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With the growing demand for multigroup covariances, the National Nuclear Data Center (NNDC) has been experiencing an upsurge in its covariance data processing activities using the two US codes NJOY-99 (LANL) and PUFF-IV (ORNL). The code NJOY-99 was upgraded by incorporating the new module ERRORJ-2.3, while the NNDC served as the active user and provided feedback. The NNDC has been primarily processing neutron cross section covariances on its 64-bit Linux cluster in support of two DOE programs, the Global Nuclear Energy Partnership (GNEP) and the Nuclear Criticality Safety Program (NCSP). For GNEP, the NNDC used NJOY-99.259 to generate multigroup covariance matrices of ^{56}Fe, ^{23}Na, ^{239}Pu, ^{235}U and ^{238}U from the JENDL-3.3 library using the 15-, 33-, and 230-energy group structures. These covariance matrices will be used to test a new collapsing algorithm which will subsequently be employed to calculate uncertainties on integral parameters in different fast neutron-based systems. For NCSP, we used PUFF-IV 1.0.4 to verify the processability of new evaluated covariance data of ^{55}Mn, ^{239}Pu, ^{233}U, ^{235}U and ^{238}U generated by a collaboration of ORNL and LANL. For the data end-users at large, the NNDC has made available a Web site which provides a static visualization interface for all materials with covariance data in the four major data libraries: ENDF/B-VI.8 (47 materials), ENDF/B-VII.0 (26 materials), JEFF-3.1 (37 materials) and JENDL-3.3 (20 materials).

I. Introduction

The nuclear data community has seen renewed interest in neutron cross section covariances in recent years. This has been largely driven by DOE-initiated programs such as the Nuclear Criticality Safety Program (NCSP), Global Nuclear Energy Partnership (GNEP), Generation IV (Gen-IV) reactor systems studies and the Advanced Fuel Cycle Initiative (AFCI). In these programs, the urgent and compelling need to reduce uncertainties in the nuclear data being used to meet target accuracies cannot be overemphasized. This revival already resulted in improved methodology for the generation of covariance data, mostly as a consequence of the utilization of advanced nuclear modeling and information merging techniques, followed by sample covariance evaluations for the new US library ENDF/B-VII.0 [1].

In the GNEP initiative, availability of covariances is crucial to the generation of a multigroup adjusted library, using a statistical adjustment method, to be used in advanced fast reactor design calculations. Emphasis of current studies is on fast, metal-cooled actinide burner reactors which would address GNEP non-proliferation objectives and also produce energy from recycled nuclear fuel.

In the NCSP, computational tools are being developed and tested, requiring an extensive amount of covariance data for all materials in the evaluated data libraries. BNL through NNDC is a member of a network of national laboratories mandated to produce nuclear data covariances which will meet the needs of criticality safety applications. In addition, NNDC serves as the linchpin for the NCSP nuclear data efforts at the other three national laboratories: LANL, ORNL and ANL.

The ENDF covariance files contain covariances of energy-dependent cross sections, as well as the covariances of resolved resonance parameters. On the other hand, end-users working in neutron-based applications usually require the covariances of multigroup-averaged cross sections, as input, for example, to sensitivity and uncertainty calculations. It is the job of processing codes to generate the required multigroup information from the energy-dependent data in the ENDF files. Advances in the processing codes and computer technology have placed in the hands of nuclear data centers, evaluators and end-users alike the unprecedented capability to generate multigroup-averaged covariances for use in neutron-based applications. This combination of factors has contributed to the upsurge in covariance processing activities in recent years.

In the succeeding sections, we will first describe the advances in the two US covariance processing codes, NJOY-99 and PUFF-IV. Then, we will discuss our results and experience in using these codes. We note that the NNDC is probably the only laboratory actively using both codes for covariance processing and thus in the best position to provide considerable feedback to code developers.

