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 formal studies and implementation of the newly proposed Unified Monte Carlo method, comparison of existing approaches (KALMAN, Monte Carlo, Backward-Forward Monte Carlo, and GANDR), establishing practical procedures for determination of covariances, and production of new covariance files. Although substantial progress has been achieved in all these directions further studies are needed to understand differences among various approaches and reach consensus on the methodology.

1 Introduction

Initial activities of the WPEC SG24 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. As the result, EMPIRE, TALYS and GNASH codes are currently capable of producing nuclear data covariances and storing them in the Evaluated Nuclear Data File Version 6 (ENDF-6) format. TALYS is using a Monte Carlo (MC) approach for drawing model parameters from uncorrelated distributions. A similar approach is also being used by Capote and Trkov. In the latter case, EMPIRE-based model covariances are used as a prior for a partitioned form of the generalized least squares code GANDR developed by Muir. A different approach is being used at the Brookhaven National Laboratory (BNL) and Los Alamos (LANL) where the EMPIRE and GNASH codes, respectively, have been coupled to the KALMAN code written by Kawano and Shibata (1997).

During the first two years SG24 efforts resulted in the considerable amount of covariances produced in support of the two major projects ? ENDF/B.VII.0 and SG26. For ENDF/B-VII.0, 12 evaluations of covariances were produced with EMPIRE-KALMAN and three with EMPIRE-MC-GANDR methodology,

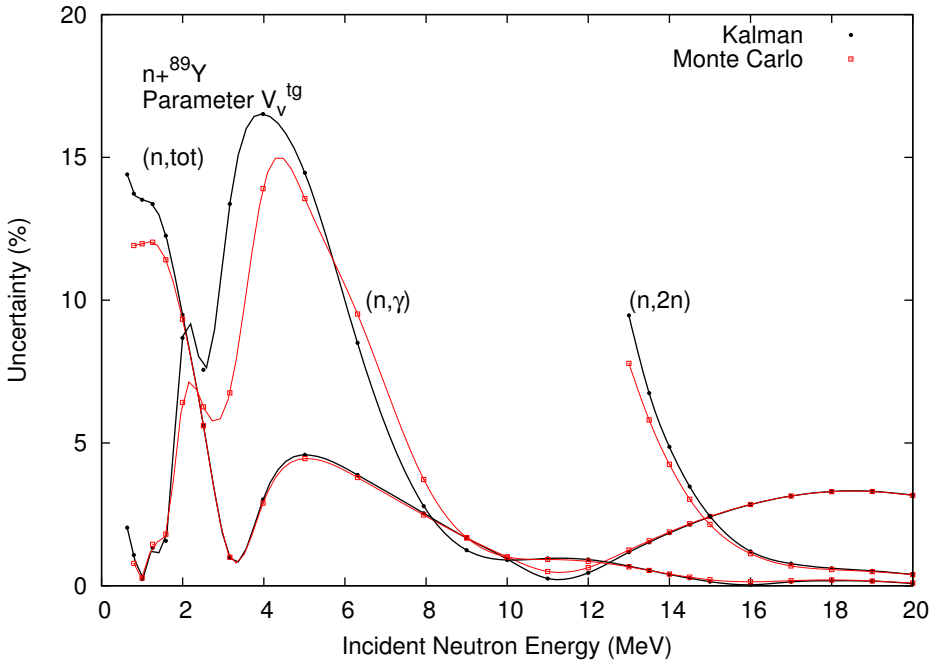

Figure 1: Comparison of the model-based cross section uncertainties obtained using Monte Carlo and KALMAN methods for various reactions. Presented uncertainties result from the uncertainty on the real depth of the optical potential.

while for SG26 the preliminary covariances for 36 materials were produced with the EMPIRE-KALMAN method and three with TALYS-MC.

In spite of these apparent successes there are still open issues such as inclusion of experimental data, understanding differences between various approaches and establishing practical procedures to be followed when determining covariances. Recent activities of the subgroup concentrated on these application critical topics.

2 Comparison of different covariance methods

2.1 Model-based covariances using Monte Carlo and KALMAN methods

The Monte Carlo (MC) sampling and the Bayesian based KALMAN approaches are, at the moment, the two most commonly used methods for determining cross section covariances in the fast neutron region. Therefore, it is of fundamental importance to compare these two approaches and understand eventual differences. Such an attempt had been already undertaken during the second year of the SG24 activity but final results were not conclusive since the inputs fed to the MC and KALMAN calculations were not exactly the same. During the last year this exercise has been repeated by Capote, Pigni, Herman and Trkov keeping inputs in both methods as close as possible. The EMPIRE code was employed to perform nuclear reaction calculations entering both approaches, thus eliminating the potential source of discrepancies, inevitable if two different reaction codes were used. Calculations were performed for total, elastic, inelastic, (n,2n), capture, (n,p) and (n,α) reactions on ^{89}Y up to the incident energy of 20 MeV. The same uncertainties on model parameters were assumed and MC drawing was performed from a Gaussian distribution. As shown in Fig. 1, there is a reasonable agreement between model-based uncertainties obtained using MC and KALMAN methods for total, capture and (n,2n). Fig. 2 compares correlation matrices for the total. Again, both methods yield essentially equivalent results - the 'chess-board' like pattern found in the correlation matrix is the same in both methods. The negative correlations localized slightly above 10 MeV in the correlation matrix obtained in the MC approach are the only difference compared to the KALMAN approach. Also, for the remaining

