Recent Advances with the AMPX Covariance Processing Capabilities in PUFF-IV

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The program PUFF-IV is used to process resonance parameter covariance information given in ENDF/B File 32 and point-wise covariance matrices given in ENDF/B File 33 into group-averaged covariance matrices on a user-supplied group structure. For large resonance covariance matrices, found for example in ²³⁵U, the execution time of PUFF-IV can be quite long. Recently the code was changed to use Basic Linear Algebra Subprograms (BLAS) routines for some of the matrix multiplications. This led to a substantial decrease in execution time. As an example, the execution time for ²³⁵U on a 238-group energy grid decreased from over a month to only 16 hours after the optimization. Actual optimization varies with BLAS implementation used and the number of processors available. If no BLAS implementation is available, PUFF-IV will revert to the un-optimized version. This faster processing capability allowed us to investigate the conversion of File 32 data into File 33 data with a larger number of user-defined groups. This conversion substantially reduces the ENDF/B file size requirements for evaluations with a large number of resonances. A covariance file containing only File 32 covariance matrices is produced, and a new tool, COVCONV, joins these covariance matrices with an existing File 33. In this conversion a tradeoff is made between the number of groups used to represent the resonance parameter covariance as a pointwise covariance matrix and the file size. We are also investigating a hybrid version of the conversion in which a File 32 resonance parameter covariance matrix is used for the low-energy region while covariance matrices for higher energies in the resolved resonance region are given as point-wise covariance matrices, using a similar method as outlined above. In addition, the processing capability for resonance parameter covariance information in Reich-Moore format (LRF = 7) was improved. The options available for the weighting function used in calculating group-averaged covariance matrices have been enhanced, and users are now able to supply any desired function. An older version of PUFF-IV is currently available in Radiation Safety Information Computational Center. We expect to release a new version containing the improvements in the near future.

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