mathrm{erfc}(a) = \frac{2}{\sqrt{\pi}} \int_a^\infty \mathrm{e}^{-z^2} dz \ . \tag{95}$$

However, when $F_n(a) \approx F_n(b)$, the difference in Eq. (90) may lose significance. In such cases, $H_n(a,b)$ can be computed by a second method based on a direct Taylor expansion of the defining integral. Write

$$H_n(a,b) = \frac{1}{\sqrt{\pi}} \int_0^b z^n \mathrm{e}^{-z} dz - \frac{1}{\sqrt{\pi}} \int_0^a z^n \mathrm{e}^{-z^2} dz = G_n(b) - G_n(a) \ . \tag{96}$$

But by Taylor's Theorem,

$$G_n(b) - G_n(a) = \frac{b-a}{1!} G_n'(a) + ... + \frac{(b-a)^m}{m!} G_n^{(m)}(a) + ... \, . \tag{97}$$

Also,

$$G_n^{(m)}(x) = \frac{d^{m-1}}{dx^{m-1}} \left[x^n \mathrm{e}^{-x^2} \right] = \mathrm{e}^{-x^2} P_n^m(x) \, , \tag{98}$$

where $P_n^m(x)$ is a polynomial with recursion relation

$$P_n^m(x) = \frac{d}{dx} P_n^{m-1}(x) - 2x P_n^{m-1}(x) \ , \tag{99}$$

with $P_n^1 = x^n$. From this point, it is straightforward to generate terms until the desired number of significant figures is obtained.

When interpreting BROADR output, it is useful to remember several important features of the Doppler-broadening process. A $1/v$ cross section remains unchanged. Contrary to "popular knowledge", the area under a resonance does not remain unchanged unless $E \gg kT/A$. In fact, each resonance develops a new $1/v$ tail. Finally, a constant cross section (for example, elastic scattering)

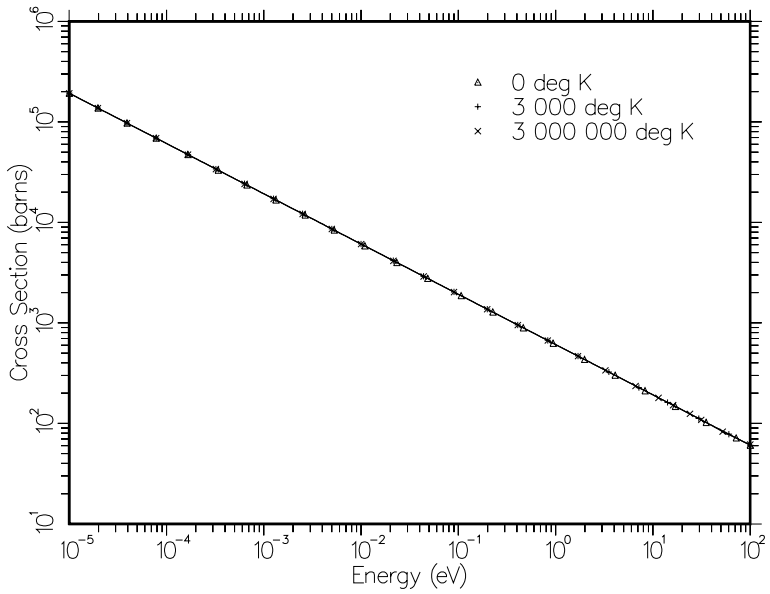

Figure 4: The (n,α) cross section for ^{10}B from ENDF/B-V for three different temperatures showing that a $1/v$ cross section is invariant under Doppler-broadening.

develops a $1/v$ tail at low energies after Doppler-broadening. These effects are shown in Figs. 4, 5, and 6; they can be best understood by noting that the Doppler process preserves reaction rate $v\sigma(v)$ according to Eq. (82), and a finite reaction rate is expected for $T > 0$K even as $v \to 0$.

