Subgroup 24: Covariance Data in the Fast Neutron Region

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Abstract

In the frame of the Subgroup 24, the two major nuclear reaction codes EMPIRE and TALYS were extended to provide covariance data for nuclear reaction cross sections in the fast neutron energy range. Several test calculations were performed and complete covariances were created for the chain of 8 Gd isotopes and for 232-Th, all included in the ENDF/B-VIIb2 library. Numerous studies are being carried out on inclusion of experimental uncertainties in the model generated covariances and comparison of different approaches.

1 Introduction

Subgroup 24 (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 nuclear reaction model codes EMPIRE, McGNASH and TALYS using:
  - Monte Carlo sensitivity method [Smi04],
  - and KALMAN (Bayesian) method [Kaw97].
- Compare results of these methods and validate the methodology against experimental covariance data.

- Address correlations between fast neutron region and neutron resonance region (low priority goal).
- Produce covariance data for a few selected materials.

SG24 members are:

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Monitor A. Koning, JEFF (NRG)

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JEFF A. Koning, JEFF (NRG), R. Capote-Noy and A. Mengoni (IAEA), A. Trkov (IAEA/JSI), Eric Bauge (CEA), H. Leeb (TU Wien), H. Vonach? (U Wien)

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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.

2 Covariance capabilities in nuclear reaction codes

2.1 TALYS

TALYS [Kon04] has been developed in a way that makes implementation of the Monte-Carlo [Smi04] method quite natural. In particular, TALYS has been ready to generate random inputs and its high speed enables hundreds or thousands of calculations in a reasonable time.

Covariance generation in TALYS is accomplished by subjecting it to a Monte Carlo method for perturbing input parameters, an approach that is now possible with the available computer power. After establishing uncertainties for parameters of the optical model, level densities, gamma-ray strength functions, fission barriers etc., random input files are produced for the TALYS code. These deliver, provided enough calculations (samples) are performed, uncertainties + all off-diagonal elements for all open reaction channels. The uncertainties of the nuclear model parameter are tuned such that the calculated cross section uncertainties coincide, to a reasonable extent, with uncertainties obtained from covariance evaluations based on experimental data.

Number of calculations were performed by A. Koning providing proof of feasibility for the Monte-Carlo method. TALYS has also been equipped with the ENDF-6 formatting routines allowing to store covariance data in MF=33 using LB=5,6,8. Actual possibilities of the code go far beyond quantities considered in the ENDF-6 format.

2.2 EMPIRE

2.2.1 KALMAN implementation

EMPIRE [Her04] code has recently been upgraded to allow generation of covariances using both Monte-Carlo [Smi04] and KALMAN methods.

KALMAN implementation was a joint effort of BNL (M. Herman) and LANL (T. Kawano). Sensitivity calculations were coded in the EMPIRE core for most of the calculated cross sections such as total, elastic, capture, and all (n,xn yp za) reactions. In order to keep size of the matrix within easily manageable limits reactions populating discrete levels are not treated explicitly. Model parameters varied in the sensitivity calculations include optical potential, dynamic deformations (Coupled Channels), level densities, fission barriers, preequilibrium strength, and emission widths for all ejectiles. A series of bash and Perl scripts have been written to automatically extract experimental data from the C4 file and prepare input for KALMAN compatible with the results of EMPIRE calculations. Covariances are produced by the KALMAN code [Kaw97] and ENDF-6 formatted (MF=33, LB=5) by appropriate scripts and FORTRAN codes.

Detailed study of the structure of the model-generated correlation matrices has been performed by D. Rochman at BNL. It can be concluded that complicated shapes of correlation surfaces are fully understood. They result from different sensitivity to various model parameters, that are often important only in the limited energy range and different reaction mechanisms contributing to specific energy regions. In certain cases (e.g., total cross section), particular dependence on certain model parameters (in case of total cross section on optical potential depths) may result in a very small uncertainties in a the close vicinity of some energy points.