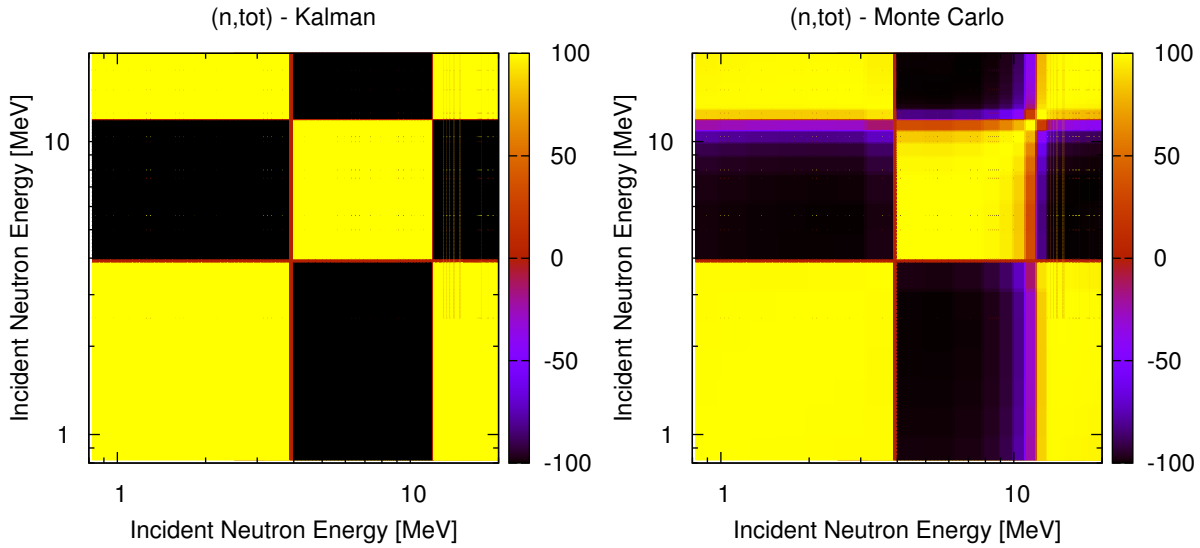

Figure 2: Comparison of the model-based correlations obtained using Monte Carlo and KALMAN methods for the total cross section. Presented correlations result from the variations of the real depth of the optical potential.

reaction channels the results obtained with KALMAN and MC are close to each other. The notable exception to this rule are the uncertainties due to the variation of the preequilibrium strength, for which non-negligible differences were noted. The reason for this discrepancy might be a relatively strong variation (20%) of the preequilibrium strength used in the calculations that together with the Gaussian distribution, allowed for values considerably far from the central value in the MC simulations. Potential non-linearity is likely to manifest itself under such extreme circumstances.

These numerical tests indicate that, in absence of experimental data, both methods are nearly equivalent. However, special care should be taken of the non-linearity (higher-order) effects in the KALMAN approach. In order to minimize the impact of non-linearity, the sensitivity matrix should be calculated using model parameter variations that are close to the parameter uncertainties. Taking these precautions the both methods yield practically identical results also in the case of the parameters for which strong non-linearity is expected, e.g., the optical model diffuseness.

2.2 Inclusion of experimental data

2.2.1 Comparison of EMPIRE-MC-GANDR and EMPIRE-KALMAN methods

Inclusion of experimental data into the covariance determination still appears to be a major issue. The KALMAN method accounts for them naturally but suffers from a typical "deficiency" of the Bayesian approaches - uncertainties tend to reach values that are considered far too small if very many experimental data are included in the analysis. One 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. In the present comparison we have refrained from resorting to this solution.

The MC approach in its classical formulation does not allow for accounting for the experimental data. In the present study the prior, obtained with the EMPIRE-MC calculations discussed above, was fed into the Generalized Least Squares code ZOTT incorporated in a more general GANDR system [1]. In the following we refer to this approach as EMPIRE-MC-GANDR or shortly as GANDR. The same nuclear reaction input was used in the EMPIRE code to produce sensitivity matrices for KALMAN and MC based priors for GANDR. The same model parameters were varied in both cases and Gaussian distributions were used in the MC approach to simulate statistical assumptions underlying the KALMAN filter. The only difference was a different energy grid, since standard GANDR energy mash is too sparse for KALMAN to operate properly.