Very early (1980s) versions of BROADR and SIGMA1 assumed that the input energy grid from RECONR could also be used to represent the Doppler-broadened cross section before thinning. The grid was then thinned to take advantage of the smoothing effect of Doppler broadening. Unfortunately, this assumption is inadequate. The reconstruction process in RECONR places many points near the center of a resonance to represent its sharp sides. After broadening, the cross section in this energy region becomes rather smooth; the sharp sides are moved out to energies where RECONR provides few points. At still higher energies, the resonance line shape returns to its asymptotic value, and the RECONR grid is adequate once more. The more recent versions of BROADR check the cross section between points of the incoming energy grid, and add additional grid points if they are necessary to represent the broadened line shape to the desired accuracy. This effect is illustrated in Fig. 7.

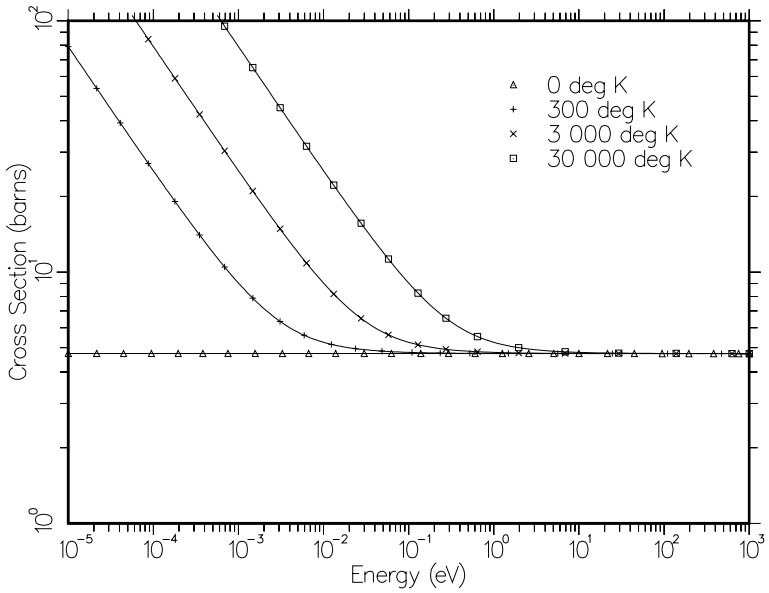

Figure 5: The elastic cross section for carbon from ENDF/B-V showing that Doppler-broadening a constant cross section adds a $1/v$ tail.

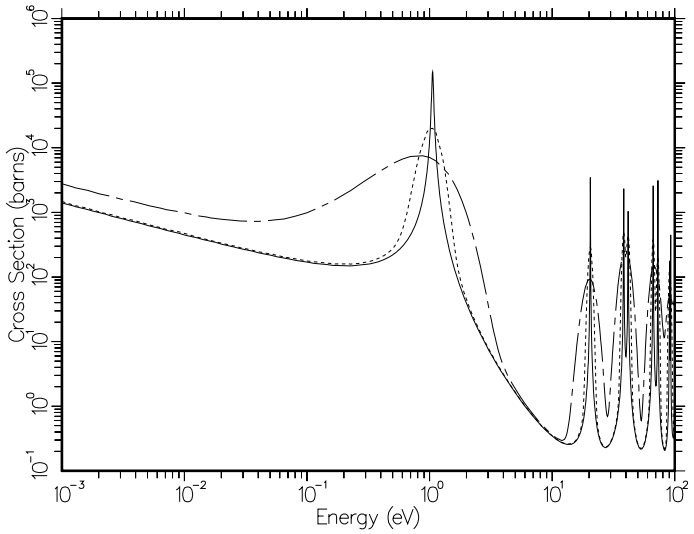

Figure 6: The (n,γ) cross section for ^{240}Pu for several temperatures showing the effects of Doppler broadening on resonances. The temperatures are 0K (solid), 30 000K (dotted), and 300 000K (dash-dot). The higher resonances behave in the classical manner even at 30 000K; note that the line shape returns to the asymptotic value in the wings of the resonance. All resonances at 300 000K (and to a lesser extent the first resonance for 30 000K) show the additional $1/v$ component that appears when kT/A is large with respect to the resonance energy.

