Working Party on International Nuclear Data Evaluation Cooperation, Subgroup 24

Covariance Data in the Fast Neutron Region

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M. Herman for SG24
National Nuclear Data Center, BNL, USA

Abstract

The second year of the project has been dedicated to testing covariance capabilities developed in the reaction codes EMPIRE and TALYS. In particular, EMPIRE has entered the production mode providing a considerable number of covariances for ENDF/B-VII.0 and for SG26. This intensive exercise allowed the code users to gain a certain experience with the EMPIRE/KALMAN methodology. In addition, several results were provided by the Monte Carlo method using both the TALYS and EMPIRE codes. Both approaches proved to generate sensible, formally correct covariances, although rigorous inclusion of experimental data continues to be a major issue. In this respect some new ideas have been proposed and will have to be developed, coded and tested during the third year of the project.

Introduction

SG24 was established at the WPEC meeting in April 2005 and charged to develop methodology and tools for producing covariance data in the fast neutron region. Specific goals of the Subgroup are:

- Develop covariance generation capabilities in the nuclear reaction model codes EMPIRE, McGNASH and TALYS using:
  - Monte Carlo sensitivity method, and
  - KALMAN (Bayesian) method.
- Compare results of these methods and validate the methodology against experimental covariance data.
- Address correlations between the fast neutron region and the neutron resonance region (low priority goal).
- Produce covariance data for a few selected materials.

SG24 members are:

Chairman	M. Herman, ENDF (BNL)
Monitor	A. Koning, JEFF (NRG)
ENDF	P. Oblozinsky D. Rochman and M. Pigni (BNL), T. Kawano (LANL), D.L. Smith (ANL)
JEFF	A. Koning, (NRG), R. Capote and A. Mengoni (IAEA), A. Trkov (IAEA/JSI), Eric Bauge (CEA), P. Talou (CEA/LANL), H. Leeb (TU Wien)
JENDL	T. Nakagawa and K. Shibata (JAEA)

BROND E. Gai, A. Ignatyuk, V. Pronyaev (IPPE Obninsk)

In the first year (April 2005 – April 2006) subgroup activities concentrated on the development of covariance capabilities within codes used for theoretical modeling of nuclear reactions and investigation of methods for including experimental data in the Monte Carlo sensitivity method.

Covariance capabilities in nuclear reaction codes

Both EMPIRE and TALYS are currently capable of producing nuclear data covariances and storing them in the ENDF-6 format. TALYS is using a Monte Carlo approach to drawing model parameters from uncorrelated distributions that are adjusted so that model generated variances reproduce experimental uncertainties and spreads of the measurements. A similar approach is also being used in EMPIRE (Capote and Trkov) although some calculations were performed using the GANDER system that derives covariances from the experimental data using model calculations as a prior. A different approach is being used at BNL where EMPIRE has been coupled to the Los Alamos KALMAN code. In the latter approach experimental data are naturally included in the procedure although large numbers of experimental data result in unphysically low uncertainties. In such cases, additional assumptions have to be invoked in order to control the magnitude of the uncertainties. More details concerning the above mentioned implementations can be found in the previous SG24 report.

New covariances

Release of the ENDF/B-VII.0 library in December 2006 and a pressing request from the SG26 accelerated practical application of the recently developed tools for generation of covariances, although some physics issues remain open. These extensive, although a bit premature, exercises exposed EMPIRE and TALYS to a severe test and allowed code users to gain experience in calculating model based covariances.

In the case of ENDF/B-VII.0, in order to obtain the sensitivity matrix with the EMPIRE code, about 10-15 of the most relevant model parameters (optical model, level density and preequilibrium strength) were varied independently, typically by about 5 % around the optimal value, to determine their effect on total, elastic, inelastic, capture, (n,2n), (n,p) and (n,gamma) cross sections in the full energy range of the evaluation. Sensitivity matrix elements were calculated by considering the change of a given reaction cross section in response to the change of a particular model parameter. A series of scripts was employed to transfer such sensitivity matrix information along with the experimental data to the KALMAN code, and to prepare adequate input.

Final uncertainties were adjusted to reproduce error bars on the best measurements by preventing errors on model parameters (initially set at 10 %) from falling below reasonable limits (3 %). This procedure was necessary since the Kalman filter tends to reduce uncertainties on model parameters if many consistent experimental data are well reproduced by the model calculations. In doing so, the Kalman filter ignores approximations inherent in the nuclear reaction models and parameter adjustments introduced during the evaluation.

In the case of 232Th and 231,233Pa, cross section covariance data for ENDF/B-VII.0 were generated by the Monte Carlo technique using the EMPIRE code. The GANDR code system

updates these nuclear model covariance results by merging them with the uncertainty information for available experimental data using the generalized least-squares technique.