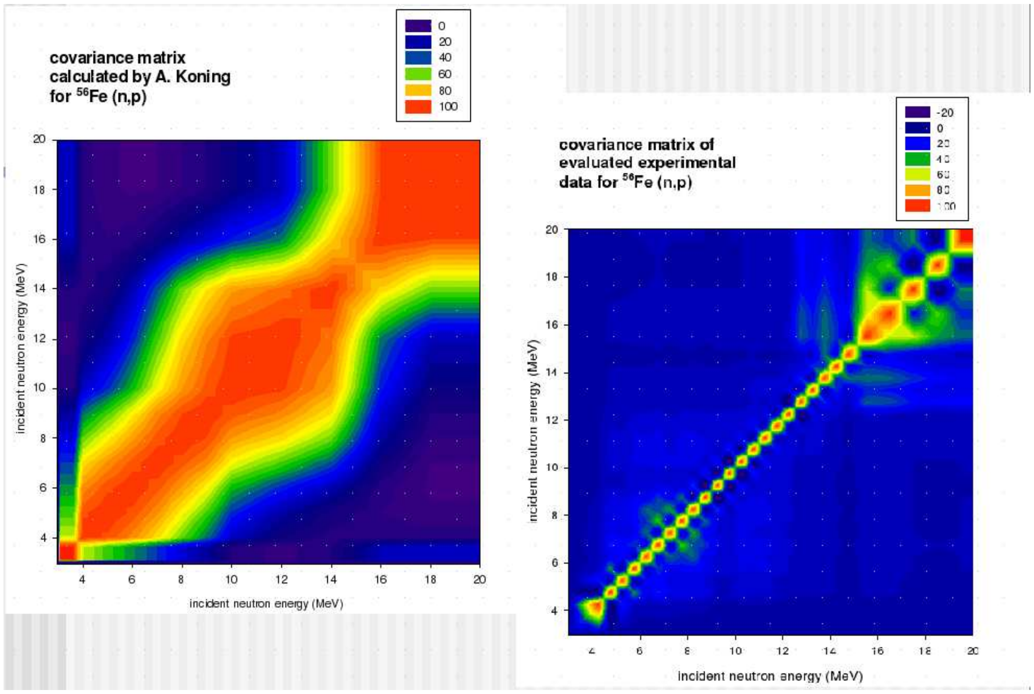

Figure 1: Comparison of self-correlation matrix for 56-Fe(n,p) reaction generated by Koning with TALYS (Monte-Carlo method) (left) and correlations obtained by Tagesen and Vonach from analysis of experimental data [Von92].

2.2.2 Monte Carlo implementation

Implementation of the Monte Carlo method in EMPIRE has been accomplished by R. Capote and A. Trkov at IAEA. The code is run number of times with specified input parameters drawn randomly from the uniform distribution. No parameter correlations are included at this stage. Dedicated codes have been developed to construct covariances and to convert them into ENDF-6 files. This implementation is analogous to the one used in TALYS.

3 Experimental data and model generated covariances

While experimental data are naturally included in the KALMAN approach they are not necessarily intrinsic to other methods. Therefore, including uncertainties obtained in real measurements is essential for producing realistic covariances with these methods. Both deterministic error propagation and Monte Carlo simulation methods are found to produce reasonable covariance information provided that the uncertainties are assumed to be based solely on model parameter errors. However, rigorous methods for also including the direct effects of experimental data and their uncertainties on an evaluation obviously need to be developed. As a first attempt, the generalized least squares algorithm has been demonstrated by D. Smith to be useful for merging the results of model parameter and experimental information in a rigorous manner. Results for a test case have been reported. This merging analysis involves two steps, and it is carried out in the space of the observable physical quantities (cross sections) rather than parameter space. Ultimately, a full Monte Carlo analysis that is simultaneously inclusive (one step) of both nuclear modeling and experimental information is sought. Development of such an approach - one that will clearly need to be based on sampling of joint probability distributions involving both nuclear model and experimental parameters - and ideas for carrying this out are now under consideration.

Recently, Monte Carlo EMPIRE calculations were coupled to the GANDER system to account for the experimental data. The preliminary results [Trk06] are very encouraging and put into evidence the role of correlations between different experiments. There are indications that inclusion of these correlations helps to avoid unphysically small cross section uncertainties.

An interesting method, called backward-forward Monte-Carlo, has been reported by E. Bauge. This method determines the model parameter covariance matrix from the Monte-Carlo (MC) sampling combined with a χ^2approach (backward MC), and then propagates the covariance of the model parameters to obtain the cross section covariance matrix by MC sampling (forward MC).

