Abstract – Computer Codes Poster Session

Computational Physics and Engineering Division

PUFF-III: A Multigroup Covariance Processing Code for the AMPX Cross Section Processing System

M. E. Dunn and B. L. Broadhead

Oak Ridge National Laboratory,[*]
P. O. Box 2008,
Oak Ridge, TN 37831-6370
(423) 574-5260
dunnme@ornl.gov

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[**]The summary is submitted for the poster session for computer codes related to the topical areas.

1. NAME AND TITLE

PUFF-III: A Multigroup Covariance Processing Code for the AMPX Cross Section Processing System

2. CONTRIBUTOR

M. E. Dunn and B. L. Broadhead, Oak Ridge National Laboratory,* P. O. Box 2008, Oak Ridge, TN 37831-6370, (423) 574-5260

3. CODING LANGUAGE AND COMPUTER

FORTRAN 90; DEC Alpha

4. DESCRIPTION OF PROGRAM OR FUNCTION

The Evaluated Nuclear Data File (i.e., ENDF), standards and formats are available to permit the communication of estimated uncertainties in the measured cross section data.[1] By including the uncertainty or covariance information, the analyst can propagate cross section data uncertainties through sensitivity studies to the final calculated quantities of interest in nuclear applications. The ENDF covariance data files provide the estimated uncertainty for the individual data as well as any correlations that may exist. Prior to using the covariance information in applications, a processing code must be used to convert the energy dependent covariance information in the ENDF library to multigroup form. PUFF-III processes the uncertainty information in ENDF Files 31, 32 and 33 and generates the desired multigroup correlation matrix for the evaluation of interest. PUFF-III has the capability to process ENDF covariances formats through version VI.

5. METHOD OF SOLUTION

In the ENDF uncertainty formats, the evaluator specifies a set of data and corresponding equations that are used to calculate the covariance between cross section x_i at energy E_i and cross section y_j at Energy E_j. As a result, the data has a histogram appearance, but the data is not considered to be multigroup covariances which would imply a covariance of one multigroup averaged quantity with another group averaged quantity. In reality, the data represents the covariance between a cross section at an energy within one interval to another energy point in another interval. Since the ENDF data represents the covariance between point energy data, PUFF-III processes the point covariance data into multigroup covariances. In particular, the cross section covariances are intended to characterize the variances of the cross sections within a specified energy range as well as the correlations between cross sections of several adjacent energy ranges. PUFF-III calculates the contribution to the multigroup covariance matrix based on the long-range correlations between cross sections over many energy ranges. PUFF-III also calculates the contribution to the specified multigroup covariance matrix based on the short-range correlations that are specified through the resonance parameter uncertainties of File 32. Subsequently, PUFF-III combines the short- and long-range contributions to obtain the specified multigroup covariance matrix throughout the energy range of interest.

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6. NEW FEATURES

Since the development of PUFF-II,[2] several new enhancements have been incorporated into PUFF-III. In particular, PUFF-III has the capability to process short range variance formats for NI type sub-subsections in File 33. Following the release of PUFF-II, lumped reaction covariance data formats were introduced into ENDF/B-V; however, PUFF-II cannot process this covariance information. Consequently, PUFF-III has been updated to process the lumped reaction covariance information that is available in ENDF/B-V and -VI. As part of the upgrade, PUFF-III has the capability to process the spontaneous fission covariances for fission neutron multiplicity or $\overline{n}$. In the previous version of PUFF, the user must visually inspect the ENDF uncertainty file and identify the covariance matrices for calculation. To reduce the amount of user interaction with the ENDF uncertainty files, PUFF-III has a directory feature that prints a directory of all explicitly and implicitly defined covariance matrices for a selected nuclide. PUFF-III also has the capability to examine the neutron cross section uncertainty file and determine the necessary cross section information for the problem. If covariance data is specified for a redundant reaction and the requisite partial cross sections are available, PUFF-III can compute the desired redundant cross sections for use in the covariance calculation. Previous versions of PUFF provide the calculated correlation matrices based on the input ENDF uncertainty information. Unfortunately, PUFF did not provide an assessment of the calculated correlation matrices. In an effort to assess the calculated results, PUFF-III determines the eigenvalues (f_i) for each calculated correlation matrix and determines if the calculated matrix is positive definite.

7. RESTRICTIONS OR LIMITATIONS

None noted.