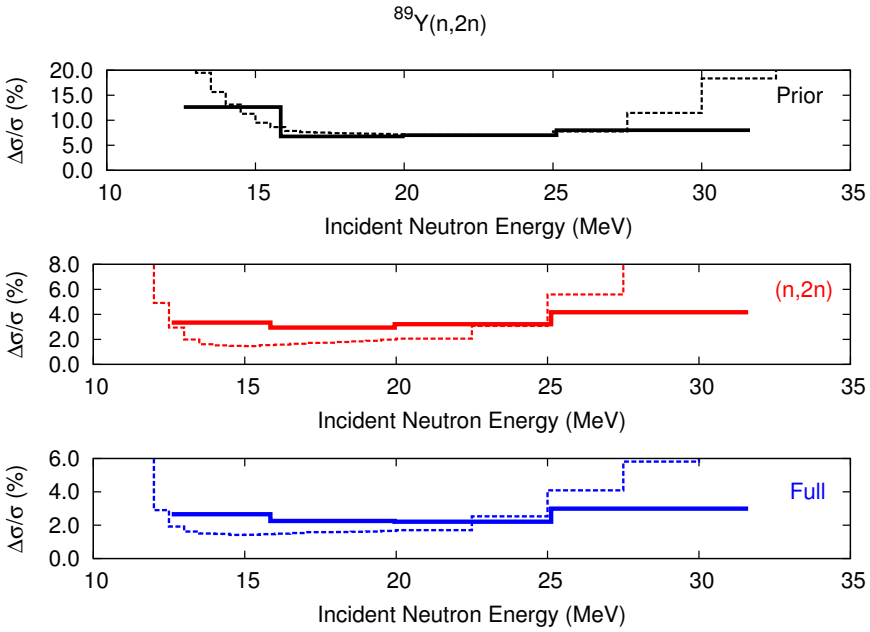

Figure 3: Comparison of uncertainties for the ^{89}Y(n,2n) reaction obtained using GANDR (solid lines) and KALMAN (dashed lines) methods illustrating the effect of including experimental data. The top panel shows default calculations and related model-based uncertainties, the middle one presents KALMAN calculations taking into account (n,2n) data only, and the bottom one shows KALMAN calculations considering experimental data for all reaction channels.

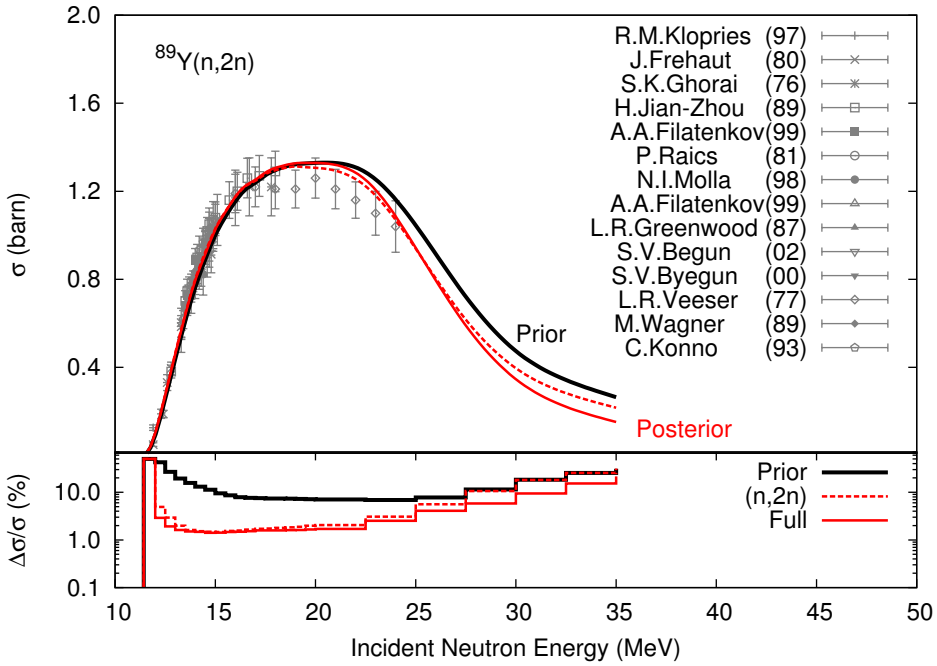

Figure 4: Comparison of the cross sections and related uncertainties for the ^{89}Y(n,2n) reaction obtained using KALMAN. Different lines illustrate effect of including experimental data: 'prior' indicates default calculations and related model-based uncertainties, '(n,2n)' represents KALMAN calculations taking into account only (n,2n) data, and 'Full' stands for the KALMAN calculations considering experimental data for all reaction channels.

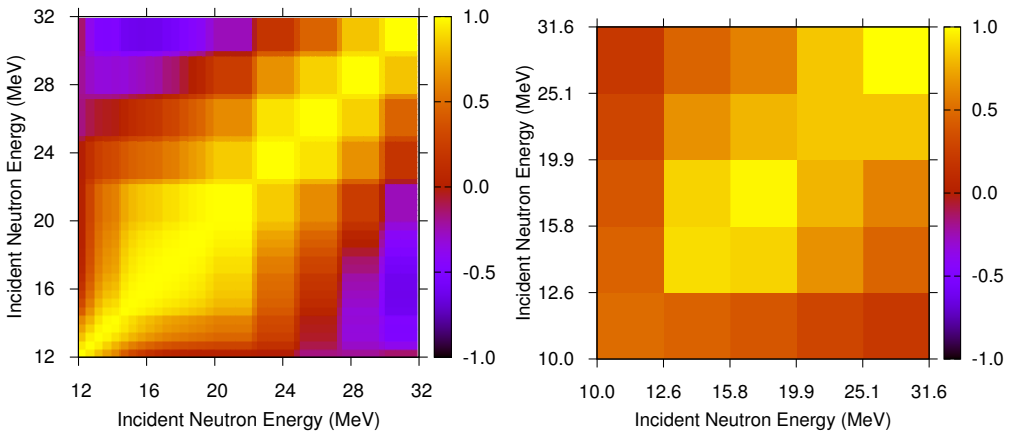

Figure 5: The correlation matrix for the ^{89}Y(n,2n) reaction obtained with KALMAN using full set of experimental data for all reaction channels.

