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Low-fidelity Covariance Project

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The Low-Fidelity Covariance Project has developed a complete set of covariance data estimates for all ENDF/B-VII.0 isotopes. Covariance data are provided for elastic scattering, inelastic scattering, (n,2n) reactions, radiative capture and fission (cross section and nubar) over the energy range from 10^{-5} eV to 20 MeV. Various approximations were utilized depending on the mass of the target, the neutron energy range, and the neutron reaction. The resulting covariance data are not an official part of ENDF/B-VII, but are available for testing in nuclear applications.

I. INTRODUCTION

This paper describes the motivation, goals, activities, and status associated with the Low-fidelity Covariance Project (“Low-Fi”). The Low-Fi project was funded in FY07-08 by the United States Department of Energy’s Nuclear Criticality Safety Program (NCSP). The project was a collaboration among Argonne, Brookhaven, Los Alamos, and Oak Ridge National Laboratories.

The motivation for the Low-Fi project stemmed from an imbalance in supply and demand of covariance data. The interest in, and demand for, covariance data has been in a continual uptrend over the past few years. Requirements to understand application-dependent uncertainties in simulated quantities of interest have led to the development of sensitivity / uncertainty and data adjustment software such as TSUNAMI [1] at Oak Ridge. To take full advantage of the capabilities of TSUNAMI requires general availability of covariance data. However, the supply of covariance data has not been able to keep up with the demand. This fact is highlighted by the observation that the recent release of the much-heralded ENDF/B-VII.0 [2] included covariance data for only 26 of the 393 neutron evaluations (which is, in fact, considerably less covariance data than was included in the final ENDF/B-VI release).

The objective of Low-Fi was to begin to correct this imbalance between supply and demand of covariance data. Quoting from the original project plan submitted to the

DOE NCSP, the goal of the work was to prepare a “complete (in energy and reaction) set of covariance data for all ENDF/B-VII isotopes that could exercise our processing methodologies and be used by the AROBCAD Program Element.” (Note: AROBCAD was then a Program Element of the NCSP.) It is important to understand what Low-Fi is, as well as what it is not. Again, quoting from the original proposal, “the goal is completeness, not high fidelity. In fact, to complete such a project in a short period requires that extremely crude approximations be made. Because of the necessarily approximate nature of the covariance data we will produce, we will not allow these data to be made available as part of a general-purpose ENDF/B release. Neither would the existence of this body of data remove at all the necessity for a more methodical and accurate evaluation of important covariance data, such as is underway at several Laboratories.” The product of our work is not complete ENDF/B format evaluations, but rather only the MF = 33 (covariance) portion of the evaluation.

Project responsibilities for the Low-Fi collaboration are now summarized. Los Alamos had responsibility for covariance data for the light isotopes (up through ¹⁹F) over the entire energy range. For all but these light isotopes, Oak Ridge was responsible for the thermal and resonance range covariances, with an upper energy defined to be 5 keV. Above 5 keV, covariances were generated at Brookhaven and Los Alamos. Brookhaven provided covariance data for all remaining materials except for the actinides and Los Alamos was responsible for the actinides. Oak Ridge consolidated the fast data with the thermal and resonance data. Argonne had lead responsibility for testing, quality assurance, and providing

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feedback. Brookhaven is the ultimate repository of these data, and will be responsible for distributing it as appropriate. Of course, if high-fidelity covariances already existed for a specific nuclide, no additional low-fidelity covariances were generated.

The Low-Fi project has been successful, in that complete covariances now exist for all 393 materials included in ENDF/B-VII.0. In general, covariance data are provided for elastic scattering, inelastic scattering, (n,xn) reactions, radiative capture, and fission (cross section and nuubar) over the energy range from 10^{-5} eV to 20 MeV.

The remaining portions of this paper are organized as follows: Section II describes the work done in the thermal and resonance regions; Section III reports on the fast covariances for non-actinides; Section IV summarizes the actinide fast-region covariances; Section V describes the light isotope work; Section VI provides the current status of the project; and Section VII provides a brief summary.