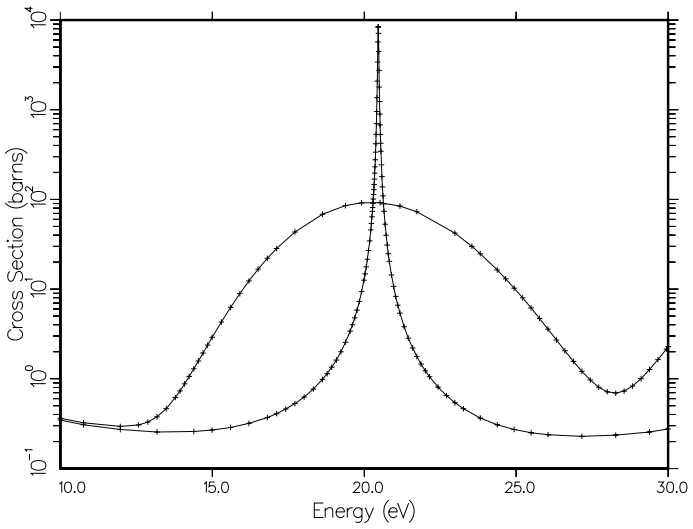

Figure 7: An expanded plot of the 20 eV resonance from Fig. 6 showing both thinning and "thickening" of the energy grid produced adaptively by BROADR. The two curves show the capture cross section at 0K and 300 000K. Note that the high-temperature curve has fewer points than the 0K curve near the peak at 20 eV and more points in the wings near 15 eV and 25 eV. Clearly, using the 0K grid to represent the broadened cross section in the wings of this resonance would give poor results.

4.2 Thermal Quantities

In thermal-reactor work, people make very effective use of a few standard thermal constants to characterize nuclear systems. These parameters include the cross sections at the standard thermal value of 0.0253 eV (2200 m/s), the integrals of the cross sections against a Maxwellian distribution for 0.0253 eV, the g-factors (which express the ratio between a Maxwellian integral and the corresponding thermal cross section), η, α, and K1. Here, η is the Maxwellian-weighted average of $(\bar{\nu})\sigma_f)/(\sigma_f+\sigma_c)$, α is the average of σ_c/σ_f, and K1 is the average of $(\bar{\nu}-1)\sigma_f-\sigma_c$. If BROADR is run for a temperature close to 293.6K (which is equivalent to 0.0253 eV), these thermal quantities are automatically calculated and displayed. Here is a sample output for ^{235}U from ENDF/B-VII:

```
thermal quantities at 293.6 K = 0.0253 eV
----------------------------------------
       thermal fission xsec:  5.8490E+02
      thermal fission nubar:  2.4367E+00
       thermal capture xsec:  9.8665E+01
```

```
      thermal capture g-factor:  9.9086E-01
      thermal capture integral:  8.6639E+01
    capture resonance integral:  1.4043E+02
      thermal fission integral:  5.0605E+02
      thermal fission g-factor:  9.7628E-01
        thermal alpha integral:  1.6828E-01
          thermal eta integral:  2.0859E+00
           thermal k1 integral:  6.4040E+02
                 equivalent k1:  7.2262E+02
    fission resonance integral:  2.7596E+02
   ----------------------------------------
```

4.3 Data-Paging Methodology

A piecewise linear representation of a reaction cross section of a resonance material may require a very large number of energy points. For example, ENDF/B-VII ^{238}U (MAT9237) requires 167 000 points for the total cross section for 0.1% precision (`errmax`=`err`). It is impractical to load all these points into memory simultaneously. However, the discussion following Eq. (86) in the theory section shows that only a limited energy range around the point of interest is required.

