ENDF/B-VII.0 library and its extension to covariances

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1. Introduction

The new ENDF/B-VII.0 library [1] was produced by the CSEWG collaboration and represents a common achievement by numerous US laboratories. The library also benefited from appreciable input from the international nuclear data community, with particular contribution by KAERI in the range of fission products. In the present paper we outline achievements of the ENDF/B-VII.0 library and indicate cross section covariances as a focus of the current and future activities leading to its successor. To some extend, our discussion is focused on the aspects in which BNL was involved.

2. ENDF/B-VII.0 library

The next generation general purpose Evaluated Nuclear Data File, ENDF/B-VII.0, of recommended nuclear data for advanced nuclear science and technology applications was released in December 2006. It contains data primarily for reactions with incident neutrons, protons, and photons on almost 400 isotopes, based on experimental data and theory predictions. Some of the principal advances over the previous ENDF/B-VI library are the following:

- New cross sections for U, Pu, Th, Np and Am actinide isotopes, with improved performance in benchmark tests;
- More precise standard cross sections for neutron reactions;
- Improved thermal neutron scattering;
- An extensive set of neutron cross sections on fission products ;
- A large suite of photonuclear reactions;
- Many new light nucleus neutron and proton reactions;
- New radioactive decay data;
- New actinide fission energy deposition;
- New methods for uncertainties and covariances, together with covariance evaluations for some sample cases.

Extensive validation, using radiation transport codes to simulate measured critical assemblies, showed major improvements:

- The long-standing underprediction of low enriched uranium thermal assemblies is removed;
- The ^{238}U and ^{208}Pb reflector biases in fast systems are largely removed;
- ENDF/B-VI.8 good agreement for simulations of thermal high-enriched uranium assemblies is preserved;
- The underprediction of fast criticality of ^{233,235}U and ^{239}Pu assemblies is removed; and
- The intermediate spectrum critical assemblies are predicted more accurately.

Unable to discuss all details of the library we choose to address fission products due to the significant contribution from KERI. Many of the ENDF/B fission product evaluations, defined as materials with Z = 31 - 68, had not been revised for a very long period of time. For a set of 74 materials, including 19 materials considered to be of priority, entirely new evaluations were performed for ENDF/B-VII.0. These new evaluations were produced by the following laboratories:

- 32 materials were evaluated by BNL-KAERI collaboration,
- 25 materials were evaluated by BNL,
- 5 materials were evaluated by BNL-JAERI collaboration,
- 8 materials were evaluated by BNL, including covariances produced by BNL-ORNL-LANL collaboration, and
- 4 materials of specific interest were evaluated by LLNL (^{74,75}As), LANL-BNL (^{89}Y) and BNL (^{90}Zr).

This evaluations were performed using the nuclear reaction model code EMPIRE [2] and in most cases benefited from the new compilation of resonance parameters performed by Mughabghab [3]. This approach enabled us to apply the advanced nuclear reaction physics and resulted in a set of consistent evaluations covering cross sections, angular distributions and energy-angle correlated cross sections for all relevant reaction channels.

3. Covariances

Neutron cross section covariances (uncertainties and correlations) are needed for several distinct types of applications. Probably the most important among them is the need to assess uncertainties of integral quantities such as design and operational parameters of nuclear power reactors. Data adjustment represents another important use of neutron covariances.

The ENDF/B-VII.0 library contains covariances for 26 materials only, i.e., for less than 7% of the materials included in the neutron sub-library. Moreover, only for 13 of these materials the covariances were determined specifically for ENDF/B-VII.0 and can be considered complete.

The issue of scarce neutron covariance data was recently addressed by the U.S. nuclear criticality safety program, which initiated the ``low-fidelity'' covariance project. The goal of this exercise was to produce rough set of covariances covering five major reaction channels, (n,el), (n,inl), (n,2n), (n,g) and (n,f) on all materials to provide a solid base for testing new tools for advanced numerical simulations employing nuclear data uncertainties and correlations. The project involved four US laboratories: BNL, LANL, ORNL, and ANL.

BNL role was to produce covariances in the fast neutron region for 307 materials from ^{19}F through ^{209}Bi. Similar covariances for actinides were determined by LANL, while ORNL provided simple but convincing estimates of the covariances in the resonance region.

The methodology, employed at BNL, in the fast neutron region is based on the nuclear reaction model code EMPIRE coupled to the LANL Bayesian filtering code KALMAN [4]. The results are almost entirely based on model calculations with marginal reference to experimental data. The EMPIRE code calculated cross sections according to appropriately selected models and model parameters, while KALMAN propagated the model parameter uncertainties into cross section (co)variances. The most relevant model parameters are those related to optical potential and nuclear level densities. These parameters were varied to calculate partial derivatives of cross sections, defining the elements of the sensitivity matrices. The calculated reaction cross sections, sensitivity matrices along with the model parameters and their uncertainties represented input quantities for the KALMAN code. Such a procedure necessarily depends on the estimation of the model parameter uncertainties and their correlations.

These massive calculations revealed the intriguing structure in cross section uncertainties and we are investigating its physics background.

The results of the ``low-fidelity covariance'' project can be used as a useful starting point for any future effort in covariances. BNL is actually involved in such an exercise aiming to provide covariances needed for the data adjustment related to the GNEP project. This real design oriented effort naturally calls for more refined modeling and more explicit use of experimental data.

3. Conclusions

The overall performance of the ENDF/B-VII.0 library is very good - noticeably better than the ENDF/B-VI.8 library released in 2001. The library has been demonstrated to contain much better physical representations of the data, to span a much greater range of nuclear data, and to perform much better than previous ENDF evaluations over a broad range of applications. This should provide a strong incentive for nuclear applications using earlier versions of ENDF to switch over to ENDF/B-VII.0 data.

Further development of the major US nuclear data library will focus on quantification of the uncertainties and their correlations, which became instrumental in advanced design calculations, data adjustment, and enhanced requirements on nuclear criticality safety. Considerable advances in computer technology and improvements in neutronics simulation codes allow refined prediction of integral quantities that start to probe the uncertainties of basic nuclear data.

The U.S. data effort is poised to continue the strong international collaboration to address future improvements in the ENDF files.

REFERENCES

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