II. THERMAL AND RESONANCE RANGE

Oak Ridge National Laboratory has taken the initiative to create approximate covariance data in the thermal and resonance regions [3]. The strategy employed was to apply integral uncertainties to differential data within the corresponding energy range. This strategy resulted from the observation that a wealth of information is available for uncertainties in measured integral data parameters in these energy ranges. Ref. [4] was used as the source of uncertainties for the integral data parameters.

The thermal energy range was defined to be energies up through 0.5 eV. Radiative capture, fission, and free-atom scattering cross sections were considered. Uncertainties in these cross sections in the thermal range were obtained from tabulated uncertainties in measured integral thermal cross sections (“integral thermal cross sections” refer to 2200-m/sec values determined by direct measurement or by activation experiments in a standard neutron field). A uniform relative uncertainty was assumed over the entire energy range, with full correlation within the energy range. It is understood that the latter assumption is an approximation for non- $1/v$ absorbers.

The resonance energy range was defined to be from 0.5 eV to 5 keV. For radiative capture and fission, uncertainties were derived from uncertainties in measured resonance integrals. Again, a uniform relative uncertainty was assumed over the entire energy range, with full correlation within the energy range. A uniform, fully-correlated uncertainty in the elastic scattering cross section was represented by the uncertainty in the potential cross section, approximated as the free-atom nuclear scattering cross section. Independent covariance data for the total reaction are not provided. These are assumed to be obtained from summing the partial reaction data (*i.e.*, cross correlations between reaction types are ignored).

In some cases the integral and differential measurements are inconsistent; defined here as having a difference

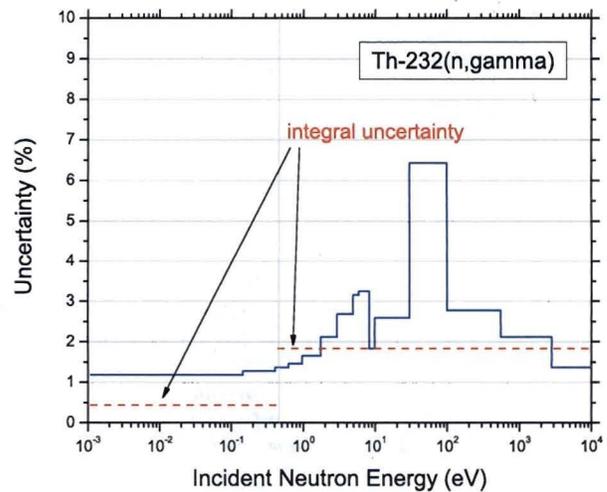


FIG. 1: Relative uncertainties of ^{232}Th capture cross sections in thermal and epithermal energy ranges: integral approximation vs. high fidelity [ENDF/B-VII].

greater than two standard deviations in the measured and computed integral parameter (*i.e.*, thermal cross section or resonance integral). In these cases the relative standard deviation is defined as half the difference, relative to the average of the measured and calculated values:

$$U = \frac{|X_I - X_D|}{X_I + X_D}; \text{ for } |X_I - X_D| > 2\Delta_I,$$

where U is the relative Low-Fi standard deviation, Δ_I is the absolute uncertainty in the integral measurement, and X_I , X_D are the measured and computed (from differential data) integral parameter. In a few instances this expression may exceed 100%. In these cases, a 100% uncertainty was assigned.

Oak Ridge has completed this work for all materials in ENDF/B-VII.0 (Low-Fi will only use those data above ^{19}F) using the most recent compilation of evaluated integral data parameter uncertainties. Figs. 1-3 show examples comparing Low-Fi results obtained using the methodology described above for several reactions with high-fidelity uncertainties previously available. General observations from a limited number of such comparisons are that the Low-Fi approximation tends to underestimate the thermal uncertainty while overestimating the resonance range uncertainty, and that the full correlations in the epithermal range appear to be overly conservative.