The strategy used is to stage the cross-section data into three "pages" of `npage` points each. Points in the center page can then be broadened using the `npage` or more points on each side of the point of interest. If $v - 4/\sqrt{\alpha}$ and $v + 4/\sqrt{\alpha}$ are both included in the three-page range, accurate broadening can be performed. If not, a diagnostic warning is printed; the user should repeat the calculation with a smaller temperature step or a larger page size.

There are many different reaction cross sections for each material. However, the cross sections for high velocities are normally smooth with respect to $32kT/A$ for any temperatures outside of stellar photospheres; therefore, they do not show significant Doppler effects. Until recently the upper energy limit for Doppler broadening was the smallest of (i) the input value `thnmax`, (ii) the upper limit of the resolved-resonance energy range, (iii) the lowest threshold, or (iv) 1.0 MeV (the default input value for `thnmax`). No Doppler broadening or energy-grid reconstruction is performed above that energy. In the past, and what users typically expect as the default action, the second condition often set the Doppler broadening upper limit.

However recent evaluated files have increasingly included threshold reactions at energies within the resolved resonance energy range. For example, recent

JENDL evaluations for ^{235}U include a resolved-resonance range upper limit of 2.25 keV, but also include non-zero cross sections for an inelastic level with a 77 eV threshold. Under the rules itemized above, Doppler broadening of these data stops at 77 eV. Other evaluations (*e.g.*, ENDF/B-VI, ENDF/B-VII and JEFF-3.1) share the same resolved-resonance range data but have zeroed out this inelastic cross section from 77 eV to 2.25 keV and so Doppler broadening of these files occurs throughout the resolved-resonance range, as most users expect.

Zeroing out non-zero data is a cludge from the past and so we have changed the Doppler upper energy limit logic so that the top of the resolved resonance range is now the default condition. This means that non-threshold reactions are also Doppler broadened. The mathematics of this operation can produce non-zero cross sections at energies below the reaction threshold. If this occurs those cross sections are zeroed.

As noted in the BROADR module source code comments, users may specify a negative value for `thnmax` to override these selection rules and force Doppler broadening to an upper energy of `abs(thnmax)` eV. This has been a long-term NJOY feature that remains unchanged in NJOY2016.

Finally, we note that the A_i and B_i factors in Eq. (88) depend only on the energy (or velocity) values and not on the cross sections. Since the A_i and B_i are expensive to compute, the code computes them only once for the points of a unionized energy grid. The sum of Eq. (88) is accumulated for all the non-threshold reactions simultaneously. This feature helps make BROADR run faster.

4.4 Coding Details

The main subroutine for BROADR is `broadr` from module `broadm`. The code begins by reading the user's input (see Section 4.5). Storage is then allocated for the `loada/finda` buffers (`ibufo` and `ibufn`) and for the scratch storage (`iscr`). The buffer length `nbuf` can be changed at will (currently `nbuf` is 1000).

The input PENDF tape is searched for the desired material (`mat1`). If the restart option is set (`istart`=1), the temperatures less than or equal to `temp1` for `mat1` are assumed to have been broadened previously, and they are copied to the output file. In either case, the files for `temp1` are copied to a scratch file on unit `nscr1`.

Next, `nscr1` is rewound and examined reaction by reaction. The energy grid from the total cross section (MT1) is saved on scratch storage using `loada`. If the input tape has not been through RECONR, the BROADR module will still

run, but at possibly reduced accuracy. The next low-threshold reaction (that is, the next reaction with a threshold less than `emin`, which is currently 1 eV) is located on `nscr1`. The energy points are retrieved from scratch file `iold` (12 or 13) using `finda`, the cross sections for this reaction are computed on this grid, and the results are stored on scratch file `inew` (13 or 12) using `loada`. The units for `iold` and `inew` are then exchanged, and the entire process is repeated for the next low-threshold reaction.