8. TYPICAL RUNNING TIME

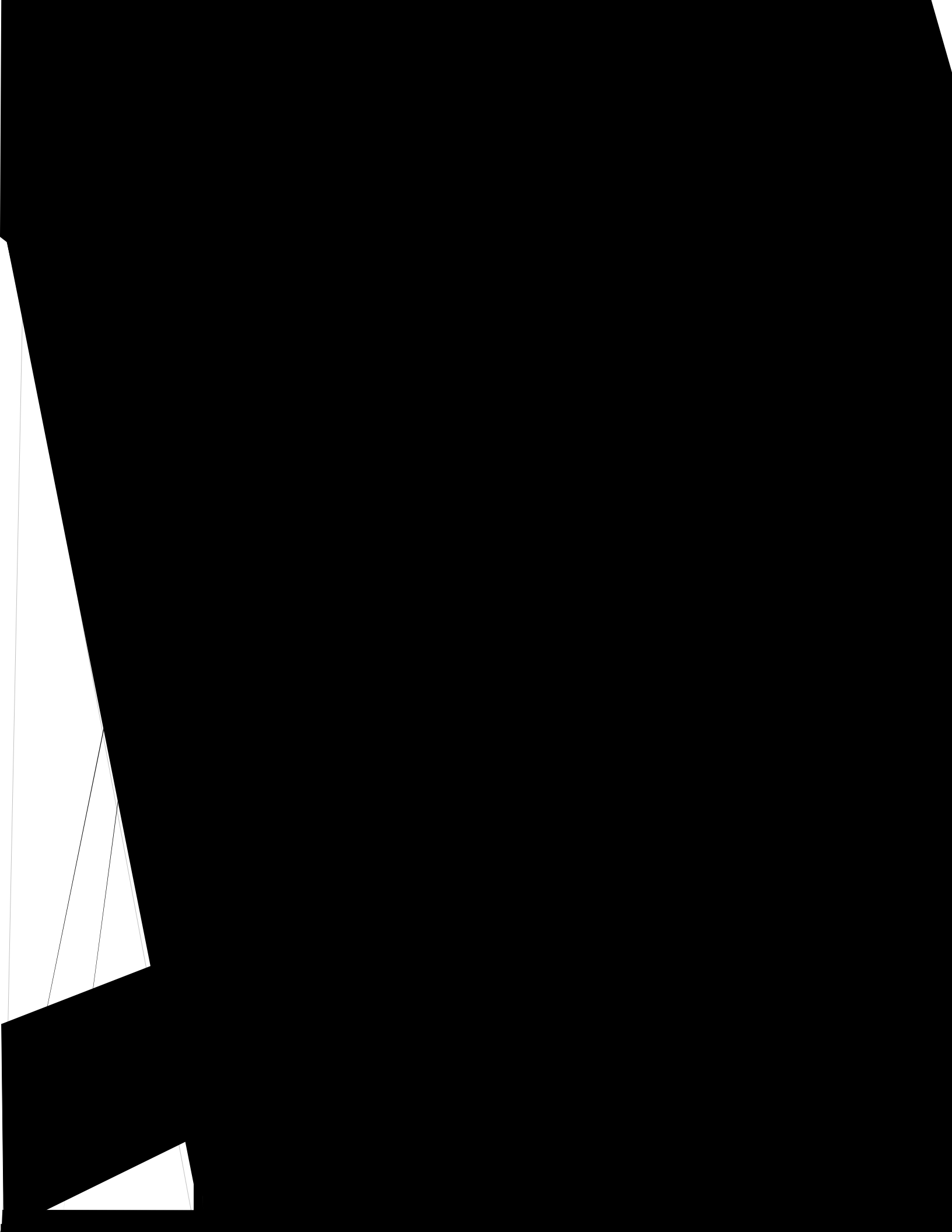
Example execution is provided in the TESTING Section.