III. FAST RANGE FOR STRUCTURAL ISOTOPES, FISSION PRODUCTS, AND HEAVY NON-FISSILE NUCLEI

Brookhaven National Laboratory was responsible for the fast (> 5 keV) covariance data for all materials from

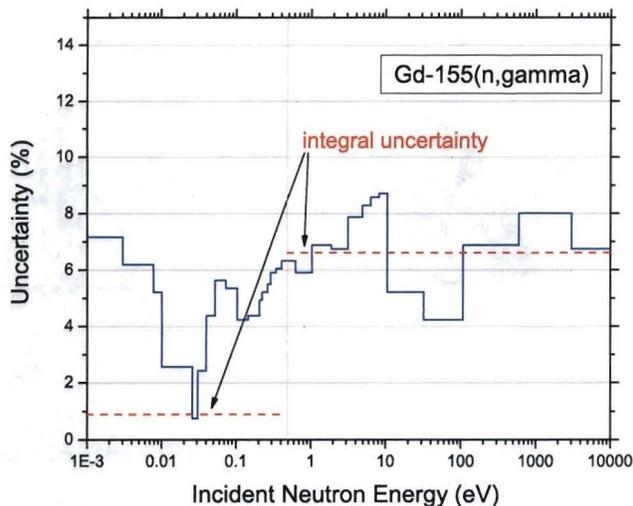


FIG. 2: Relative uncertainties of ^{155}Gd capture cross sections in thermal and epithermal energy ranges: integral approximation vs. high fidelity [ENDF/B-VII].

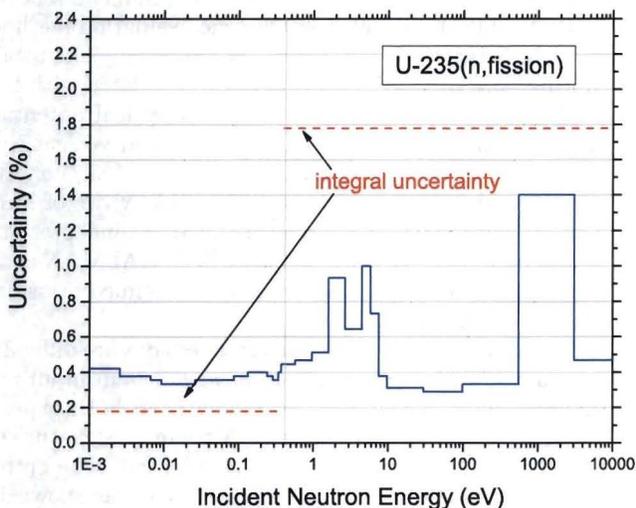


FIG. 3: Relative uncertainties of ^{235}U fission cross sections in thermal and epithermal energy ranges: integral approximation vs. high fidelity [ENDF/B-VII].

^{19}F through ^{209}Bi . In order to accomplish this large task, there was minimal utilization of experimental data. Rather, a well-grounded, although necessarily approximate, methodology was established that was conducive to “mass-production” of this substantial quantity of data [5].

The EMPIRE code [6] was used to calculate reaction cross sections. A global set of models and model parameters were utilized for all materials. Sensitivities to a total of 18 model parameters were also determined from EMPIRE calculations, for each nuclide, at a total of 30 incident energies. Estimates for the uncertainties of these 18 model parameters were based on past work and expert

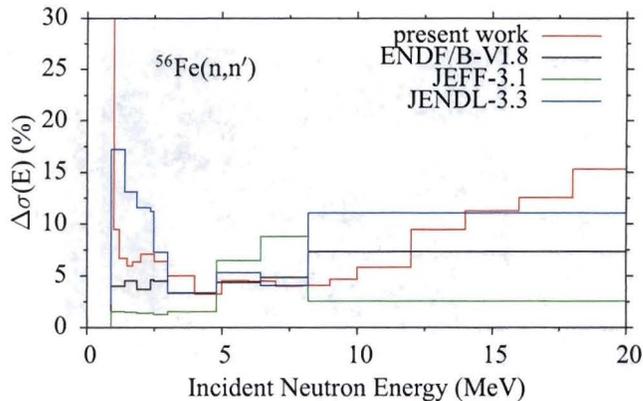


FIG. 4: Relative uncertainties of $^{56}\text{Fe}(n,n')$ cross sections compared to three major nuclear data libraries.