Figs. 3 illustrates effect of including experimental data on the uncertainties of the ^{89}Y(n,2n) reaction estimated using EMPIRE-KALMAN and EMPIRE-MC-GANDR methods. The pure model-based predictions are very similar, as discussed before (flat behavior of the GANDR results at higher energies is believed to be an artifact). As expected, adding experimental data reduces uncertainties in both methods, but reduction in KALMAN is stronger than in GANDR. One should note, however, that cross-correlations between different experiments were considered in GANDR but not in KALMAN. Inclusion of the experimental data for all the remaining channels (especially nearly 1000 points for total) reduces (n,2n) uncertainties by about 30%. in GANDR. In KALMAN this difference is practically negligible around 14-15 MeV, i.e., in the range in which many (n,2n) measurements are available as can be seen in Fig. 4. The same figure shows also the effect of including all experimental data on the posterior cross sections. Additional experimental points constrain model parameters so that the fit is slightly worse than in the case of using (n,2n) data only. Still it is improved compared to the prior calculations. On the other hand, there is a considerable advantage of reproducing all reaction channels simultaneously with the same set of model parameters, which is not the case if data are restricted to a specific reaction. Additional advantage (or disadvantage) of this approach are cross correlations among various reaction channels.

Figs. 5 presents correlation matrices obtained with the two methods. The comparison is to some extend obscured by the low energy resolution in the case of GANDR but general structure of the two matrices can be considered similar. In the KALMAN matrix one notes relatively week correlations below 15 MeV that is related to the large number of experimental data available in this region. At higher energies, the correlations are stronger as expected for the model dominated cases. The anticorrelations observed above 28 MeV can be explained as due to the preequilibrium emission that decreases (n,2n) cross sections in the maximum of the excitation function and increases them in the high energy tail. The same effect is not seen in the GANDR correlation matrix, most likely to the too coarse energy grid.

Finally, in Fig. 6 we show effect of adding experimental data on uncertainties of the total cross section using the KALMAN method. We note, that 2.8% systematic error was assumed for all experiments but no cross correlations were allowed. Using extended set of Abfalterer (more than 400 points) the uncertainties are of the order of 1.5%. Adding about 200 points by Foster brings them down to about 1%, and including all the experiments causes further reduction to about 0.75%. Most experimentators would consider such low uncertainties unrealistic. It is intriguing why, the formally correct, Bayesian approaches tend to produce too low uncertainties. Neglect of the intrinsic model uncertainties is considered a possible explanation. Hopefully, the work by Pigni and Leeb will shed light on this problem.

2.2.2 Comparison of Backward-Forward- MC and GNASH-KALMAN methods

An alternative method to predict cross sections, uncertainties, and covariance data uses the European TALYS reaction modeling code and a Backward-Forward Monte-Carlo uncertainty quantification technique. This

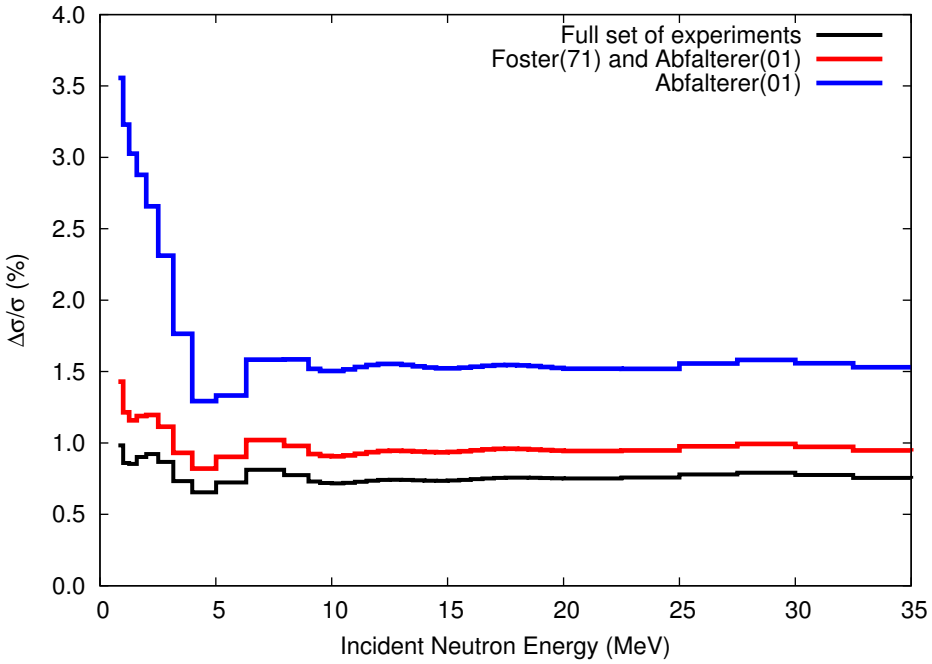

Figure 6: Uncertainties on n+^{89}Y total cross section obtained with KALMAN using (i) full set of experimental data for all reaction channels, (ii) removing all (n,tot) experiments except Foster and Abfalterer, (iii) removing all (n,tot) experiments except Abfalterer.

approach uses a microscopic optical model, together with Hauser-Feshbach and preequilibrium reaction mechanisms, and the underlying model parameters and their uncertainties and correlations are determined through a Monte-Carlo filtering method based on comparisons with measured cross section data. The results obtained using this approach are compared with the GNASH-KALMAN method in the recently published paper [2].