4 Results

A. Koning has been using Monte Carlo method in TALYS to generate covariance data for a number of reactions on various targets. These include comparison with a careful experiment-based covariance evaluation performed by Vonach et al. [Von92] for 56-Fe. The widths of the model parameters were adjusted such that reasonable agreement with the uncertainties of Vonach et al. was obtained. This comparison, shown in Fig. 1, demonstrates a striking difference between the two approaches that is due to different 'type of knowledge' being used in both cases. Model calculations naturally predict strong correlations since individual model parameters tend to affect broad energy ranges, while measurements are believed to be quite indepen-

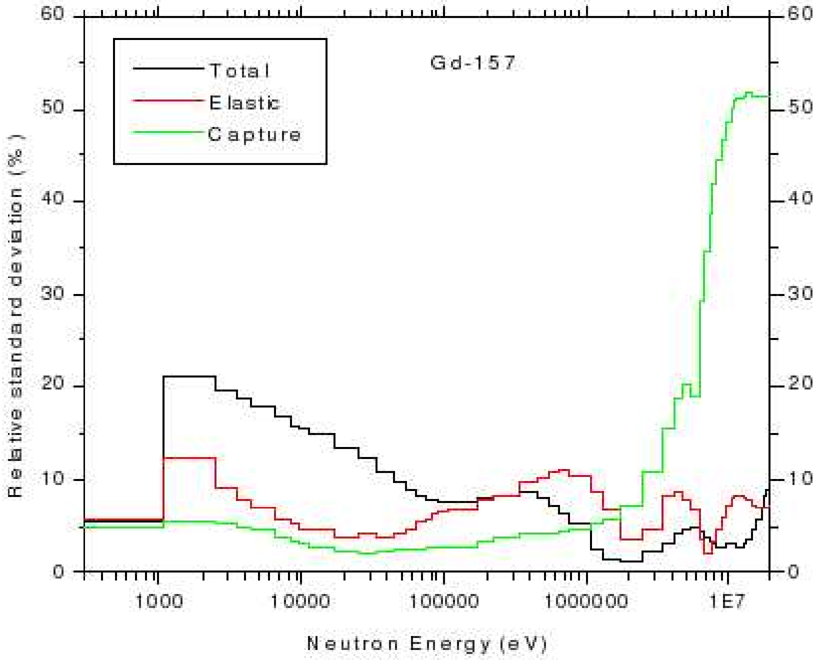

Figure 2: Uncertainties for total, elastic and capture cross sections on 157-Gd obtained with EMPIRE/KALMAN [Roc06].

dent from each other, i.e., long range correlations (systematic errors) are assumed to be relatively weak. We should expect that bringing both sources of knowledge together should produce intermediate result for the correlation matrix and... lower uncertainties.

We also note relevant study of uncertainties of optical model potential performed by A. Koning (using Monte Carlo method implemented in TALYS) that indicates about 3% uncertainty for the most important parameters.

Complete set of covariances was generated by D. Rochman et al [Roc06] for the chain of 8 Gadolinium isotopes using KALMAN method and EMPIRE code. These evaluations make part of the ENDF/B-VIIb2 release and are accessible at [ENDF]. Sensitivity matrices were calculated taking into account 15 model parameters including real and imaginary depths of optical model potentials for neutrons and protons, level density parameters for compound, target, as well as (n,2n) and (n,p) residues, tuning of compound nucleus emission widths for gammas, neutrons and protons, free

