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Abstract

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New Capabilities for Processing Covariance Data in the Resonance Region

D. Wiarda, M. E. Dunn, N. M. Greene, N. M. Larson, and L. C. Leal

Oak Ridge National Laboratory, P.O Box 2008, Oak Ridge, TN 37831-6354, USA*

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AMPX [1] is a modular system of FORTRAN computer programs that relate to nuclear analysis with a primary emphasis on tasks associated with the production and use of multigroup and continuous-energy cross sections. The PUFF-III module within the AMPX code system handles the creation of multigroup covariance data from ENDF information. The resulting covariances are saved in COVERX format [2].

We recently expanded the capabilities of PUFF-III to include full handling of covariance data in the resonance region. The new program has been named "PUFF-IV." The PUFF-III code can process some types of resonance data covariances using a sensitivity analysis but does not handle newer ENDF file formats. To our knowledge, PUFF-IV is the first processing code that can address both the new ENDF format for resolved resonance parameters and the new ENDF "compact" covariance format. The existing code base was rewritten in Fortran 90 to allow for a more modular design. Results are identical between the new and old versions within rounding errors. Automatic test cases have been added to ensure that consistent results are generated.

Processing of the resolved resonance region is done analytically. Partial derivatives with respect to the resonance parameters are calculated using a library developed by N. M. Larson, the author of the R-Matrix fitting program SAMMY [3], as an aid to developers of processing codes for generating cross-sections and derivatives with the new ENDF formats. The library calculates the derivatives for Reich-Moore parameters. Even if the resonance data are given in terms of Single-Level or Multi-Level Breit-Wigner formalism, the Reich-Moore formulae are used to calculate the derivatives. Although this calculation is an approximation, nevertheless it should be quite good. For situations in which the Breit-Wigner approximations are adequate, they give nearly the same cross sections and derivatives as does the Reich-Moore approximation. The derivatives are calculated on a dense energy grid. The grid may be calculated by the AMPX POLIDENT module, which calculates point-wise cross-section data and creates the corresponding energy grid. The variation of partial derivatives across grid boundaries is monitored, and the user is alerted if too coarse a grid is used. The covariance for the point-wise cross section in terms of the covariance information between the resonances parameters is

$$\langle \delta\sigma_m(E_i)\delta\sigma_l(E_j) \rangle = \sum_{kn} \frac{\partial\sigma_m(E_i)}{\partial P_k} \langle \delta P_k \delta P_n \rangle \frac{\partial\sigma_l(E_j)}{\partial P_n},$$

where m and l denote different reaction types and k and n denote resonance parameter indices. The covariance matrix elements $\langle \delta P_k \delta P_n \rangle$ are specified in the ENDF files, and the partial derivatives are calculated as described above. The group-averaged covariance can then be calculated as

$$\langle \delta x_I^m \delta x_J^l \rangle = \frac{1}{\Phi_I \Phi_J} \int_{I,J} \Phi(E_i) \langle \delta\sigma_m(E_i)\delta\sigma_l(E_j) \rangle \Phi(E_j) dE_i dE_j,$$

where x_I^m denotes the group-averaged cross section for group I and reaction type m . The function $\Phi(E_i)$ denotes the specified weighting functions and

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$$\Phi_I = \int_I \Phi(E_i) dE_i \approx \sum_I \Phi(E_i) \Delta E_i,$$

where the approximation is valid if the energy grid is sufficiently dense. For the calculation of the group-averaged cross-section data, the integral is also approximated by a sum and can be calculated as

$$\langle \delta x_I^m \delta x_J^l \rangle = \sum_{kn} D_{Ik}^m \langle \delta P_k \delta P_n \rangle D_{Jn}^l$$

with

$$D_{Ik}^m = \frac{1}{\Phi_I} \sum_I \Phi(E_i) \frac{\partial \sigma_m(E_i)}{\partial P_k} \Delta E_i.$$

If the energy range for a group extends beyond the resolved resonance region, then contributions from the higher-energy regions are added to the above formulae.

Results calculated with the above approach for the resolved resonance region were compared with results calculated using the SAMMY R-matrix fitting program, which can also generate group-averaged covariance data. Results agreed within rounding errors for all formats considered. When necessary, SAMMY was instructed to use the same approximation; i.e., calculate via the Reich-Moore formulae even though the ENDF file specifies Breit-Wigner.

For comparison, we used a modified JENDL 3.2 ^{158}Gd file and calculated the resolved resonance region covariance data only, using PUFF-IV, ERRORJ [4], and SAMMY. ERRORJ has similar capabilities to PUFF-IV, using a sensitivity evaluation of the resonance data, but does not support all ENDF formats supported by PUFF-IV. Results obtained by the three programs should be comparable. Figure 1 shows the correlation matrix for total cross-section data for the three programs. The results are nearly identical and vary only within rounding errors (all differences $< 5 \times 10^{-5}$).

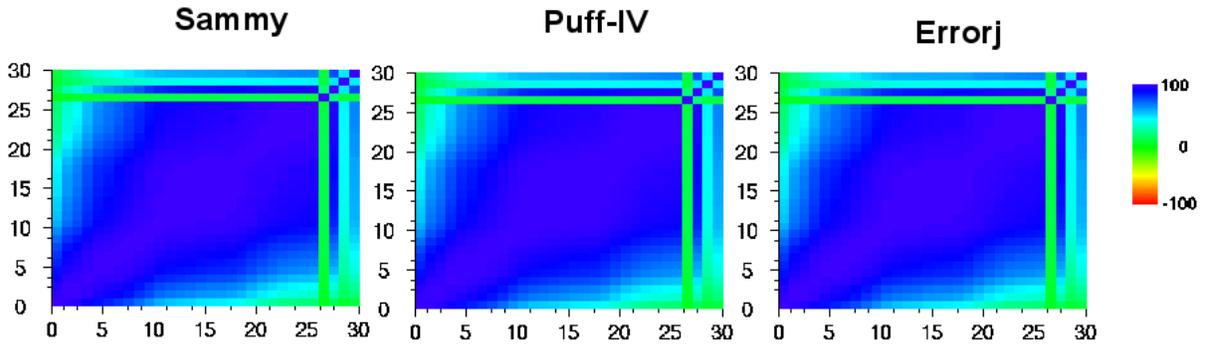


Figure 1. The correlation matrices for total cross-section data in ^{158}Gd calculated by the PUFF-IV, SAMMY and ERRORJ programs. The 30 upper (lower-energy) groups of the 44 group structure in the SCALE [5] code that represent the resolved resonance region for ^{158}Gd were used for the comparison.

References

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