Figure 7 compares the relative uncertainties in the (n,2n) reaction cross sections given by the BFMC and GNASH-KALMAN methods. The correlation matrices for the ^{89}Y(n,2n) reaction cross section are plotted in Fig. 8; the top panel shows the result of BFMC, and the bottom panel is for GNASH-KALMAN method.

Comparison of these results with the exercise discussed in section 2.2 indicates reasonable agreement between uncertainties obtained with GNASH-KALMAN, EMPIRE-KALMAN and EMPIRE-MC-GANDR methods. The important value of the uncertainty around 14 MeV is 2%, 1.6% and 2.2% respectively. As far as the correlation matrices are concerned there is a close resemblance between those obtained within the GNASH-KALMAN and EMPIRE-KALMAN approaches, which is not surprising considering that the two calculations differ only in the reaction codes involved in the determination of the sensitivity matrices. Both codes, are essentially equivalent within the scope of this comparison.

2.3 Theoretically formulated prior for parameter uncertainties

Evaluated nuclear data files are consistent sets of cross sections and spectra (primarily of neutron induced reactions) which should represent the best knowledge of the corresponding observable. The evaluation process is a mathematically well defined procedure based on Bayesian statistics [3], which provides the fundamental relationship for the modification of the probability distribution due to new experimental information,

$$p(\underline{x}|\underline{\sigma}, M) = \frac{p(\underline{\sigma}|\underline{x}, M)}{p(\underline{\sigma}|M)} p(\underline{x}|M)\,. \tag{1}$$

Here $p(\underline{x}|\underline{\sigma}, M)$ is the conditioned probability distribution of the parameters $\underline{x}$ for a given set of experimental cross sections $\underline{\sigma}$ and for a given model M. The experimental information enters via the likelihoood function

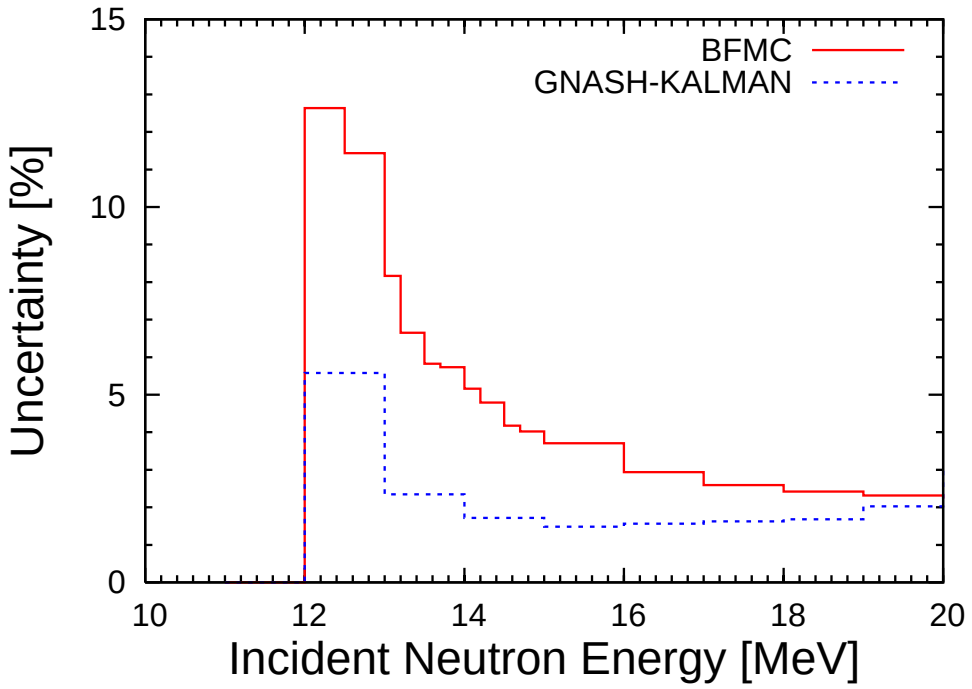

Figure 7: Relative uncertainties in the n + ^{89}Y(n,2n) reaction. The solid line is for the BFMC method, and the dotted line is for the GNASH-KALMAN method.

$p(\underline{\sigma}|\underline{x}, M)$, which is essentially a normal distribution with well defined center and width. The most intriguing quantity is the a-priori distribution $p(\underline{x}|M)$ which describes the probability distribution of the parameters in a given model. There was a longstanding debate about the proper choice of this so-called prior. A breakthrough has been achieved by Jaynes in 1968 [4] who demonstrated that the prior associated with complete ignorance can uniquely be deduced from invariance properties of the problem.