II. Advances in the Processing Codes

A. LANL code NJOY-99

For many years, the LANL code NJOY-99 [2] has had the capability to process ENDF covariance data from File 31 (nubars) and File 33 (cross sections) with the ERRORR module, including limited capabilities to process File 32 (resonance parameters). Recently this module was extracted from NJOY, and an improved version, ERRORJ, was created by Go Chiba, JAEA [3]. ERRORJ expanded upon ERRORR to include processing of resolved resonance parameters in the Reich-Moore formalism (File 32), angular distribution (File 34) and energy spectra (File 35) covariance data.

A preliminary merge of ERRORJ-2.3 into NJOY-99 was performed in 2006 prior to the release of ENDF/B-VII.0. More recently, NJOY-99.259 with fully incorporated ERRORJ-2.3 was officially released to the user community.

A suite of five test problems were executed to verify that ERRORJ was correctly merged into NJOY-99. Two of these

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problems are from the historical NJOY test suite available at http://t2.lanl.gov/codes/NJOY-99/index.html. The first of these test problems processes ENDF/B-V ^{235}U File 31 and File 33 data. The second problem processes ENDF/B-V ^{nat}C File 33 data, including execution of the COVR and VIEWR modules to produce covariance plots. The output files generated by NJOY-99.259 were identical to those produced by earlier NJOY-99 versions that contain the original ERRORR module.

In addition, three new test problems were developed by Go Chiba. These require processing of various JENDL-3.3 neutron files. The first problem processes covariance data from ^{238}U Files 31, 33, 34 and 35. This job follows the usual sequence of producing Doppler broadened pointwise data with the RECONR and BROADR modules. These data are then group averaged with GROUPR prior to executing the ERRORJ module. The second new test problem only uses RECONR and BROADR before executing ERRORJ, thereby testing the capability to produce the necessary group average data to then process Files 31 and 33. Again, the JENDL-3.3 ^{238}U file provides the basic nuclear data input. The final new test job processes the three major actinides, ^{235,238}U and ^{239}Pu. Pointwise, room temperature data are created using the RECONR and BROADR modules which is subsequently group-averaged with GROUPR. The three GROUPR output files are merged onto a single tape with MODER and ERRORJ is executed to process file ^{238}U including cross material covariances for MT18 (the fission cross section) with ^{235}U and ^{239}Pu. The output files created by NJOY-99.259 agreed well with those provided by Go Chiba with only occasional differences observed in the least significant digit of various output quantities.

Additional visualization capability for covariance matrix data is still required. Covariance matrices developed from Files 31 and 33 only may be visualized using the COVR and VIEWR modules; a limitation consistent with the processing capability of the original ERRORR module. Visualization of File 34 and File 35 derived matrices remains a future option.

B. ORNL code PUFF-IV

In early 2006, PUFF-III had only limited capabilities to process the resonance parameter covariance data (File 32) of the new ENDF/B-VII.0 library. To address this deficiency, ORNL completely rewrote PUFF-III in Fortran 90 and released PUFF-IV which has the built-in capability to fully process ENDF/B-VII.0 File 32 data in the resonance region. This made PUFF-IV the only code at the time which could handle both the Reich-Moore ENDF-6 format for resolved resonance parameters and the new ENDF-6 “compact” covariance format.

An important new feature in PUFF-IV is the capability to process ENDF data files which do not contain File 33. PUFF-IV will automatically recognize which covariance data (File 31, 32, and/or 33) are present and process them according to user input specifications.

We note that while NJOY-99 uses numerical methods for calculating resonance sensitivities, the PUFF-IV code uses analytical methods. These sensitivities are needed to determine cross section uncertainties and correlations.

In early 2007, ORNL released an upgrade for PUFF-IV from 1.0.3 to 1.0.4. Among the many improvements was the resolution of the “step-size underflow” problem which would lead to the generation of “0.0” cross sections in cases wherein the user supplied an energy group structure having boundaries not monotonically increasing.