The final result of this process is a list of `nreac` low-threshold-reaction types in `mtr` (usually MT2, MT18, and MT102), the threshold value for the first high-threshold reaction (or the input value) in `thnmax`, and scratch file `iold` containing the energy grid and all the low-threshold reactions (there are `n2in` points).

Now that the number of reactions to be broadened simultaneously is known (`nreac`), storage for data paging can be assigned. The total amount of storage available is `namax`. The value of `namax` should be as large as possible (current value is 15 000 000). This space is divided up into the largest possible page size, `npage`. An overflow region `nstack` is also allocated. Now that the page size is known, the code allocates three pages for energies (`e`), three pages for each reaction cross section (`s`), one extended page for the broadened energy grid (`eb`), and three extended pages for the broadened cross section (`sb`). This system is designed to use the available storage with maximum efficiency.

The cross sections on `iold` are now broadened by `bfile3` (see below) and the results are written on scratch unit `inew` using `loada`.

The directory from `nscr1` is revised to reflect any thinning or thickening and written on the output PENDF tape (`nout`). Note that the new temperature is written into the first word of the Hollerith data record to simplify later searching.

The broadened cross sections are now converted into ENDF TAB1 records and merged with the unbroadened cross sections on `nscr1`. The total cross section (and sometimes nonelastic, inelastic, fission, (n,2n), or charged-particle reactions) is reconstructed to equal the sum of its parts. The new Doppler-broadened "MAT" on `NOUT` is a legal PENDF file with the same MAT number as the original data but with a new temperature.

The process is now repeated for each of the `ntemp2` final temperatures `temp2` requested. Note that after each step `inew` contains the new data and `iold` contains the previous data. If the "bootstrap" option is set (`istrap`=1), these units are interchanged. For this option, `stemp2(it)` is always obtained from `temp2(it-1)`. Because of the thinning effect of Doppler-broadening, the broadening runs faster at each step. The accumulation of error is usually not a prob-

lem. For istrap=0, temp1 is used for the starting temperature every time.

The broadening and energy-grid reconstruction are directed by bfile3 . The routine loads data into the appropriate memory pages from scratch file iold and then either calls broadn to broaden it (with thinning or thickening of the grid as necessary) or calls thinb to thin it without broadening. The results are written onto scratch file inew.

In broadn, the energy grid points just loaded into e by bfile3 are converted to the dimensionless variables x and y [see Eq. (87)]. An adaptive reconstruction of the Doppler broadened cross section is then performed for the energy range in the center page using an inverted stack algorithm like the one described for RECONR. The upper limit of each panel is taken to be a point from the input grid, but in order to allow for thinning, up to nmax=10 of the input grid points can be skipped before the actual upper limit is selected. In addition, the energy of the upper limit cannot be more than step=2.01 times the energy of the preceding point. The cross sections are now computed at the midpoint of the top panel in the stack using bsigma. If the results differ from the values obtained by interpolation by more than the specified tolerance, the new point is added to the stack, and the tests are repeated. Otherwise, the top point in the stack is converged. A backward check is made to see if some of the previous points can be removed based on the new value, the new value is stored in the output array, and the height of the stack is reduced by one. The routine now tries to subdivide the new panel at the top of the stack in the same way. When the stack has been reduced to one element, a new upper limit is chosen from the input energy grid as described above, and the entire process is repeated. The reconstruction logic in BROADR uses the same integral tests as RECONR. Refer to the RECONR chapter for more details.

Subroutine bsigma is used to calculate the actual broadened cross section at an energy point using the data in the three pages. First, the routine locates the energy panel containing the desired energy en. It then loops over intervals below the current point adding in contributions to $\bar{\sigma}$ from the $V-v$ term of Eq. (84) until the contributions to the cross section become small. If the lower limit of the bottom page is reached before convergence, a warning message is issued. The routine then loops over intervals above the current point until convergence. Once again, a warning is issued if necessary. Finally, the low-energy term [the one involving $V+v$ in Eq. (84)] is added, if applicable.