In nuclear data evaluations, which strongly rely on model calculations, the proper choice of the prior is important for the reliability of the generated file. This is particularly true for the extension of the energy range beyond 20 MeV where experimental data are scarce. It was therefore the primary goal to develop a unique and well defined procedure for the determination of the prior in nuclear data evaluation. Following the concept of maximum information entropy [5] and including invariance properties of Jaynes [4] a method was established which contains, besides mathematical constraints, the physics knowledge on the parameters as a-priori information [6, 7]. Especially, criterions for the admissible ranges of the depths and the geometry of the optical potential have been worked out [7, 8]. The corresponding a-priori probabilities of the parameters are calculated from the approximate equations for maximum information entropy via numerical means. Using these probability distributions of the parameters the covariance matrices for the cross sections associated with the model parameter uncertainty is obtained by Monte Carlo simulation.

In the following the example of the prior determination for basic n-Pb reaction data in the energy range between 10 and 60 MeV[7] is given, which is based on TALYS [**?**] calculations with default parameters. The method provides the a-priori probability distributions of the parameters of the model. In Fig. 9 the probability distribution of the half density radius and the diffuseness of the real part of the optical potential are shown. The obtained cross section correlations

$$\frac{\langle \Delta\sigma(E)\Delta\sigma(E')\rangle}{\sqrt{\langle \Delta^2\sigma(E)\rangle\langle \Delta^2\sigma(E')\rangle}} \tag{2}$$

are displayed in Fig.10 for the total and the elastic cross section.

The feasibility of the method has been shown for several examples. However, it accounts only for the covariance matrices due to parameter uncertainties. Procedures to estimate also the model defects and the

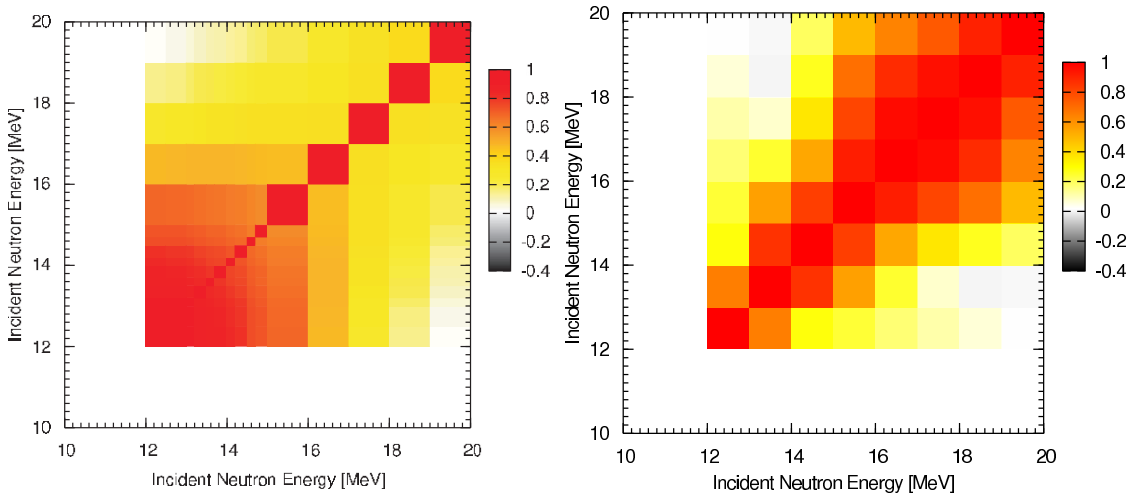

Figure 8: In-channel correlation matrices for the (n,2n) channel. The top panel shows the result of BFMC, and the bottom panel is for GNASH-KALMAN.

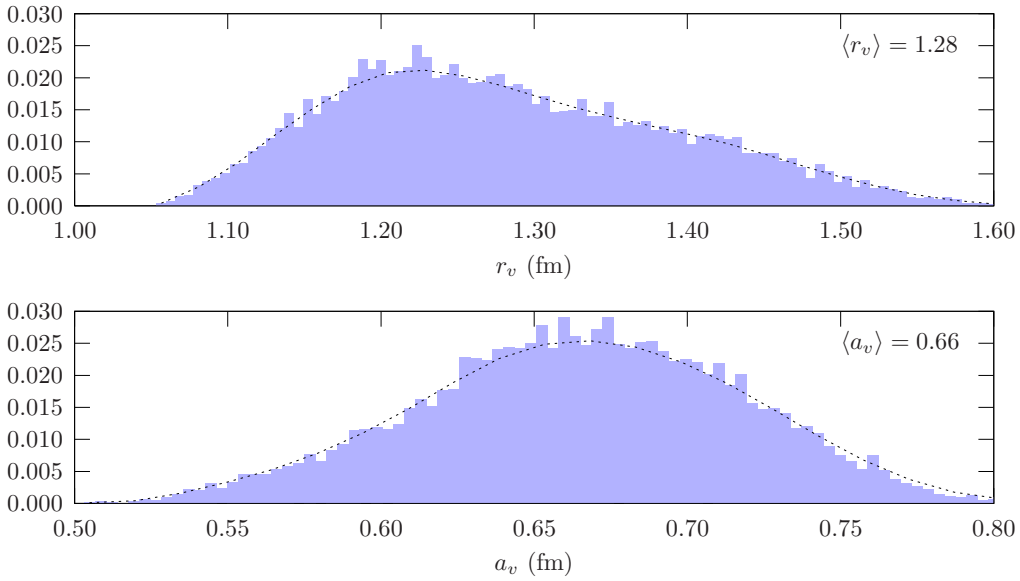

Figure 9: The prior distributions of the optical model parameters for a sampling of 1000 sweeps. The reduced half density radius r_v and the difuseness a_v are shown.

associated correlations are in progress.