In April 2007, new ORNL-LANL covariance evaluations of ^{233,235,238}U and ^{239}Pu were released to the nuclear data community for testing. These evaluations were stored in huge data files due to their large resonance parameter covariance matrices which required unprecedented amount of PUFF-IV processing time. To address this issue, ORNL overhauled PUFF-IV’s matrix multiplication modules to take advantage of the efficiencies in the Basic Linear Algebra Subprograms (BLAS) routines when available on a computing system. As a result, significant reduction in processing time was achieved as reported by D. Wiarda [4]. However, the latest version has not yet been released for distribution through RSICC.

To date, PUFF-IV still cannot process the covariances of angular and energy distributions of secondary neutrons (File 34 and File 35) as well as covariance data for the production of radioactive nuclei (File 40) [5].

III. Processing Covariances for GNEP

As part of the data adjustment project, the GNEP core group headquartered in Idaho National Laboratory has been conducting rigorous testing on the validity of a new algorithm which allows collapsing an integral parameter’s fine-group (reference) covariance data to a coarse group while preserving the uncertainty calculated in the fine group structure. For the integral parameters to be used in the investigation, they used: 1) the neutron multiplication factor (k_{eff}) in different fast neutron systems with different fuels, coolants and reactivity coefficients, and 2) reactivity coefficients [6]. These tests will help INL to asses whether the use of the collapsed matrices will have an impact on the statistical adjustment procedure.

To enable the GNEP core group to conduct the tests, NNDC provided them with multigroup covariance matrices of ^{56}Fe, ^{23}Na, ^{239}Pu, ^{235}U and ^{238}U generated by NJOY-99.259 from the JENDL-3.3 library using the 15-, 33-, and 230-energy group structures and the constant weighting function. Fig. 1 shows a general schematic diagram on the flow of processing. The 230-energy group structure served as the reference group representation in the study. Furthermore, the processed covariance matrices covered the five reaction channels of interest: elastic, inelastic, (n,2n), fission, capture, and total for redundancy.

The processed covariance matrix files are by default voluminous because of the generation of cross correlation matrices for every combination of reaction types available for an isotope. To address this issue, the COVR module in NJOY-99.259 was used to confine the generation of plots and numeric data files to include only the five reaction types of interest to GNEP.

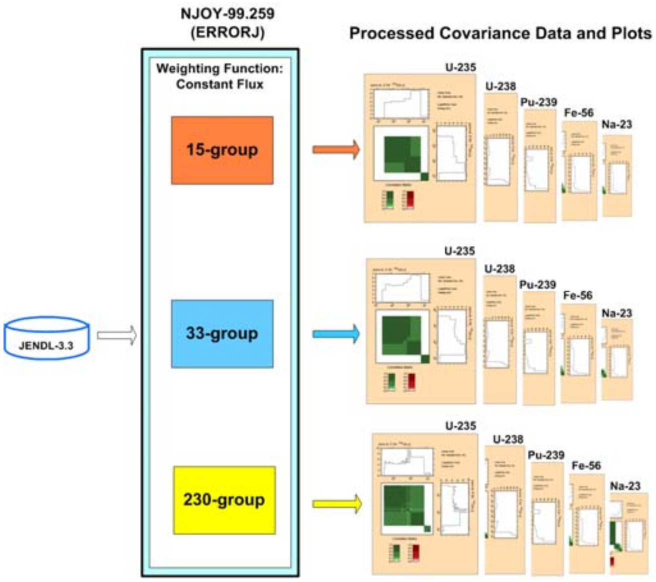

FIG. 1: Generation of multigroup covariance matrices for ^{56}Fe, ^{23}Na, ^{239}Pu, ^{235}U and ^{238}U using NJOY-99.259 and 15-, 33-, and the 230-energy group structures. Evaluations were taken from JENDL-3.3.

IV. Processing Covariances for NCSP

NNDC provides technical support to the Criticality Safety Support Group. As the U.S. clearinghouse for nuclear data we are tasked to check the processability and completeness of covariance data files before they are stored in the ENDF/A repository, see *http://www.nndc.bnl.gov/exfor/4web/ENDF-A/complete -evaluations/*.