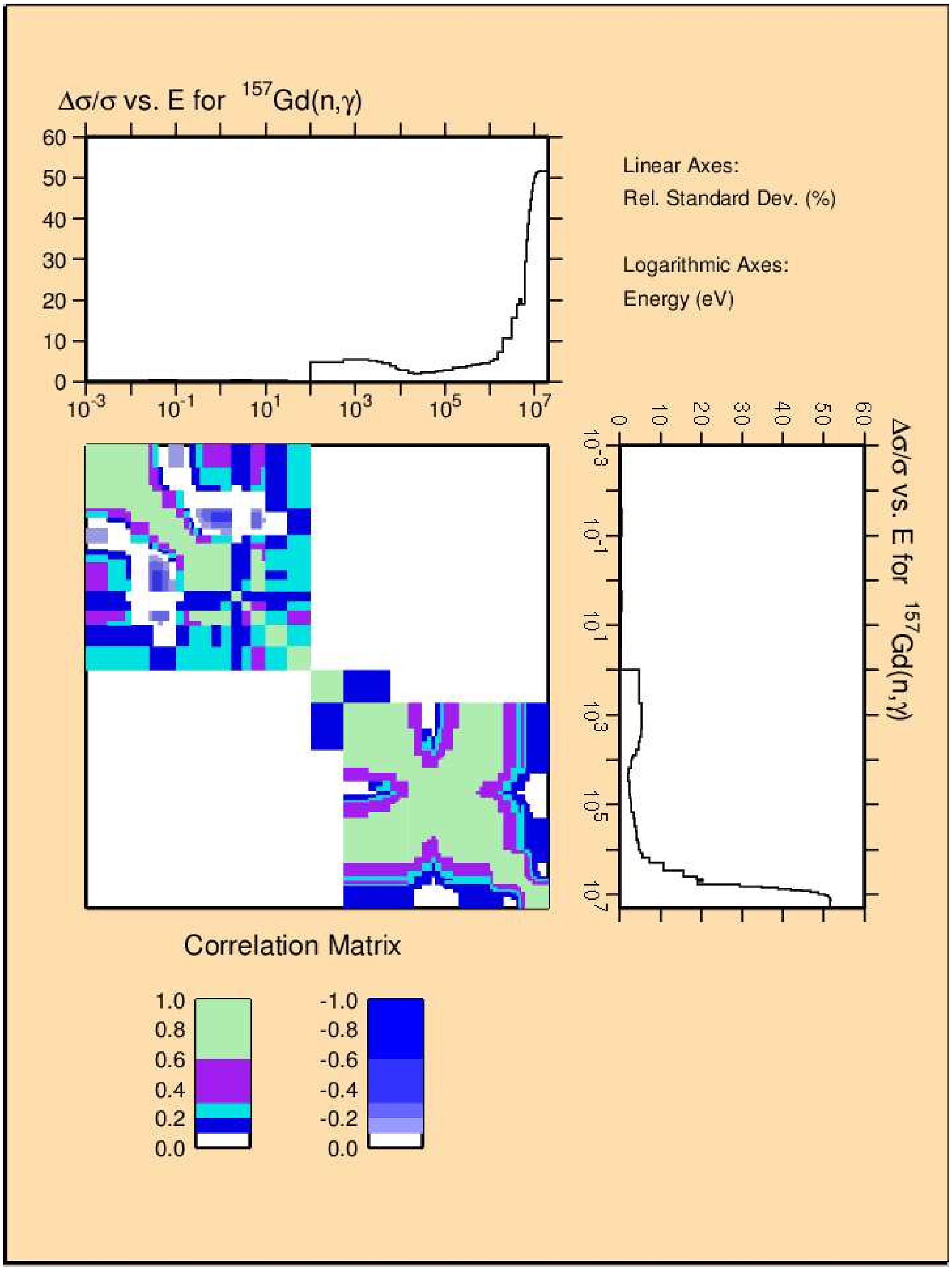

Figure 3: Multi-group correlation matrix and uncertainties for neutron capture on 157-Gd produced by processing ENDF/B-VIIb2 evaluation with ERRORJ [Roc06].

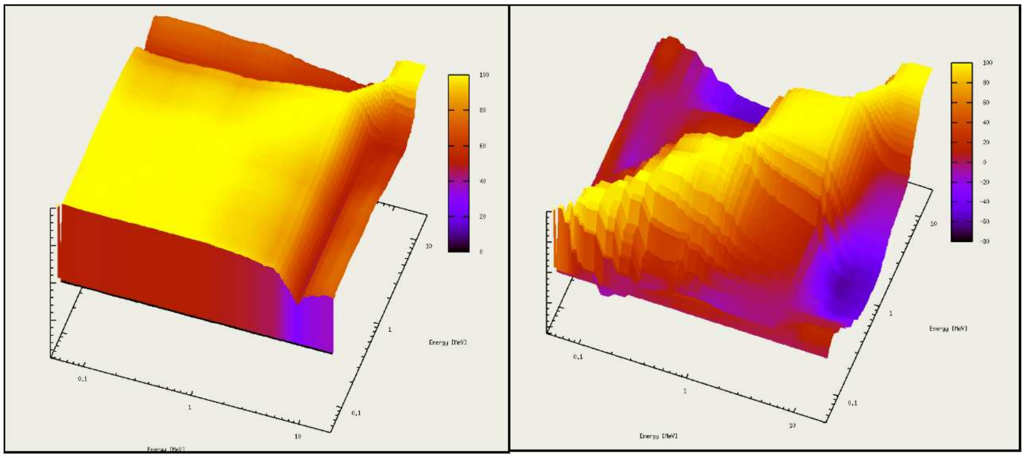

Figure 4: Effect of experimental data for covariance determination using KALMAN method [Roc06]. Left plot shows correlation matrix for neutron capture on Gd-157 obtained purely from model calculations while the right plot was obtained with experimental data taken into account.