3 Development and testing of the Unified Monte Carlo approach

Applications of Bayes Theorem and the Principle of Maximum Entropy lead to the generation of a multi-variable probability density function whose random variables correspond to those nuclear data quantities one seeks to evaluate. According to statistics, the best estimators for these physical quantities, as well as their associated covariance matrix, are defined in terms of the first and second moments of this probability function. This function incorporates information from nuclear modeling as well as experiment in a "unified" manner. This explains the choice of the word "unified" in describing this new method. The well-known

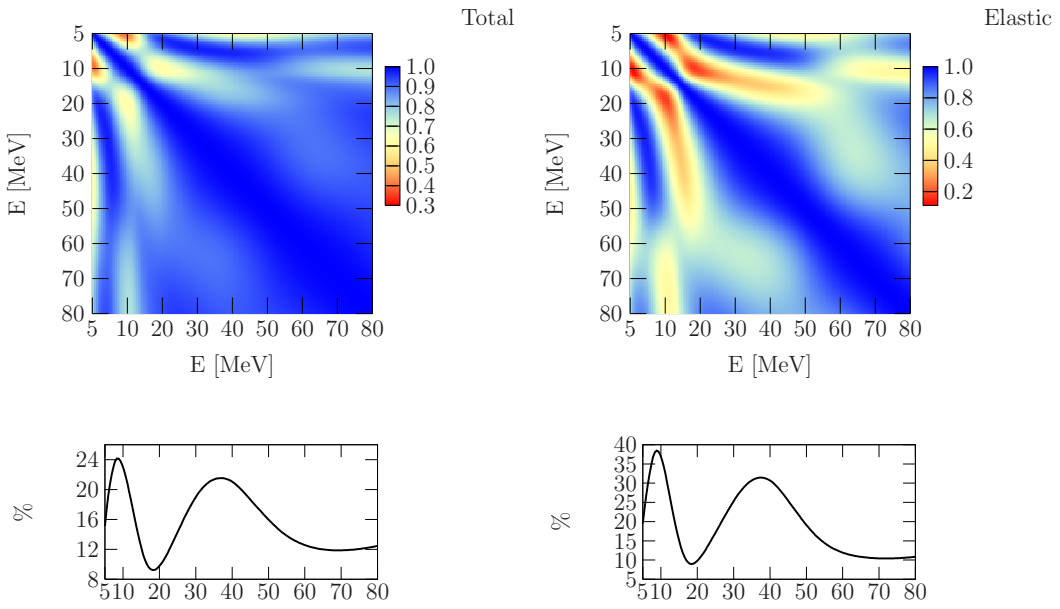

Figure 10: The energy correlations of the simulated cross section within a reaction channel. The covariance matrix is normalized according to Eq. (2). The cross section uncertainty (%) is shown below each contour plot.

generalized least-square method (GLS) is an effective procedure for locating the peak of this probability distribution. Furthermore, if this distribution is truly normal (Gaussian), then these peak values of the variables are also the best estimator values as defined above. However, if the distribution is not normal but is skewed, for example as would be the case if ratio or possibly integral experimental data are included in the evaluation process, then the distribution will not be exactly normal and the GLS solution will be somewhat biased and thus not truly equivalent to the one defined in terms of the actual moments of the distribution. The UMC method aims to calculate these true moments of the probability distribution directly, regardless of whether or not it is normal. In principle, these moments involve multi-dimensional integrals that are difficult to calculate deterministically. However, this difficulty can be circumvented in principle by applying the Monte Carlo technique. In so doing, one also avoids the necessity for knowing the exact normalization of the probability density function. The essence of the UMC method is therefore this application of Monte Carlo simulation to evaluation of the above mentioned moment integrals for the probability density function.

The concept of UMC was mentioned briefly at the 2007 SG24 meeting. This introduction was followed by a more detailed exposition of the method and demonstration of its feasibility during the late spring and early summer of 2007. An informal memorandum was circulated in late May and the concept was reported formally at the AccApp'07 Conference in Pocatello, Idaho, in late July. A more detailed report, ANL/NDM-166, which is essentially a polished version of the original memorandum, was issued in January 2008. This report can be found on the Internet at the following Web address:
http://www.ne.anl.gov/capabilities/nd/reports/ANLNDM161.html.