In late 2007, NNDC began processing new ORNL-LANL evaluations of ^{233,235,238}U and ^{239}Pu with NJOY-99 and PUFF-IV. The new evaluated data files were the largest ever received by the NNDC because they contained huge covariance matrices of resonance parameters (File 32). For instance, the ^{235}U File 32 contained more than 21 million lines resulting in a file size of 1.7 GB. As a consequence, NNDC had to modify the ERRRORJ module in NJOY-99.259 to successfully process ^{233,238}U and ^{239}Pu but failed with ^{235}U. On the other hand, PUFF-IV 1.0.4 was able to successfully process all of these materials but required an enormous amount of computer time. For instance, it took our Linux cluster (3.2-GHz Intel Xeon, 4-GB RAM per CPU) 29 hours to process ^{235}U using the 44-energy group structure and the 1/E weighting function.

In March 2008, NNDC received from ORNL updated covariance evaluations of ^{233,235,238}U and ^{239}Pu with File 32 data converted into File 33 using a method developed at ORNL. As a result of the conversion, the data files were significantly smaller than the immediate preceding evaluations and thus were more manageable and much faster to process with PUFF-IV.

To roughly assess the impact of the conversion, we compared the uncertainties of the File 32 with that of the original (unconverted) data file. Figs. 2 and 3 show the comparison plots for ^{235}U and ^{239}Pu fission cross sections. Observed discrepancies should be attributed to changes in the evaluations rather than conversion. The processing washed out fine details, requiring some caution when comparing group-wise uncertainties with the pointwise values at the thermal energy taken from S. Mughabghab 2006 [7].

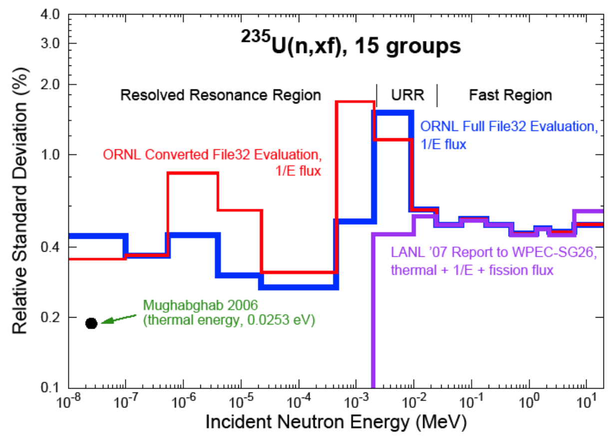

FIG. 2: Relative uncertainties in ^{235}U fission cross section processed by PUFF-IV in the 15-energy group structure. ORNL supplied resolved resonance and URR data, while LANL covered fast region. Shown are various stages of the evaluation process, the final result being in red. Also shown is the thermal pointwise value [7].

In Fig. 2, the purple curve represents the LANL evaluation of ^{235}U fission cross section uncertainties in the fast energy region. This was integrated with the ORNL covariance evaluation in the resolved and unresolved resonance regions as shown by the blue curve. To address the file size issue, ORNL converted the File 32 covariances, after some improvements in the evaluation, into the File 33 shown by the red curve. The final covariance data file was verified by the NNDC for and included in the ENDF/A library.

As shown in Fig. 3, the evaluation of ^{239}Pu fission cross section uncertainties underwent the same series of stages. LANL performed the evaluation for the fast energy region (purple curve), ORNL handled the evaluation for the resolved and unresolved regions and then integrated the LANL and ORNL evaluations (blue curve), and ORNL converted File 32 data into the File 33 representation (red curve) to reduce the file size. The final covariance data file was verified by the NNDC and included in the ENDF/A library.

Wiarda and Leal [4] emphasized that great care must be taken in selecting the energy group structure to use in the conversion process in order to achieve good agreement. For a detailed description of the impact of the conversion process on multigroup covariances, see Ref. [8].

