

V.C.2. Bondarenko-Weighted Averages

The general definition of the flux-weighted multigroup cross section is

$$\bar{\sigma}_{x,i} = \int_{E_i^l}^{E_{i+1}^g} \sigma_x(E) \Phi(E) dE \bigg/ \int_{E_i^l}^{E_{i+1}^g} \Phi(E) dE \quad , \quad (\text{V C2.1})$$

in which subscript x indicates the particular type of cross section (e.g. capture, fission, total). (Superscript g on the energy limits is used to distinguish these energies from the energies E_i of the experimental grid.) The flux $\Phi(E)$ is the energy-dependent neutron flux. Since this flux is not known, the Bondarenko narrow-resonance scheme [IB64] is often used. This scheme is defined as

$$\bar{\sigma}_{x,i} = \int_{E_i^l}^{E_{i+1}^g} \frac{\sigma_x(E) C(E)}{\sigma_{tot}(E) + \sigma_0} dE \bigg/ \int_{E_i^l}^{E_{i+1}^g} \frac{C(E)}{\sigma_{tot}(E) + \sigma_0} dE \quad , \quad (\text{V C2.2})$$

in which σ_{tot} is the total cross section, σ_0 is an energy-independent constant, and $C(E)$ is a smooth function of energy. Currently in SAMMY, $C(E)$ may be expressed as a piece-wise linear function of energy; see Section VI.F.1 for input options.

(The limit in which C is constant and σ_0 is effectively infinite, while it has little practical application, may be useful for comparison purpose. This limit may be written as

$$\bar{\sigma}_{x,i} = \int_{E_i^l}^{E_{i+1}^g} \sigma_x(E) dE \bigg/ \int_{E_i^l}^{E_{i+1}^g} dE \quad ; \quad (\text{V C2.3})$$

this is the form discussed in Section V.C.3 as the “unweighted energy average” option. While a large value of σ_0 and constant C can be used with the Bondarenko option to calculate this quantity, that method is highly inefficient. Instead, it is recommended that the option described in Section V.C.3 be used.)

Evaluation of the integrals in Eq. (V C2.2) is performed in similar manner to that described in Section III.A for numerical integration of the Doppler and resolution-broadening functions. However, unlike the integrations needed for those operations, here the integrand does not approach zero at the end points. The integration scheme is therefore modified at the end points to use the exact limit.

In addition to the calculating the multigroup cross sections, it is also necessary to generate the associated covariance matrix. This is accomplished by first taking small increments

$$\delta \bar{\sigma}_{x,i} = \sum_k \frac{\partial \bar{\sigma}_{x,i}}{\partial u_k} \delta u_k \quad , \quad (\text{V C2.4})$$

where u represents the resonance parameters. The covariance matrix is then found by taking expectation values

$$\begin{aligned} C_{xx'ij} &= \langle \delta \bar{\sigma}_{x,i} \delta \bar{\sigma}_{x',j} \rangle = \sum_{k,k'} \frac{\partial \bar{\sigma}_{x,i}}{\partial u_k} \langle \delta u_k \delta u_{k'} \rangle \frac{\partial \bar{\sigma}_{x',j}}{\partial u_{k'}} \\ &= \sum_{k,k'} \frac{\partial \bar{\sigma}_{x,i}}{\partial u_k} M_{kk'} \frac{\partial \bar{\sigma}_{x',j}}{\partial u_{k'}} , \end{aligned} \quad (\text{V C2.5})$$

in which

$$M_{kk'} = \langle \delta u_k \delta u_{k'} \rangle \quad (\text{V C2.6})$$

is the (known) covariance matrix for the resonance parameters.

Derivatives of the multigroup cross sections with respect to the resonance parameters are found using the chain rule, in the usual fashion.

Input needed to generate Bondarenko-weighted averages (multigroup cross sections) and the associated covariance matrix using SAMMY is described in Section VI.F.1 of this document. Examples are given in test cases tr083 and tr085; included in these examples are validity tests where the Bondarenko scheme of Eq. (V C2.2) is used to mimic the energy-average scheme of Section V.C.1 and the unweighted average of Section V.C.3.