Covariance Data in the Fast Neutron Region Subgroup 24 report to the WPEC meeting

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Abstract

Recent activities carried out under auspices of the WPEC Subgroup 24, or those closely related to the subgroup, are summarized. The major efforts were addressing establishing practical procedures for determination of covariances, and ensuring their credibility. In support of these investigations the Workshop on Neutron Cross Section Covariances was organized by the NNDC. The present report includes a short summary of the relevant ideas and conclusions that resulted from the Workshop.

1 Introduction

The third year of the SG24 activity was dedicated to the consolidation of the covariance generation methodology developed in the first two years of the subgroup activity, and addressing unsolved issues that raised concern of the evaluation and user communities. In particular, we refer to unrealistically low uncertainties resulting from the commonly recognized analytical methods based on solid statistical foundations. Implementation of the covariance capabilities in the major nuclear reaction codes (EMPIRE, McGNASH, and TALYS) opened possibilities for massive production of covariances using advanced theoretical modeling supported with experimental data. Let us mention here major covariance projects executed recently such as 'low-fidelity', WPEC Subgroup 26, and TENDL. This vast experience, accumulated over the relatively short period of time, enabled broader scrutiny of the applied methods and critical review of the results.

The most popular methods for determining covariances in the fast neutron region can be classified in three cathegories: (i) deterministic (e.g., KALMAN filter by **T. Kawano** [2] and the closely related Generalized Least Square Method (GLSM)), (ii) stochastic ones that involve Monte Carlo calculations using random sets of model parameters, and (iii) hybrid approaches that combine features of the deterministic and stochastic treatments. All these methods have their advantages and drawbacks and it is expected that all of them will play a role in future studies and practical evaluations of covariances.

The deterministic methods are based on the Bayesian updating procedure and propagate nuclear model parameter uncertainties to the cross sections. They require, generally, less sweeps of reaction calculations than Monte Carlo approaches, being thus more manageable than their stochastic counterparts. The major advantage of the deterministic methods is their capability of including experimental data and propagating experimental results and their uncertainties back to the reaction model parameters. In this sense, deterministic approaches constitute a comprehensive and powerful evaluation tools that allow to adjust model calculations to fit experimental data and produce recommended cross sections producing simultaneously cross section covariances, improved model parameters and parameter covariances. The drawbacks of the deterministic procedures are their implicit assumption of the linear dependance on the parameters and Gaussian distribution of the results. None of these conditions is actually fulfilled in the real evaluation practice. In addition, deterministic methods are not able to cope with the uncertainties of discrete quantities such as number of nuclear levels, spins and parities.

The stochastic methods are virtually not affected by the above mentioned shortcomings of the deterministic methods. They do not require 'a priori' assumptions regarding probability distribution of the result and can easily deal with the discrete quantities. The major drawback of the currently used stochastic methods is their inability of incorporating experimental data in a rigorous manner. Only the recently proposed by **D. Smith** Universal Monte Carlo (UMC) approach offers a possibility of including experimental data in a mathematically correct way. This formalism is, however, computationally intensive and has not yet been implemented at the level allowing for practical use in the nuclear data evaluation. It was expected that the Subgroup 24 advances the UMC method to the point to make its use feasible.

A simplified variant of the stochastic approach is being employed by the TALYS team. First, the optimal set parameters, which reproduces experimental data, is searched. Then hundreds or thousands of reaction calculations with random sets of model parameters are performed and stored. The experimental data and their uncertainties are accounted for by accepting those calculations that are within a prescribed limit from the optimal cross sections and rejecting all those which do not fulfill this condition. Standard statistical analysis can then be used on the accepted set of calculations to obtain cross section as well as parameter covariances. The natural extension of this approach is to follow the reaction calculations with ENDF-6 formatting, processing, and transport calculations to compare results directly with the integral experiments observables. Calculations of this type were successfully carried out by the TALYS developers. The approach offers several clear advantages: it eliminates non-linearity issues, and does not require new formats or processing capabilities. It ensures also that the cross section uncertainties follow common-sense since this is the way they were imposed. The latter advantage is at the same time the major formal drawback of the approach since, in spite of the advanced modeling and tremendous calculation effort involved, the actual uncertainties are essentially left to the 'ad-hoc' judgment of the evaluator. In addition, the complete procedure does not allow for convenient storing of the covariance information, although the intermediate results (before data processing and transport calculations) can be converted into standard MF33 files.