Subroutine thinb is provided for cases where the input cross section set is to be thinned only. This routine uses the original SIGMA1 method. The first

input point is always kept. The routine then loops over higher energy values. For each grid point, all the points from there back to the last accepted point are checked for their deviation from a straight line. If they all can be removed without violating the specified tolerance, the interval is extended to the next higher point and the tests are repeated. If any point in the range is too far from the linear approximation, the last point in the range is accepted as an output point, and the testing process is repeated starting from this new lower limit. The procedure terminates when all of the points in the middle page have been thinned, and control is returned to `bfile3` to get the next page of data. Thinning may have been a necessary feature in the past when computing resources were limited but is a rarely used feature today.

Subroutine `hunky` has been modified from the original SIGMA1 version to implement the alternate $H_n(a,b)$ calculation when necessary (see `hnabb`). When using the direct method, F_n values from the previous step are used in the difference of Eq. (90), and `funky` is called to get the new values. The A_i and B_i of Eq. (88) are related to the `s1` and `s2` here.

Subroutine `funky` evaluates $F_n(a)$ by the recursion formula of Eq. (94) using the very accurate SLATEC version of the reduced complementary error function from the NJOY2016 math module.

Function `hnabb` implements the alternate calculation described by Eqs. (96)-(99). The series expansion is continued until about six significant figures are guaranteed (see `eps` and `hnabb`). Currently, `hnabb` is called when only four significant figures are reliable in `hunky` (see `toler` in `hunky`).

4.5 User Input

The following input instructions have been copied from the comment cards at the start of BROADR.

```
!---input specifications (free format)--------------------------
!
! card 1
!    nendf    input endf tape (for thermal nubar only)
!    nin      input pendf tape
!    nout     output pendf tape
!
! card 2
!    mat1     material to broadened and thinned
!    ntemp2   number of final temperatures (default=1)
```

```
!    istart   restart (0 no, 1 yes, default 0)
!    istrap   bootstrap (0 no, 1 yes, default 0
!    temp1    starting temperature from nin (default=0K)
!
! card 3
!    errthn   fractional tolerance for thinning
!    thnmax   max. energy for broadening and thinning
!             (default=1 MeV)
!    errmax   fractional tolerance used when integral criterion
!             is satisfied (same usage as in reconr)
!             (errmax.ge.errthn, default=10*errthn)
!    errint   parameter to control integral thinning
!             (usage as in reconr) (default=errthn/20000)
!             set very small to turn off integral thinning.
!      (A good choice for the convergence parameters
!       errthn, errmax, and errint is the same set of
!       values used in reconr)
!
! card 4
!    temp2    final temperatures (deg Kelvin)
!
! card 5
!    mat1     next MAT number to be processed with these
!             parameters.  Terminate with mat1=0.
!
!---input options-------------------------------------------------
!
! The output tape will contain the ntemp2 final temperatures
! specified.  It is necessary to have temp1.le.temp2(1).
! if temp2.eq.temp1, the data will be thinned only.
!
! restart    Continue broadening an existing pendf tape.  All
!            temperatures are copied through temp1.  Additional
!            final temperatures are added by starting with the
!            data at temp1.
!
! bootstrap  If bootstrap is not requested, each final tempera-
!            ture is generated by broadening directly from temp1
!            to temp2.  If bootstrap is requested, each final temp-
!            erature is broadened from the preceding temperature.
!            Bootstrapping is faster due to the thinning in the
!            previous step.  However, errors accumulate.
```

```
!
! thnmax     A possible upper limit for broadening and thinning.
!            The actual upper limit is the lowest of (i) this input
!            value; (ii) the end of the resolved resonance range;
!            (iii) the lowest reaction threshold; or (iv) 1.0 MeV.
!
!            A negative value for thnmax forces the Doppler
!            broadening upper limit to be abs(thnmax) irrespective
!            of the other conditions.
!
!            Caution:  this may cause one or more threshold
!            reactions to be broadened.  The magnitude of
!            thnmax must be chosen to keep the number of
!            broadenable reactions less than or equal to the
!            maximum of ntt (160).
!
!            Caution: for use in transport codes, it is recommended
!            to use the program default.  We don't know how
!            to compute the spectrum of scattered neutrons from
!            a broadened inelastic level in the current generation
!            of codes.  Broadened cross sections for threshold
!            reactions may be useful for other purposes.
!
!-----------------------------------------------------------------
```