NNDC also processed with PUFF-IV 1.0.4 a new evaluation of ^{55}Mn from ORNL in March 2008. ^{55}Mn is an important material from the point of view of the criticality safety of reactor fuel stored in thick stainless steel (constituents Fe, Ni, Cr, Mn) cans or inserts. Covariances for this material were subject to past and also recent interest, providing a rare possibility to compare a rich variety of existing covariance results.

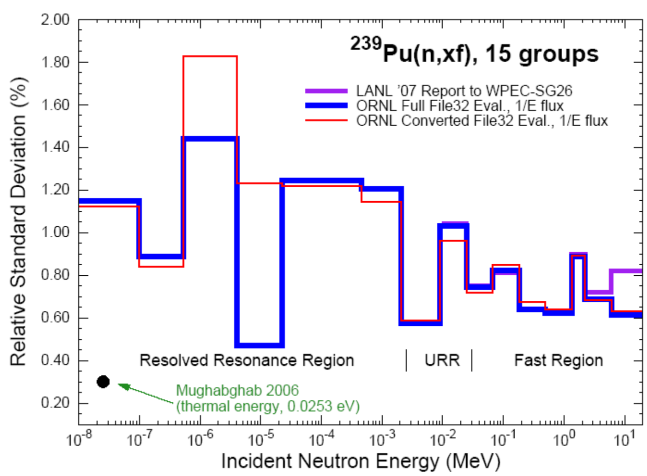

FIG. 3: Relative uncertainties in ^{239}Pu fission cross section calculated by PUFF-IV using the 15-energy group structure. See also the text in Fig. 2.

Shown in Fig. 4 are plots of the relative uncertainties of ^{55}Mn neutron capture cross sections. In the processing, we used the 44-energy group structure and the 1/E flux. Presently, the new high-fidelity evaluation contains covariance data in the resolved resonance region (ORNL 2008), while the evaluation by BNL/KAERI represents an intermediate quality result in the entire energy region. To determine the significance of these new results, we compared them with the recent low-fidelity estimate by ORNL-BNL. Legacy evaluations from ENDF/B-VI.8, IRDF-2002 and JENDL-3.3 are also shown to illustrate the impact of new data and new evaluation techniques and methods on uncertainty estimation and analyses.

V. Covariances Web Page

For the last few years, there has been a frequent request from the data end-users at large for a capability to enable a quick glance of available covariances in the nuclear data libraries. In response to such a request, the NNDC developed a Web page which provides a static covariance data visualization interface for the four major evaluated nuclear data libraries: ENDF/B-VI.8 (47 materials), ENDF/B-VII.0 (26 materials), JEFF-3.1 (37 materials) and JENDL-3.3 (20 materials).

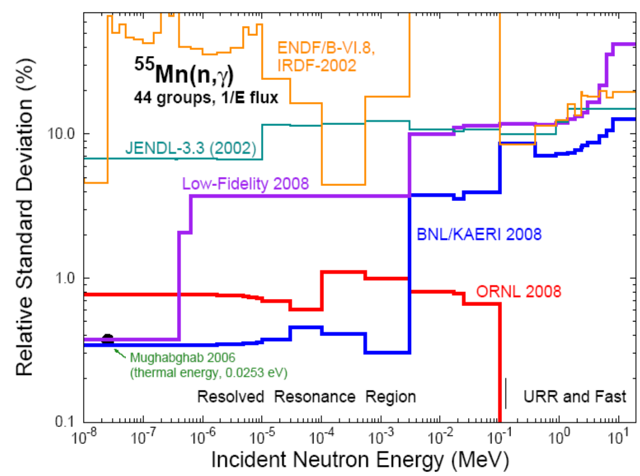

FIG. 4: Relative uncertainties in ^{55}Mn capture cross section processed by PUFF-IV using the 44-energy group structure and 1/E flux. Recent evaluations are marked as Low-Fidelity 2008, followed by the intermediate quality BNL/KAERI 2008, and the new high-fidelity ORNL 2008. Shown for comparison are legacy evaluations in ENDF/B-VI.8, adopted by IRDF-2002, and JENDL-3.3.