Another stochastic approach that has been reported the SG24 meetings is the forward-backward Monte Carlo. This formalism has a capacity of including experimental data into Monte Carlo calculation but is computationally complex and SG24 has used it only for the case of 89Y.

A sort of a hybrid approach has been proposed by **D. Muir** in the GANDR code. Here, Monte Carlo reaction calculations with a reaction model code (e.g., EMPIRE) are used to produce informative cross section prior and the related covariance matrix. Then, this prior is combined with the experimental data through the GLSM fitting. This compromise brings experimental data into analysis preserving some of the advantages of the stochastic methods (e.g., ability to consider uncertainties of the discrete quantities) but invokes linearity assumption in the GLSM fitting phase and loses possibility of providing feedback on the model parameters and their covariances.

All the above mentioned approached have been implemented directly or indirectly in the existing nuclear reaction codes such as CoH, EMPIRE. McGNASH, and TALYS. The fervent activity carried out in various labs over the last three years produced enough results for defining and understanding strengths and weaknesses of current covariance methodology and its implementation:

- Basic capabilities for generating nuclear data covariances in the fast neutron range have ben developed and implemented in the nuclear reaction codes used for data evaluation.

- Capabilities to generate covariances in the fast neutron region have been established in several laboratories world-wide (e.g., BNL, LANL, IAEA, JAEA, IPPE Obninsk, NRG Petten)

- Inter-comparison of methods has been carried out in the frame of the SG24 and understanding of advantages and disadvantages of different methods has been achieved.

- Nuclear reaction theory plays central role in the determination of covariances in the broad energy range for a complete set of reaction channels and observables. Theory constraints provide also major source of cross-correlations among different reaction channels as well as among different isotopes.

- For the nuclei or reaction channels for which no measurements are available any estimates of covariances must resort to the nuclear reaction theory, since propagation of the model parameter uncertainties is the only viable possibility. For such cases, uncertainties of the model parameters become critical as the only source of information for generating cross section covariances.

- It is recognized that preparation of the covariances is, to a large degree, affected by subjective evaluator's judgement such as the selection of the method, choosing experimental data and the way these data are treated in the evaluation procedure (e.g., estimation of the systematic uncertainties and correlations among experiments). These factors might cause uncertainties recommended by different evaluators to differ by as much as 100%.

- It has been noted that many uncertainty estimates are unrealistically low that rises justified concern of the users who, as a matter of principle, lose confidence in practical usability of the covariances. Addressing this issue is fundamental for the future of the field as well as for the further development of nuclear techniques and applications that need realistic and reliable estimates of security margins.

- For some nuclei with A lower than 100 strong fluctuations are observed in a few MeV region. These fluctuations cannot be described by model calculations. There is no consensus nor clear guidelines on how such cases should be treated if covariances are based on the model calculations.

- SG24 activities were focused on the nuclear reaction mechanisms that are statistical in nature, such as optical, compound nucleus, and preequilibrium models. This choice excludes from considerations light nuclei that must be treated within totally different approaches.

Recognizing open issues in the current covariance methodology the NNDC has organized the Covariance Workshop in Port Jefferson in June 2008. This workshop, intended as support for the SG24, stimulated scientific discussions and brought a number of contributions that are relevant to the issues mentioned above. The proceedings of the Workshop were published in the special issue of the Nuclear Data Sheets in December 2008. In the following, we will summarize those salient points of the discussion, which are relevant to the SG24 mandate.

2 Covariance workshop at Port Jefferson

A Workshop on Neutron Cross Section Covariances was held from June 24 - 27, 2008, in Port Jefferson, New York. This Workshop was organized by the National Nuclear Data Center, Brookhaven National Laboratory, to provide a forum for reporting on the status of the growing field of neutron cross section covariances for applications and for discussing future directions of the work in this field. The Workshop focused on the following four major topical areas: covariance methodology, recent covariance evaluations, covariance applications, and user perspectives. Attention was given to the entire spectrum of neutron cross section covariance concerns ranging from light nuclei to the actinides, and from the thermal energy region to 20 MeV. The papers presented at this conference explored topics ranging from fundamental nuclear physics concerns to very specific applications in advanced reactor design and nuclear criticality safety.

This Workshop was attended by 53 registered participants. Of these, 37 represented the United States and 16 were foreign visitors from 10 countries as follows: Austria, Belarus, France, Germany, Israel, Japan, Netherlands, Slovenia, South Korea, and the United Kingdom. There were 39 separate contributions presented; of these 32 were oral talks and 7 were posters. The breakdown of these presentations by topic is as follows: covariance methodology (12), recent covariance evaluations (12), covariance applications (7), and user perspectives (4).