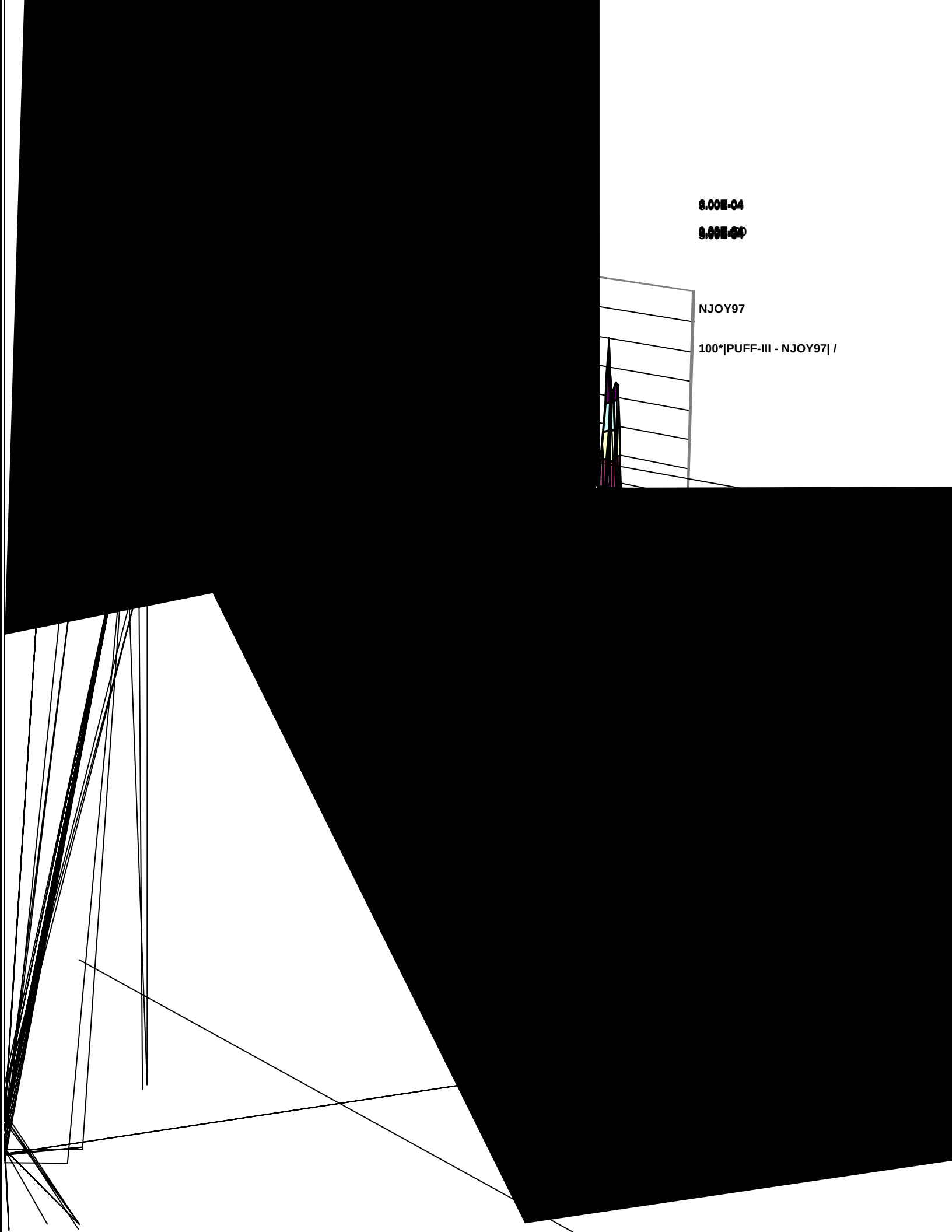
9. MACHINE REQUIREMENTS

PUFF-III has been developed on a DEC Alpha AS 500/500 workstation using a FORTRAN 90 compiler.

10. TESTING

In an effort to test the code, the ENDF/B-VI covariance data for ^{56}Fe was processed using PUFF-III. Since an AMPX generated multigroup library based ENDF/B-VI data does not currently exist, NJOY97[3] was used to generate a multigroup library for ^{56}Fe using the 44 group energy structure. Subsequently, the AMPX module SMILER was used to convert the NJOY data to an AMPX master library format. Using the 44 group cross sections for ^{56}Fe, multigroup covariance matrices were calculated for each explicitly and implicitly defined covariance matrix. PUFF-III was executed on a DEC Alpha AS 500/500 workstation, and the CPU time required for the calculation is 32 seconds. To illustrate the results, the covariance between the total and elastic scattering cross sections for ^{56}Fe (i.e., <1, 2>) is provided in Figure 1. In an effort to verify the calculated results, the covariance data for ^{56}Fe was processed using the ERRORR module of NJOY. Since the same multigroup cross sections are used in PUFF-III and ERRORR, any differences in the calculations can be attributed to the covariance processing modules as opposed to the cross section data. The percent difference between the ERRORR calculated covariance matrix and the PUFF-III covariance matrix is provided in Figure 2. Based on the results in Figure 2, the differences between PUFF-III and ERRORR are negligible. With the development of PUFF-III, a new and improved multigroup covariance processing code is available to process ENDF/B-VI covariance data for nuclear applications.

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100*|PUFF-III - NJOY97| /

11. REFERENCES

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2. J. D. Smith III, "Processing ENDF/B-V Uncertainty into Multigroup Covariance Matrices," ORNL/TM-7221, Union Carbide Corporation, Oak Ridge National Laboratory, June 1980.
3. R. E. MacFarlane, "NJOY97.0 Code System for Producing Pointwise and Multigroup Neutron and Photon Cross Sections from ENDF/B Data," Los Alamos National Laboratory, April 1998.

12. DATE OF ABSTRACT

August 1999

KEYWORDS: AMPX, COVARIANCE DATA, CROSS SECTION, ENDF/B-VI, MULTIGROUP, PUFF-III, RESONANCE PARAMETERS, UNCERTAINTY