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TITLE: Current Status of Fusion-Relevant Covariance Data

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DISCLAIMER

Current Status of Fusion-relevant Covariance Data

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ABSTRACT

The following review of the current status of formatted data covariance files and their multigroup processing is a contribution to the IAEA Advisory Group Meeting on "Improved Evaluations and Integral Data Testing for FENDL." to be held at the Max-Planck-Institut für Plasmaphysik, Garching, Germany, 12-16 September 1994. The draft agenda of this meeting lists as Item 6 the "assessment of present status and role of uncertainty files, their processing and sensitivity studies related to FENDL." We conclude that this is an important and timely topic and recommend needed actions in this field.

Requirements for Data Covariances

There two potentially important applications of processed data covariances in the design of any large nuclear facility such as ITER. In a project of this size and cost, it is only prudent to include in the overall design process a "data assessment," which is a determination by some means of whether or not the nuclear data being employed in the prediction of such quantities as radiation dose to operating personnel, radioactive waste generation, tritium production, etc., are sufficiently accurate to achieve program objectives. The final result of a "data assessment" is a simple yes or no. The estimated uncertainty due to the basic data either is either acceptable or unacceptable. If unacceptable, some action is required to improve the data, such as some combination of new measurements, new calculations, or new evaluations (of the data or of the covariances of the data).

The ITER project is fortunate to be the beneficiary of over a decade of work by the data evaluation community to characterize the quality of their distributed nuclear data evaluations by means of formatted data covariance files, starting with the famous "File 33" of ENDF. Both the formats and the contents of the ENDF covariance files have, since their inception, undergone major improvements in quality of the information presented and the level of detail covered.[1] Thus we are, at least in principle, in a position to quantitatively estimate the uncertainty in the prediction of almost any neutronic property of the ITER blanket and shield due uncertainty in the basic data that go into such a prediction. However, as discussed below, some problems remain to be addressed.

The second major application of data covariances is a more active one, where one tries to improve the quality of the entire package of neutronic tools by confronting specific neutronic predictions with the results of integral measurements in relevant geometries. The major question to answer here is "Are the predictions consistent with the integral measurements?" To answer this seemingly simple question requires four different types of information:

(1) the integral data (some detector response in some assembly); and
(2) uncertainty in the integral data due to the measurement process; and
(3) the predicted response; and
(4) uncertainty in the predicted response due to uncertainties in the basic data employed.

Item 4 requires, of course, the very same data and methods that are required in the "data assessment" activity discussed in the previous paragraph. The kind of "consistency analysis" just described implies the need to collect much more information, namely, Items 1-3 in the list above. The benefits of integral experiment analysis are also larger—at the end of the analysis, one may be able to uncover errors in any of the information of types 1 through 4. In particular, errors in the transport code (or in the way the code is being employed by the analyst) can often be identified by analyzing integral experiments.

Status of Covariance Processing

The specific aim of this paper is review the current status of our ability to quantitatively estimate the uncertainty of computed neutronic properties due to the uncertainty in the basic data. This is practically the whole problem in "data assessment" and a major part of the problem in integral experiment "consistency analysis." Unfortunately, to move from a statement about the uncertainty of the basic data (as in contained in File 33 and related files of ENDF) to a statement about the data-related uncertainty of a engineering prediction requires considerable labor. Traditionally, the first step of such an analysis is to employ the ENDF data together with a processing program to compute the uncertainty of multigroup cross sections. The second step is to compute the sensitivity of the desired neutronic quantity to individual multigroup cross sections. The third step is a simple matrix multiplication of the uncertainties with the sensitivities, to obtain the desired uncertainty by the law of "propagation of errors."

The most advanced tool available for multigroup processing of ENDF-formatted covariances is the ERRORR module[2] of NJOY. ERRORR currently processes all of the cross-section covariance data in the "pointwise" File-33 format into a user-specified multigroup structure. The biggest remaining deficiency of ERRORR is that most of the newer ENDF-6 formats for representing uncertainties of energy and angle emission spectra are not yet processed. For example, no processing is yet

done for File 30, which G. Hale, for example, plans to use to describe all ^{1}H covariances (also see further comments below about File 30), nor for File 34, which the European Fusion File uses to describe ^{56}Fe angular distribution uncertainties, nor for the proposed File 36, which H. Vonach plans to use in the near future to describe uncertainties in multiplicities and emission spectra in File 6. Although of reduced importance for fusion, the processing of resonance-parameter covariances (File 32) is possible only for a the most commonly used File-32 options. In particular, R. Peelle's new format allowing correlations between the parameters of different resonances is not handled.