The Workshop highlighted the fact that several very positive developments are taking place related to nuclear data covariances. First, the strong cooperative interaction between the data producer and data user communities is unprecedented in this field! Second, great progress is being made in developing, testing, and applying new evaluation methodologies. Third, the new evaluations being produced for inclusion in the major nuclear data libraries include extensive covariance information. Finally, use of the techniques of sensitivity analysis, coupled with recently developed covariance information, is leading to the design of "smart" experiments that will offer the possibility for obtaining new information that will improve the evaluated libraries significantly rather than just representing repeats of measurements that provide little or no beneficial impact. Ultimately, this approach will lead to major cost savings and faster convergence to target accuracy levels for the nuclear databases used in basic and applied nuclear science.

Most of this report follows fast neutron range related contributions that were presented during the Workshop.

3 Avoiding unreasonably small uncertainties

Major issue, often encountered analyzing covariances in the evaluated files, are uncertainties that are far too small to be credible. This happens , in spite of the fact that mathematically rigorous statistical methods, such as Bayesian approach, are being used. The problem is aggravated with increasing number of experimental points available for a given reaction. In addition, simultaneous inclusion of many reaction channels into the analysis leads to further reduction of the uncertainties. This issue was a major target of the SG24 in the reported year. Although we don't claim to have solved the problem definitely, we have identified three reasons that significantly contribute to lowering final uncertainties: (i) intrinsic model uncertainties, (ii) correlations within and among the experiments, and (iii) hidden systematic errors in the experiments. Below we outline each of these issues along with the suggested solution.

3.1 Intrinsic model uncertainties

We illustrate the problem within the Kalman filter method following **M. Herman *et. al*** in [1], but the conclusions also apply to other methods relying on theoretical modeling of nuclear reactions. Quite often, Kalman filter analysis involving a vast amount of experimental data results in uncertainties that are far lower than systematic uncertainties even of the most precise measurement. This happens in spite of the fact that proper experimental covariances, accounting for systematic uncertainties, are supplied as an input to the KALMAN code.

One of the sources of the problem is the implicit Kalman filter assumption that the model itself is perfect. Thus, any uncertainties in model calculations are only due to the uncertainties of the model parameters. Often, the shape of a calculated excitation function is constrained, *i.e.*, even with a substantial variation of model parameters it is not possible to alter the shape or the absolute value of the function in an arbitrary fashion.

For example, any variations of the optical potential parameters do not provide for scaling of the absolute value of the total cross section. Such scaling is actually the degree of freedom that would be needed to accommodate systematic uncertainties in the measurements that in most cases amount to scaling cross sections up and down without changing the shape. Lack of this possibility might have a dramatic effect on parameter uncertainties - any scaling of the cross section appears incompatible with the model calculations since it cannot be reproduced by any sensible variation of the model parameters. If the model were perfect we would have to conclude that the systematic experimental uncertainties are overestimated. It is very difficult to argue, however, that the models are accurate within less than 1%. Thus, to avoid such the unrealistic reduction of systematic errors one may introduce intrinsic model uncertainty by defining a fictitious model parameter that multiplies model predicted cross sections. The prior value of this scaling parameter is one and its variation allows to preserve systematic uncertainties in the experiment.

A more formal approach to the problem was presented by **H. Leeb *et. al*** in [1]. These authors distinguish between 'scaling' type of the model deficiency, essentially equivalent to the one described above, and 'remodeling' that includes also certain flexibility of the energy dependance. In other words, while the first approach allows for the change of the absolute value of the cross sections preserving the the shape of the excitation function the second one goes further and also allows for the modification of the shape. Complete simultaneous relaxing of the both constraints would naturally result in complete elimination of the reaction modeling from the covariance determination. In order to prevent 'throwing out the baby with the bath water' authors derive the methods to establish covariance matrices for the model deficiencies from the analysis of the data for the neighboring nuclei.

3.2 Correlations within and among experiments

It is well known that systematic uncertainties in the experiment cause correlations among experimental points measured in the same experiment. These correlations are critical for determining covariances, especially if a single experiment contains a large number (N) of points that, if uncorrelated, lead to the reduction of the uncertainty at the rate of $\sqrt{N}$. The systematic uncertainty sets the limit for this reduction. The proper way of including such a constraint is to allow for the correlations among experimental points. Such correlations are determined by the ratio of systematic and statistical uncertainties. This brings an important issue of proper documenting and storing the sources of uncertainties in the measurements.