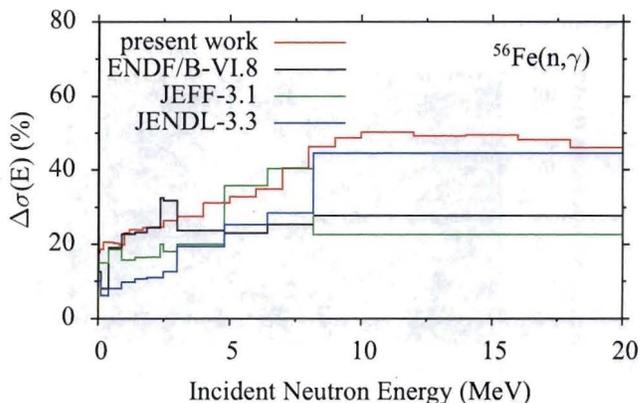


FIG. 5: Relative uncertainties of $^{56}\text{Fe}(n,\gamma)$ cross sections compared to three major nuclear data libraries.

judgment.

Calculated reaction cross sections, sensitivity matrices, model parameters, and model parameter uncertainties were provided as input to the KALMAN Bayesian filtering code [7]. KALMAN was used to calculate the covariance matrices for each nuclide. Reactions considered were total, elastic scattering, inelastic scattering, radiative capture, and $(n,2n)$.

Brookhaven has completed this work for a total of 307 nuclides. In a few cases, resulting uncertainties have been compared with measured data to provide confidence in the methodology. Additionally, comparisons of the resulting Low-Fi uncertainties have been made with existing high-fidelity uncertainties for a few reactions. See, for example such comparisons for reactions on ^{56}Fe in Figs. 4 and 5. Finally, plots have been made of global results. Figs. 6 and 7 show uncertainties for elastic and inelastic scattering respectively, over the entire fast energy range, for all 307 materials evaluated by Brookhaven. Insight into the patterns observable in Figs. 6 and 7 arises from characteristics of the optical model.

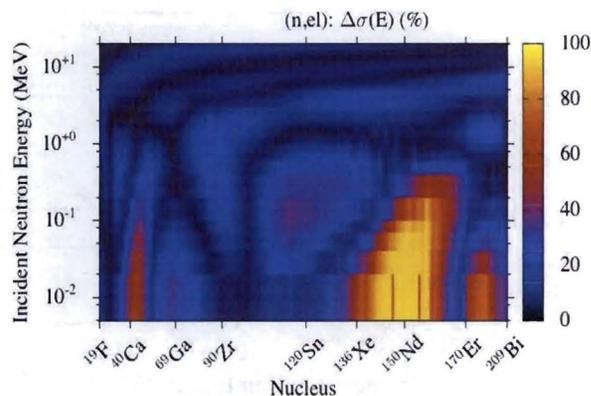


FIG. 6: Relative uncertainties for the elastic scattering cross sections on 307 materials obtained with the EMPIRE-KALMAN method in the fast neutron energy region.

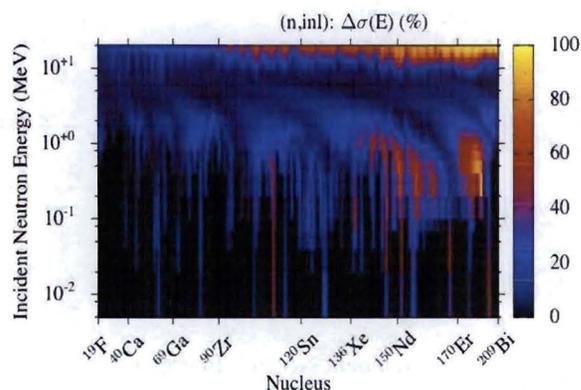


FIG. 7: Relative uncertainties for the inelastic scattering cross sections on 307 materials obtained with the EMPIRE-KALMAN method in the fast neutron energy region.

IV. FAST RANGE FOR ACTINIDES

Los Alamos was responsible for fast energy region actinide covariance data. Such data were obtained from other existing sources for several materials. High-fidelity covariances of major actinide data (^{232}Th , $^{233,235,238}\text{U}$ and ^{239}Pu) above the resonance range have been reported see, for example, Ref [8]. Also, full energy range cross section and $\bar{\nu}$ covariance data were obtained for 14 actinides ($^{234,236}\text{U}$, ^{237}Np , $^{238,240,241,242}\text{Pu}$, $^{241,242m,243}\text{Am}$, and $^{242,243,244,245}\text{Cm}$) from the work of WPEC Subgroup 26 [9]. The uncertainty in thermal data tends to be overestimated with the WP-26 approach, which is based on propagation of resonance parameter uncertainties. Hence ORNL replaced the WP-26 thermal covariance data with integral uncertainties as described in Section II. The other 47 actinide covariances, from ^{225}Ac to ^{255}Fm were evaluated at LANL with a simplified technique, which is based on empirical estimates of the nuclear reaction model parameters or cross sections themselves.