A second category of problem has to do with the output format of the processed multigroup covariances. At present all multigroup covariances computed with the ERRORR module of NJOY are post-processed by the COVR module[3] into BOXR format, which is the cross-section covariance input format employed in the SENSIBL code[4]. If a different sensitivity system/covariance format will be used by the ITER team, then the corresponding formatting capability should be added to COVR. The changes should be relative straightforward to implement, once the target sensitivity system is specified by the ITER team.

Uncertainty of Neutron and Photon Emission Spectra

An important technical aspect of the neutronic analysis of ITER is the geometric complexity of the ITER design, caused by such necessary features as vacuum-pumping ports, divertors, and channels for the insertion and removal of experimental modules. This geometric complexity is compounded by the extremely anisotropic scattering of 14-MeV neutrons in their interactions with structural materials. Even the secondary neutrons and gamma rays from 14-MeV neutron interactions are often higher in energy (hence, scatter more anisotropically) than the radiations typically found in fission systems. Predicting the behavior of superconducting and other sensitive materials in this (very 3-dimensional) radiation environment is, in itself, a daunting task. It is very important to note that the geometrical complexity of this problem will also very likely place new demands on the tools used in sensitivity and uncertainty analysis. For example, the very commonly made assumption that all uncertainty resides in the cross section values (or, equivalently, that all secondary angle-energy emission spectra are perfectly known) is almost certain to be an unacceptable approximation in this application.

In view of this, it is important to point out that we are now on the verge of solving a long-standing problem in the representation of emission spectrum uncertainties, namely, how to describe, in a practical way, the "covariance matrix of a transfer matrix." This has been attacked in the past by the SED-SAD approach, which arbitrarily enforces an additional, very coarse multigroup structure on the problem. Somewhat similar approaches are employed in the existing ENDF File 35 and the proposed File 36. It is difficult to see how to evaluate the covariances to put into

such a "super-coarse" structure or, more to the point, how a processing module such as ERRORR can sensibly re-bin such coarse covariances into other user-specified structures. The basic problem here is that coarse-group covariance data are already integrated over energy and angle, and this integration cannot be undone by a processing code.

File 30 solves the problem of describing the "covariance matrix of a transfer matrix" by factoring this impossibly large covariance matrix into a triple product involving two much smaller matrices. The first is covariance matrix describing a relatively small number (30-50) of underlying parameters, assumed to be responsible for the most important cross-section and emission-spectrum uncertainties. In a particular evaluation scenario, the appropriate choice of parameters might be a subset of the parameters that were input to a statistical nuclear model code in computing the data near 14 MeV. The second matrix contains the sensitivities of each element of the transfer matrix to each "uncertain" parameter. Thus, for example, instead of storing a 100,000 x 100,000 matrix somewhere, one only needs to store (for 40 parameters) a 40 x 40 matrix and a 40 x 100,000 one. Existing sensitivity analysis systems will need some slight modifications to handle covariances in this factored form before sensitivity calculations based on the File-30 method can actually be carried out.

Conclusion

To summarize, a three-pronged attack is needed: first the ERRORR covariance processing module of NJOY (the ERRORR module) requires updating to permit the processing several new version-6 covariance formats that are of interest in fusion; secondly, we may need to update the COVR module to output data in the exact form specified for ITER analyses; and thirdly, the data community needs to work with sensitivity specialists to update the sensitivity codes selected for ITER analyses to accommodate File-30 type factored covariances.

References

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2. "ERRORR," Chapter X of R. E. MacFarlane and D. W. Muir, "The NJOY Nuclear Data Processing System, Version 91" Los Alamos National Laboratory report LA-12740-M, to be published (1994).

3. "COVR," ibid., Chapter XI.

4. D. W. Muir, J. W. Davidson, D. J. Dudziak, D. M. Davierwalla, C. E. Higgs, and J. Stepanek, "A Benchmark-Problem Specification and Calculation using SENSIBL, a One- and Two-Dimensional Sensitivity Analysis Code of the AARE System." Fusion Eng. and Design 10, 79-85 (1989).