The same considerations can be extended onto correlations of uncertainties among different experiments (**H. Leeb *et. al*** in [1]). In the typical Bayesian analysis subsequent updates are done under the assumption that various experiments are uncorrelated. Thus systematic uncertainties in a set of experiments are treated as statistical leading to the reduction of the final uncertainty as discussed above for a single experiment. In practice, it is quite typical to face cases in which several experiments are correlated, e.g., due to the use of the common standard. In order to include such correlations in the Bayesian approach, the correlate experiments must be lumped into a singe 'meta-experiment' that allows to construct correlation matrix with cross-experiment terms. While formally possible, such procedure may lead to impractically large matrices that would not be possible to handle even with modern computers. **H. Leeb *et. al*** in [1] have proposed an approximate method that preserves the convenience of the Bayesian update while allowing for taking cross-experiment correlations into account.

3.3 Hidden systematic errors in experiments

In the previous section we pointed out the importance of systematic errors in the experiments. It is widely acknowledged that systematic uncertainties must be included and handled correctly in order to obtain reasonable estimates of evaluated cross section covariances. Some evaluators retain that experimentalist often underestimate systematic uncertainties or miss certain sources of such uncertainties. An approach currently used in Russia to generate covariances for neutron cross section evaluations is based on the unrecognized error estimation concept (**E. Gai and A. Ignatyuk** in [1]). In this technique, the average deviations of experimental data from the evaluation are considered to establish the systematic uncertainties, which are then assigned to the individual experiments.

4 Implementation of the UMC method

Recently, a new approach to nuclear data evaluation called Unified Monte Carlo (UMC) has been suggested. As the title indicates, this approach aims to handle both theoretical modeling and experimental data uncertainties by Monte Carlo. It is not limited to any particular energy range and can be applied broadly in neutron cross section evaluations. Detailed properties of UMC have been studied using “toy” examples, *i.e.*, hypothetical data sets that nevertheless exhibit key features of realistic situations encountered in nuclear data evaluations (**R. Capote and D. Smith** in [1]). Significant differences between UMC and GLS were reported for cases involving ratio experimental data, while the validity of GLS for those situations that involve only “simple”, linear data/parameter relationships has been upheld through the reported comparisons between GLS and the more rigorous UMC approach for these cases. While simple brute force applications of the Monte Carlo approach offer a straightforward means to propagate uncertainties or perform evaluations by UMC, this can be very computationally intensive. An alternative way to do this in UMC involves using the more efficient Metropolis sampling scheme.

The significant progress has been achieved in understanding practical issues related to the implementation of the UMC approach and it is believed that there are no real obstacles on the way to practical use of the method in evaluations. However, due to manpower limitations, the Subgroup was not in a position to develop software general enough to go beyond limited scale testing.

5 Model parameter uncertainties in RIPL-3

With nuclear reaction modeling assuming major role in the covariance determination methodology the adequate 'a-priori' knowledge of the uncertainties of the model parameters becomes an issue of primary importance. These uncertainties constitute the only source of information for constructing covariances for the nuclei which were not investigated experimentally. In general, uncertainties of the model parameters, along with model deficiencies, define constraints that are imposed by the nuclear reaction theory.

Parameter uncertainties were one of the objectives of the recent release of the Reference Input Parameter Library (RIPL-3) prepared in the frame of the IAEA coordinated research project. Accordingly, RIPL-3 includes uncertainties for the critical model parameters such as optical potential, level densities, γ-ray strength functions, and nuclear masses. These parameters are practically always derived from the experimental data that are independent from the neutron cross section measurements. Therefore, they can be treated as genuine additional information when preparing covariances for the evaluated files, providing valid constraints.

6 Understanding OMP minima

Large-scale evaluations of covariances from nuclear modeling have been facilitated by recent neutron cross section evaluation code enhancements. For example, distinct maxima and minima in evaluated neutron total cross section uncertainties have been observed in recent large scale EMPIRE calculations with the spherical optical model (**M. Pigni** *et al.* [3]; **M. Herman** *et al.* in [1]). These effects can be understood physically as resulting from S-wave sensitivity crossing zero at lower energies, partial wave interference phenomena at a few MeV range as well the Ramsauer effect at higher energies. Furthermore, this newly gained insight may provide a useful approach for exploring the origins of certain systematic features of these uncertainties that possibly stem from the inevitable deficiencies that are inherent to the physics models which are used for nuclear data evaluation purposes.