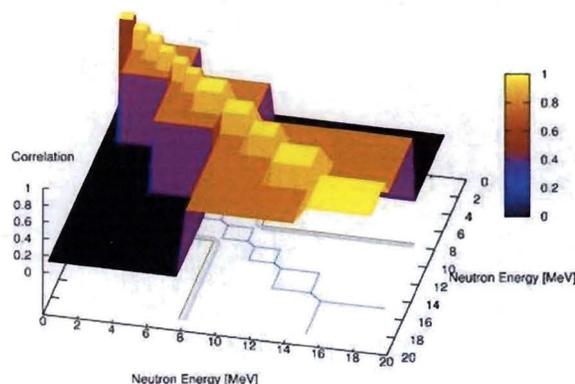


FIG. 8: The common structure of correlation matrix for fission cross sections of minor actinides.

Covariance data for existing nuclear data files were evaluated retroactively; therefore, understanding how the old evaluations were performed was crucial. The covariance estimate is guided by the comment section (MF=1, MT=451) that describes the evaluation method and which reactions cross sections are given. The total, capture, and (n,xn) cross sections are calculated with the CoH and GNASH codes with a global optical potential of Koning and Delaroche [10], and the relative sensitivities of the potential parameters are calculated. For the capture and (n,xn) calculations, the sensitivities of level density parameters, E1 strength function, and precompound parameter are also included. The KALMAN code gives cross section covariances from an assumed prior parameter covariance matrix.

Global calculations of fission cross sections are difficult, as a calculated fission cross section with default input parameters often deviates substantially from both experimental data and evaluated data. A common structure of fission cross section covariance was adopted. The entire energy range is divided into several blocks, as shown in Fig. 8, and the uncertainty in each block is assigned in an empirical manner, typically in the 15-30% range.

The uncertainty for $\bar{\nu}_{\text{prompt}}$, the average number of prompt neutrons emitted from fission, was simply estimated at 20% with full correlation over the entire incident energy range (10^{-5} eV to 20 MeV). No uncertainty was provided for $\bar{\nu}_{\text{delayed}}$. The uncertainty for $\bar{\nu}_{\text{total}}$ should therefore be the same as that prescribed for $\bar{\nu}_{\text{prompt}}$.

V. LIGHT ISOTOPES

Los Alamos evaluated the covariance data of 16 materials from ^1H through ^{19}F over the entire energy region — from 10^{-5} eV to 20 or 150 MeV depending on the maximum energy of the current ENDF/B-VII.0 evaluation (the ^7Li covariances were taken to be those from the current ENDF/B-VII.0 evaluation). A wide range of

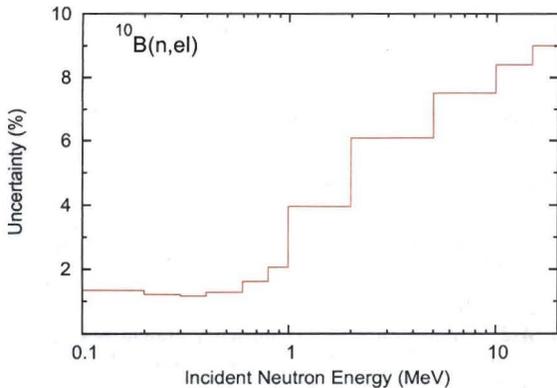


FIG. 9: The uncertainties in ^{10}B elastic scattering.

