V.A. RECONSTRUCTING POINT-WISE CROSS SECTIONS

SAMMY'S main purpose is to analyze neutron-induced cross section data by fitting to R-matrix parameters; in that mode, the user provides an energy grid (the experimental grid) from which an auxiliary grid can be constructed as discussed in Sections III.A.1 and III.A.2. To calculate a cross section directly from the resonance parameters without any pre-defined energy grid, one would use a nuclear data processor code such as AMPX [MD02], NJOY [RM82], or PREPRO [DC04]; these codes were designed to create energy grids that would describe the unbroadened cross sections with sufficient accuracy for essentially any purpose.

Occasionally, however, it is desirable to have SAMMY generate point-wise cross sections without a pre-existing energy grid. SAMMY has two methods of accomplishing this, as described below. The user should be aware that the energy grids generated in SAMMY will provide a means of viewing the cross sections but are not intended to be highly accurate representations of all the structure in the cross sections.

Method 1

The first method, borrowed almost directly from the processing code NJOY [RM82], uses a convergence algorithm to choose an energy grid sufficiently dense to properly define total, elastic, and capture cross sections, as well as fission if needed. The output ODF (plot) file SAMMY.ODF contains energies in Section 1, total cross section in Section 2, elastic cross section in Section 3, capture cross section in Section 4, and reaction cross section in Sections 5 if needed; Section 6 holds the absorption cross section (sum of capture plus reaction cross sections). These cross sections are unbroadened (zero temperature). To invoke this option, include the phrase

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RECONSTRUCT CROSS SEctions from resonance parameters
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in card set 3 of the INPut file (see Section VI.A of this report). SAMMY will ask for the data file name, as always, but a dummy name may be given since that information is never used.

Caveat: This method makes use of the Reich-Moore approximation to R-Matrix theory. It cannot be used with MLBW or SLBW resonance parameters.

Several criteria are used in the RECONSTRUCT option to assure that the energy grid is sufficiently dense. An initial grid consists of beginning and ending points plus all resonance energies within the specified energy range. Beginning at the lowest energy, each pair of points $\sigma_a = \sigma\left(E_a\right)$ and $\sigma_b = \sigma\left(E_b\right)$ is examined to see whether these two points alone can describe the midpoint between those two points $\sigma_m = \sigma\left(E_m = \frac{1}{2}\left(E_a + E_b\right)\right)$. Convergence is assumed only if each type of cross section (elastic, capture, and reaction) separately meets one of the criteria.

Criterion # 1. If both σ_a and σ_b are smaller than SIGMIN, points *a* and *b* are sufficient. The value for SIGMIN is an input parameter whose default is 10^{-6} barns.

Criterion # 2. For large changes in the cross sections ($\sigma_a > 1.4\sigma_b$ or $\sigma_b > 1.4\sigma_a$), the midpoint is added to the energy grid.

Criterion # 3. Let $\sigma_{m,\text{int}}$ represent the interpolated cross section at E_m; $\sigma_{m,\text{int}}$ is given by

$$\sigma_{m,\text{int}} = \frac{E_b - E_m}{E_b - E_a}\sigma_a + \frac{E_m - E_a}{E_b - E_a}\sigma_b \quad . \qquad \text{(V A.1)}$$

If σ_m is smaller than both σ_a and σ_b (so that the mid point is near a minimum in the cross section), the convergence requirement is

$$\left|\sigma_b - \sigma_{b,\text{int}}\right| \le \left|\sigma_b\right| \times \text{ERRXC2}/10 \quad . \tag{V A.2}$$

where ERRXC2 is an input parameter whose default value is 0.005.

Criterion # 4. If σ_m is not smaller than both σ_a and σ_b, the criterion is less stringent.

$$\left|\sigma_b - \sigma_{b,\text{int}}\right| \le \left|\sigma_b\right| \times \text{ERRXC2} \quad . \tag{V A.3}$$

The convergence parameters ERRXC2 and SIGMIN may be specified by the user to have different values from the default values of 0.005 and 10^{-6} barns respectively. See card set 7 of the INPut file (Table VI A.1).

Method 2

SAMMY's second option for generating point-wise cross sections without specifying an energy grid *a priori* makes use of SAMMY's ability to choose an auxiliary grid that properly defines the unbroadened cross section (see Section III.A). The user must provide some kind of a "data file," but it need not necessarily be appropriate for the nuclide(s) being considered; it is used only as a starting point for the auxiliary grid. SAMMY first sets up a grid of NEPNTS from EMIN to EMAX; NEPNTS is specified on card set 2 of the INPut file (see Table VI A.1). This grid is evenly spaced in velocity space (i.e., in the square root of energy). SAMMY then chooses additional points for the auxiliary grid as though broadening were to occur.

To invoke this option include the phrases

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ARTIFICIAL ENERGY GRid is needed
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and

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PUT UNBROADENED CROSs sections into plot file
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in the INPut file. An output plot file SAMMY.UNB contains energies in section 1 and cross section in section 2. (Note that the name of this file is no longer SAMXAC.ODF, to avoid confusion about which file is produced when.) A second file, SAMMY.DAT, contains the same information in SAMMY's TWENTY data format.

Unlike the RECONSTRUCT method of generating an energy grid, this method evaluates only the one type of cross section specified in the INPut file. Also unlike the first method, any of the several R-matrix approximations may be used, as specified in the INPut file.

Both methods

Examples of reconstructing point-wise cross sections using both of these methods can be found in several test cases. See, specifically, tr037 for "pure" reconstruction, and tr042, tr049, and tr175 for reconstruction followed by computation of stellar (Maxwellian) averages (see Section V.D).

Finally, it should be noted that, prior to release 7.0.1 of the SAMMY code, the implementation of method 1 would occasionally produce unrealistic values of stellar averages.