Comparison of different approaches for covariance determination

A small meeting, involving a few members of the SG24, was held in July 2006 at Los Alamos. The discussion concentrated on different approaches to covariance determination and some related technical aspects. Kawano presented a comparison of the Monte Carlo and Kalman methods using a simple model – the Lorentzian function. The main characteristics of both methods are:

- KALMAN Method
    - Error propagation with the first order Taylor expansion
    - Calculation is fast
    - Second order effects are not taken into account
    - Experimental data are combined using Bayes theory
- Monte Carlo Method
    - Error propagation by means of the random sampling technique
    - Calculation is slow
    - Higher order effects are included
    - Including experimental data is not straightforward - might be possible by random sampling in the data space

The numerical test, involving calculation of uncertainties and correlation matrices with both methods, produced very close results indicating that, in absence of experimental data, both methods are equivalent. It was decided that a more realistic comparison will be performed taking 89Y as a test case. These results will be presented at the SG24 meeting in Paris, May 18, 2007.

Inclusion of experimental data

At the current stage, inclusion of experimental data into the covariance determination appears to be a major issue. The KALMAN method accounts for them naturally but suffers from the general 'deficiency' of all Bayesian approaches – uncertainties tend to reach values that are considered far too small if many experimental data are included in the analysis and the representation of experimental systematic errors and their correlations is missing or inadequate. So far, the only practical remedy to this problem is to prevent uncertainties on the model parameters to fall below some sensible limit (say 3%). While this procedure is simple and effective it introduces a highly arbitrary component into the estimation of uncertainties.

The Monte Carlo method, in its original formulation by D. Smith, has no explicit provision for experimental data. A conceptually simple way to work around this is to reject Monte Carlo samplings that produce results lying outside a reasonable band defined by the experimental data. Alternatively, one may adjust parameter sampling intervals in a way to ensure that final results are within the above mentioned band. This procedure, successfully used by A. Koning in TALYS, provides useful results on parameter uncertainties but lacks mathematical rigor and is affected by arbitrary judgment (width of the band). The Monte-Carlo plus GANDR formalism is more rigorous than these two *ad hoc* approaches to merging modeling and experimental results, but it represents a hybrid approach rather than a full Monte-Carlo treatment of the evaluation process.

An interesting method, called backward-forward Monte-Carlo, has been developed by E.

Bauge. This method determines the model parameter covariance matrix from the Monte-Carlo (MC) sampling combined with a chi-squared approach (backward MC), and then propagates the covariances of the model parameters to obtain the cross section covariance matrix by MC sampling (forward MC). Application of this elegant method, however, is limited to relatively simple cases since more complex ones are difficult to handle.

Recently, a new idea, based on random sampling from both, model and experimental, distributions has been proposed by D. Smith. R. Capote and A. Trkov have refined the method by including weighted averages that seem to fulfill all expected limiting cases. The method was finally made feasible by the availability of the SAMPAR code (written by Soo-Youl Oh) that generates random numbers from some typical (normal, lognormal, and uniform) multivariate distributions. The first results obtained by using this method are expected to be presented at the SG24 meeting in May 2007. They will be compared with the study of 89Y performed specially for this purpose at BNL using the KALMAN method.

We also note that, the search for the invariants (general measures) in covariances was performed by E. Gai and V. Pronyaev. These invariants are certain conserving quantities obtained from covariance matrices of the evaluated data which are practically not dependent on a model used in the fit. Introducing the general measures of the uncertainties allows to verify whether the least-squares fit was done for a given sets of experimental data and to compare the covariance matrices of the evaluated uncertainties obtained in different fits, which often look very differently.

Based on these general measures and related integral quantities, Gai and Pronyaev conclude that the uncertainties obtained in the course of the international evaluation of the neutron cross section standards are realistic while the CSEWG estimate of the corridor of errors based on the "modern day experimental possibilities" is pessimistic. Any estimation considering uncertainties assigned to the individual experiments should give lower uncertainties.

5. Conclusions

During the second year of activity, SG24 successfully applied covariance capabilities developed in the two main reaction codes - TALYS and EMPIRE. This effort resulted in the considerable amount of covariance data produced in support of the two major projects – ENDF/B.VII.0 and SG26. For the ENDF/B-VII.0, 12 evaluations of covariances were produced with EMPIRE/KALMAN and 3 with EMPIRE/MC methodology. The numbers are even more impressive in the case of SG26 for which preliminary covariances for 36 materials were produced with the EMPIRE/KALMAN method and 3 with TALYS/MC.

In spite of the fact that many covariances were produced using the EMPIRE and TALYS codes, one should keep in mind that there are issues that still should be resolved. The most pressing one is the treatment of experimental data in both, KALMAN and Monte Carlo, methods. There is a hope that the new concept of weighted drawing from the multivariate distributions might be an answer.

Determination of covariances for materials without experimental data will necessarily rely on model calculations. To this end we need reliable estimates of uncertainties and correlations for model parameters – an issue that goes beyond the mandate of SG24. However, this

important activity could be considered within the scope of the IAEA RIPL project. Finally, there is urgent need to clean the EXFOR data base of experimental data from mistakes, misprints and obviously wrong data so that it can be safely used as a reference in large scale, automated model calculations aiming at the determination of covariances for cross sections and model parameters.