Note that `temp1` need not occur on `nout` if `istart`=0. The restart option (`istart`=1) enables the user to add new temperatures to the end of an existing PENDF tape. This option is also useful if a job runs out of time while processing, for example, the fifth temperature in a job requesting six or more final temperatures. The job can be restarted from the `nout`. The first four temperatures will be copied to the new `nout` and broadening will continue for temperature five. The bootstrap option speeds up the code by using the broadened result for `temp2(i-1)` as the starting point to obtain `temp2(i)`. The `thnmax` parameters can be used to speed up a calculation or to prevent the broadening of inappropriate data such as sharp steps or triangles in an evaluated cross section (for example, ENDF/B-V lead).

The following example prepares a broadened PENDF file for ^{235}U from ENDF/B-VII at two temperatures. The line numbers are for reference only; they are not part of the input.

```
1.  broadr
2.  20 21 22/
3.  9228 2/
4.  .001/
5.  300. 1200./
6.  0/
```

On line 2, unit 20 should contain the ENDF file and unit 21 should a RECONR-generated ASCII PENDF file of 0K cross sections for the isotope. Two materials will be generated on unit 21 with 0.1% accuracy. First will be the 300K data, followed by a MEND record, followed by the 1200K data, followed by MEND and and TEND records. Best results are obtained when the error tolerance `errthn` and the optional integral-thinning controls `errmax` and `errint` are the same as those used for the RECONR run.

4.6 Error Messages

`error in broadr***nin and nout must be same mode`
: Use coded to coded, or blocked binary to blocked binary. The latter is faster due to the several tape copies performed in BROADR.

`error in broadr***max. energy too large ...`
: The user requested Doppler broadening to an energy beyond the maximum energy in the ENDF file.

`error in broadr***too many low threshold reactions`
: The current limit is set by the global parameter `ntt`=180. Check `tt`, `mtr`, and `ntt` in `broadr`, `tt` in `bfile3`, and `sbt` in `broadn`.

`message from broadr--desired mat and temp not on tape`
: Check the input PENDF file and the user input.

`message from broadr--no broadenable reactions`
: No low threshold reactions were found.

`error in broadr***storage exceeded`
: Insufficient storage to update directory. Increase `nwscr`=1000 in `broadr`.

`message from stounx--sigma zero data removed ...`
: The input PENDF tape already contained a special unresolved section in File 2. It has been removed. Rerun UNRESR if necessary.

`message from bsigma--broadening truncated at a=--`

The page is too small for the temperature difference requested. Increase total storage available (`namax`) or repeat the calculation with smaller temperature steps and `istrap`=1. The normal maximum size of `a` is 4.0 and `a` is inversely proportional to $T_i - T_{i-1}$.

4.7 Input/Output Units

The following units are used for input and output by BROADR.

10	`nscr1` in BROADR. Contains the ENDF/B data at the initial temperature.
12/13	`iold/inew` in BROADR. Contains union grid and low threshold reactions.
20-99	User's choice for `nin` and `nout` to link with other modules.

Units 12 and 13 will always be binary. Unit 10 will have the same mode as `nin` and `nout`.

4.8 Storage Allocation

All storage is divided in the most efficient way possible. The container array size `namax` should be made as large as possible. The value of `nbuf` can be increased or decreased at will — larger values will give faster execution. The value for `nwscr` depends on the size of the ENDF/B dictionary, and 1000 words is sufficient for all current evaluations.