To build this Web page, NNDC processed with NJOY-99.259 all materials which have covariance information using constant flux in the 44- and 187-energy group structures. Fig. 5 depicts the flow of the processing. Plots of relative uncertainty (%) versus incident neutron energy (eV) and their associated correlation and cross correlation matrices were generated and posted on the Web page.

The above covariance Web page should be viewed only as a stop-gap solution. It is intended as a precursor to the dynamic visualization capabilities to be provided by the Sigma ENDF Retrieval and Plotting System. This new Web interface will provide powerful but easy-to-use viewing functionalities such as the ability to view uncertainties and covariance matrices directly from any text file [9]. In the near future, data end-users will be able to view unprocessed File 33 (cross sections) covariances and later also File 32 (resonance parameters) covariances where pre-processing would be necessary.

VI. Conclusion

With the recent advances in the processing codes, NJOY-99 and PUFF-IV have proven to be invaluable tools in generating multigroup uncertainties and correlation matrices for use in DOE-initiated programs such as GNEP and criticality safety. In the development of the first extensive covariance Web page, NJOY-99 provided the processing and plotting capabilities to build a static covariance data visualization interface for the major evaluated data libraries.

Active use of these two US codes by the NNDC appeared to be crucial in checking and verifying new covariance evaluations. In this process we also provided considerable feedback to code developers. Close collaboration between the NNDC and the processing code developers will remain to be an important element in the current US effort to develop new covariances, with the ultimate goal being their inclusion into the future ENDF/B-VII.1 library.

Acknowledgments

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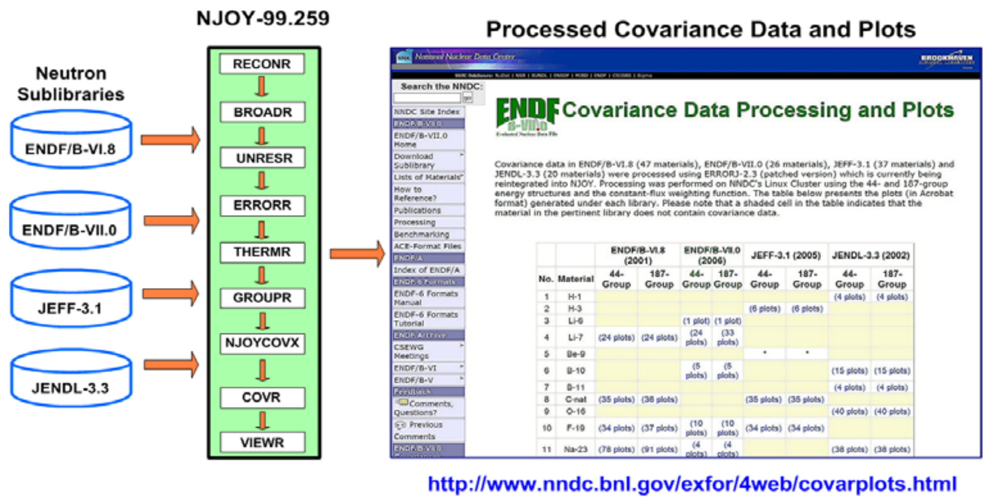

FIG. 5: Processing of covariance data from the four major evaluated nuclear data libraries using NJOY-99.259. The constant flux and the 44- and 187-energy group structures were used. For each reaction channel, plots of relative uncertainty versus incident neutron energy and their associated correlation and, in very few cases, also cross correlation matrices can be accessed.

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[9] B. Pritychenko and A. Sonzogni, "*Sigma: Web Retrieval Interface for Nuclear Reaction Data,*" see this issue of Nuclear Data Sheets.