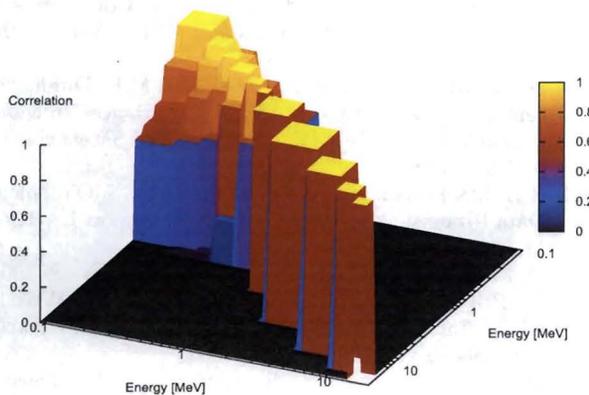


FIG. 10: The correlation matrix of ^{10}B elastic scattering.

methods were used in this effort. At one extreme, full high-fidelity R-matrix analyses were performed for certain reactions on ^1H , ^6Li , and ^{10}B [11]. Other, more approximate techniques included least-squares fitting to experimental data, statistical model calculations often adopted at higher energies, or even just a simple estimation [12]. The method employed depended substantially on the availability of experimental data.

As an example, the uncertainty of ^{10}B elastic scattering is shown in Fig. 9. Fig. 10, which shows the correlation matrix, demonstrates a strongly correlated part below 1 MeV that comes from the R-matrix analysis. At higher energies, the block correlation method similar to that shown in Section IV for fission cross sections was adopted.

VI. CURRENT STATUS AND FUTURE PLANS

All high-energy MF = 33 covariance files generated at Brookhaven and Los Alamos have been transmitted to Oak Ridge. ORNL developed an automated utility program to combine these high-energy data with their thermal and resonance covariance data into a single MF =

33 for each nuclide. Note that there are no correlations in Low-Fi across the three energy ranges (thermal, resonance, fast). As an initial test of the merged files, ORNL processed them with PUFF-IV [13] to ensure they conform to ENDF/B formats and procedures.

The files have been distributed to Argonne for additional quality assurance and testing. This work is in progress and to date has identified a small number of “issues” to be corrected in the Low-Fi files. NJOY [14] processing has identified data entry errors (resulting in unreasonably large uncertainties) in a small number of files. An eigenvalue analysis of each of the symmetric LB-5 sub-subsections identified that forty of the materials have significant negative eigenvalues, beyond what is normally attributed to round-off [15]. All issues uncovered during this phase will be communicated and resolved. The processing and review of these files by both PUFF and NJOY (ERRORJ) at several of the labs has already led to improvements not only in the Low-Fi files but also in the processing codes for the covariance data. Tools to visualize covariance data are useful in the QA process; in addition to capabilities embedded in the major processing systems, recent enhancements to Sigma at Brookhaven are also very promising [16].

Ultimately, the MF = 33 covariance files for each nuclide will be archived and made available by the NNDC at Brookhaven. It is not planned to merge the Low-Fi covariance data with the released ENDF/B-VII.0 evaluations. It is certainly possible that, over time, some of this work could form the basis for MF = 33 covariance files that formally become a part of future ENDF/B-VII releases for some evaluations.

It is expected that application libraries will be created using data from Low-Fi. Of necessity, these application libraries will mix evaluated cross sections and covariances for some materials that arise from different, and inconsistent, sources. As long as the source of all data for these application libraries is documented, we believe that the value in testing Low-Fi covariances justifies these efforts. Initial versions of such application libraries that derive a substantial portion of covariance data from Low-Fi have, in fact, already been documented [17, 18].

One obvious benefit of having complete Low-Fi covariance data is the opportunity to assess results from practical applications. One outcome should be the identification of materials for which high-fidelity covariances are required. Members of the Low-Fi collaboration would count it as a success, if, over time, the results of this work became obsolete as they were supplanted by high-fidelity covariances.

VII. SUMMARY

In summary, the Low-Fi project was sponsored by the US DOE Nuclear Criticality Safety Program and involved a collaboration among Argonne, Brookhaven, Los Alamos, and Oak Ridge National Laboratories.

Complete, in energy and reaction, covariances have been produced for all 393 materials in ENDF/B-VII.0 using a variety of methods. The product of this work should enhance sensitivity/uncertainty capabilities and studies

for a variety of nuclear applications.

Support of the DOE US Nuclear Criticality Safety Program is gratefully acknowledged.

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