path in the exciton model, and multiplicative factor on the response functions in the Multistep Direct model. Covariances were produced for total, elastic, capture, total inelastic (MT=4), (n,2n), (n,p) and (n,alpha) reactions. Experimental data, cleaned from the obvious discrepancies, were used as an input to KALMAN. 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%). Calculations have been extended throughout the unresolved resonance region. Fig. 2 shows total, elastic and capture uncertainties obtained for 157-Gd. All Gd files were successfully processed through NJOY and ERRORJ to produce group-wise covariance data. Example plots of cross section self-correlations and associated uncertainties created by ERRORJ are shown in Fig. 3.

We note, that comparison of EMPIRE/KALMAN calculations with and without experimental data is consistent with conclusions drawn from the comparison of TALYS results with experimental-based covariances. Fig. 4 shows that EMPIRE/KALMAN calculations without accounting for experimental data produce very strong long range correlations that are significantly reduced when experimental results are included in the analysis. In the latter case, correlation matrix reveals more complicated structure with high correlations aligned within a relatively narrow band along the diagonal; a picture that is intermediate to the two extremes previously shown in Fig. 1.

R. Capote and A. Trkov produced full set of covariances for the new 232-Th evaluation, this time, using Monte Carlo method implemented in EMPIRE. Also in this case calculated results were converted into ENDF-6 formated file and successfully processed by NJOY and ERRORJ to produce group-wise data. The results, although included in the ENDF/B-VIIb2 library, will be revised before the final release of the library. Current results used GANDER system to account for experimental data within the Monte Carlo method. The resulting uncertainties turn out to be rather low and this deficiency has been ascribed to the neglected of correlations between different experiments. Preliminary results, obtained while including these correlations, were reported to eliminate the problem [Trk06].

5 Challenges and future developments

Number of important issues regarding reliability of the fast neutron covariances is being studied. Large scale generation of covariance data requires that the following issues are clarified and settled:

- inclusion of experimental data in the methods based exclusively on model calculations - it has been shown that model generated covariances tend to show very strong correlations while those determined solely from experimental data tend to account only for a short range correlations leading to the nearly diagonal matrix. We need to include both sources of information in order to produce covariances that reflect our 'full knowledge' of the problem.

- determination of model parameter uncertainties - is essential for predicting covariances for reactions lacking any experimental data. A considerable effort would have to be undertaken to achieve this goal, definitely outside the scope of SG24. On the other hand, parameter uncertainties have to be kept under control since Bayesian methods tend to underestimate them.

- understanding the effect of correlations among experimental points and different measurements - it is a general tendency that Bayesian methods, helped by the reaction model constrains, tend to produce unrealistically small uncertainties if many experimental points are involved (e.g., total cross sections with thousands of measurements). There are indications that this problem can be controlled by including experimental correlations and realistic uncertainties on model parameters.

- effect of uncertainties intrinsic to the model itself - this effect, addressed by H. Leeb, is difficult to be included explicitly in any statistical analysis, however, it might be instrumental in preventing unphysically small uncertainties produced in certain cases (see the point above).

- comparison of different methods - we seem to be in a position to perform such a comparison during the forthcoming year.

6 Conclusions

During the first year of activity, SG24 concentrated on building covariance capabilities in the two main reaction codes TALYS and EMPIRE. Both codes reached a stage that enables their testing in real evaluations. The first attempts with EMPIRE resulted in covariances for a full chain of Gd isotopes and for Th-232, all included in the recent release of the ENDF/B-VIIb2 library [ENDF]. Numerous, often encouraging, efforts were dedicated to the inclusion of experimental uncertainties in the model generated covariances. Further activities will address comparison of various methods and establishing procedures that should ensure physically meanigfull uncertainities.

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