7 Covariances for prompt fission neutron spectra

Work on producing covariances is extending beyond neutron cross sections to consideration of uncertainties associated with important fission neutron spectra due to their potentially significant influence on reactor system response uncertainties as well as on other applications such as neutron dosimetry.

If fission neutron spectra are represented by parameterized models, then spectrum uncertainties can be estimated by propagation of the parameter uncertainties. Such a study has been carried out using the Watts and Kornilov spectrum formulations, with a Monte Carlo method used to propagate the spectrum model parameter uncertainties (**I. Kodeli** *et al.* in [1]). A group from LANL reported on its work devoted to estimating uncertainties for prompt fission neutron spectra and neutron multiplicity. Their investigation incorporates the prior parameters and uncertainties associated with the Los Alamos spectrum model, and then merges experimental values and uncertainties using the Kalman filter approach (**P. Talou** *et al.* in [1]). When propagating fission spectrum uncertainties to system response uncertainties, it is important that the spectrum be normalized and that all rows and columns of the covariance matrix sum to zero. According to work reported from Argonne National Laboratory (ANL), caution is also needed in calculating sensitivity coefficients to obtain reliable system parameter uncertainties (**W. Yang** *et al.* in [1]).

8 Covariances for light nuclei

Light nuclei were, so far, not considered in the SG24 activities since the physics of the fast neutron induced reactions on these nuclei is very different from the reaction mechanisms use for the heavier nuclei. Namely, statistical approaches are not valid and the few-body approaches must be invoked. The omission was also justified by the fact that advanced, mathematically rigorous, methods are already in place in the context of the R-matrix code EDA (**G. Hale** in [1]).

Subgroup 24 inspired a novel approach to the covariances for the light nuclei based on the 'ab-initio' few-body calculations using realistic nucleon-nucleon interaction and the Refined Resonating Group Model as discussed by (**H. Hofmann** in [1]). Preliminary calculations have been performed for the n+d system producing excellent results for incident neutrons with energies up to about 10 MeV. Higher energies would require considerable expansion of the model space which would be possible but not very practical.

9 Experimental covariances

Uncertainties in evaluated non-elastic cross sections (˜ 5-10%) are usually seen to be much larger than those for total cross sections. Work at Lawrence Livermore National Laboratory has led to the development of a procedure to reduce these uncertainties based on considering the relationship between total, elastic, and non-elastic cross sections as well as the physical constraint provided by Wick's limit on the forward elastic scattering cross section (**F. Dietrich** in [1]).

Reliable evaluation of minor actinide neutron cross sections is extremely difficult to do and guidance from measurements is frequently non-existent. An investigation at Joint Institute of Nuclear Energy Research, Minsk-Sosny, Belarus, is examining the manner in which the more extensive and better known information on major actinides can be used to provide reasonable estimates of minor actinide cross sections and their uncertainties. The importance of performing evaluations and determining uncertainties using good nuclear models as a means to reduce the assumed parameter uncertainties is emphasized (**V. Maslov** in [1]). This paper also discusses potentially negative influences of "tuning" major actinide evaluations to agree with data from integral criticality experiments on estimating reasonable cross section uncertainties and correlations for minor actinide nuclei.

10 Conclusions

SG24 has been working towards the final objective of establishing credible, scientifically justified and practically feasible methodology for determining covariances in the fast neutron region. The original scope focusing on cross sections has been enlarged to include fission neutron spectra, and neutron multiplicities. Although there has been a substantial progress in understanding differences among different methods of estimating covariances the methodology is not yet fully mature to ensure unique answer if the same set of data is processed by different evaluators. Estimation of covariances still involves a significant portion of an arbitrary judgement regarding choice of the method, selection of the experimental data and the way the latter are treated. Although UMC method is computationally intensive it still might be the most adequate approach in cases involving measurement ratios and strong non-linearities. Thus, practical implementation of the new UMC concept should be considered the priority issue.

In spite of the various difficulties, there has been pressing request from the users for a consistent set of covariances to be used with the current nuclear data libraries. In response to these needs, many covariances were produced using the EMPIRE, GNASH and TALYS codes using methods outlined in this report.

One of the most remarkable achievements of the SG24 is sensitization of the evaluation community to the necessity of providing covariances with each new evaluation, which recently became almost a rule.

References

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