An investigation of the performance of the UMC method in comparison with the GLS method has been undertaken by Capote and D. Smith who applied both methods to simple examples with few input values that have been selected to explore various features of the evaluation process that impact upon the quality of an evaluation. Among the issues to be explored are: i) convergence of the UMC results with the number of Monte Carlo histories and the ranges of sampled values; ii) a comparison of Monte Carlo sampling using the Metropolis scheme and a brute force approach; iii) the effects of large data discrepancies; iv) the effects of large data uncertainties; v) the effects of strong or weak model/experimental correlations; and vi) the impact of ratio data and integral data. We employed two distinct Monte Carlo sampling schemes to generate random values for the probability distribution function (pdf) $p(\sigma)$ of interest for the present investigation. The first of these is referred to as the "brute force" (BF) method. The second sampling approach is the Metropolis algorithm. Use of a Monte Carlo sampling scheme with good efficiency and high fidelity is essential for

success in using the UMC approach.

It was concluded that the UMC method yields results which compare favorably, to within acceptable precision, with the GLS results thereby establishing the UMC approach as a viable alternative to GLS. In the studied cases, the Metropolis sampling is two orders of magnitude more efficient than a brute force sampling approach. In situations involving only direct cross sections relationships the GLS method is more straightforward and less computationally intensive than the UMC method. Since the methods are theoretically comparable when only direct experimental cross sections are considered (unitary relationship), GLS is the preferable choice. However, the situation could be very different if ratio of cross sections, or more complex relationships are involved. Further studies are under way.

4 Fission spectra covariances

Talou, Madland and Kawano are currently working on producing covariance matrices for the prompt fission neutrons chi-matrices for the ENDF/B-VII.0 files U235, U238 and Pu239. The methodology follows closely the one used for assessing cross-section covariance matrices in the fast energy region. Model calculations (using the Los Alamos model) are combined with experimental data using a Kalman filter (Bayesian updating technique) to produce the covariance matrices.

Kodeli, Trkov and Capote have applied a new Monte Carlo (MC) method to produce covariance matrices of the prompt fission neutron spectra (PFNS) for ^{235,238}U and ^{239}Pu neutron induced fission. Parameters of the model describing the PFNS were sampled randomly within the given uncertainty intervals, assuming normal distribution. The covariance matrix for the Watt spectrum generated by the MC method was validated by comparison with the matrix derived analytically. Furthermore it was shown that the matrices produced in this way comply with the zero-sum rule as prescribed in the ENDF-6 manual. Analytical derivation is appropriate in case of linear dependence of the spectra on the underlying parameters, whereas in the MC approach the extension to more complex models is straightforward: PFNS covariance matrices were obtained both for the Watt model and for the phenomenological parameterization of the fission neutron spectra proposed by Kornilov et al. [9].

Derived covariance data were used in the cross section sensitivity and uncertainty analyzes of several KRITZ UO2 and MOX critical configurations performed in the scope of the OECD international benchmark exercise. Two different approaches to calculate the sensitivity coefficients of k_{eff} relative to the fission spectra were used as a means to check and assure the mathematical correctness of the matrices. The sensitivity method using the normalization of the coefficients was found very efficient in correcting the covariance matrices which do not fulfill exactly the ENDF-6 format rules. The use of the method is recommended to assure the formal correctness of the matrices used. Comparison of uncertainties based on the unnormalised and normalized methods provided a verification of the generated matrices. Uncertainties in k_{eff} for different KRITZ benchmarks, estimated from these covariance matrices were found to be consistent with the differences between the k_{eff} values based on different models for prompt fission spectrum of relevant actinides, i.e. ENDF/B-VII, Watt and Kornilov models.

5 Covariance evaluations

5.1 'Low-fidelity' project

Simple estimates of cross section covariance data were generated at NNDC and LANL for all materials in the neutron sublibrary of ENDF/B-VII.0 in the energy range of 5 keV - 20 MeV. This large-scale project was initiated by the U.S. Nuclear Criticality Safety Program to provide a low-fidelity but complete set of covariances that could be used to exercise processing methodologies and tools. The covariance matrices cover light nuclei, structural materials, fission products, heavy non-fissile nuclei and actinides. These results represent an attempt to provide model-based and consistent estimates of covariance data for nuclear criticality safety applications. The evaluation methodology combines the nuclear reaction model codes EMPIRE (at NNDC) or GNASH (at LANL), which calculate sensitivity of cross sections to the perturbation of nuclear reaction model parameters, and the Bayesian code KALMAN that propagates uncertainties of the model parameters to cross sections. The varied parameters affect optical model potential, level densities, radiative

widths and strength of the pre-equilibrium emission. Taking into account large number of materials, only marginal reference to experimental data was made. Essentially, measurements on a few selected isotopes were used to guide the choice of uncertainties on the model parameters. This work is the first attempt to generate neutron cross section covariances on such a large scale.

In Fig. 11 'low-fidelity' results for the inelastic scattering on ^{56}Fe are shown. The uncertainties turn out to increase at the threshold region and at energies above 10 MeV, while at energies between 1 and 10 MeV they are generally lower than 10%. This might be considered overoptimistic when compared with the spread of experimental data in Fig. 11. However, the next plot (Fig. 12) shows that the 'low-fidelity' results are comparable to other 'high-fidelity' evaluations. In this particular case, the global constraints of the model based approach bring results which are surprisingly close to the more elaborated approaches based on the detailed analysis of the experimental data. In general, however, the 'low-fidelity' uncertainties are on the conservative side and tend to be higher than those obtained in the detailed analysis.

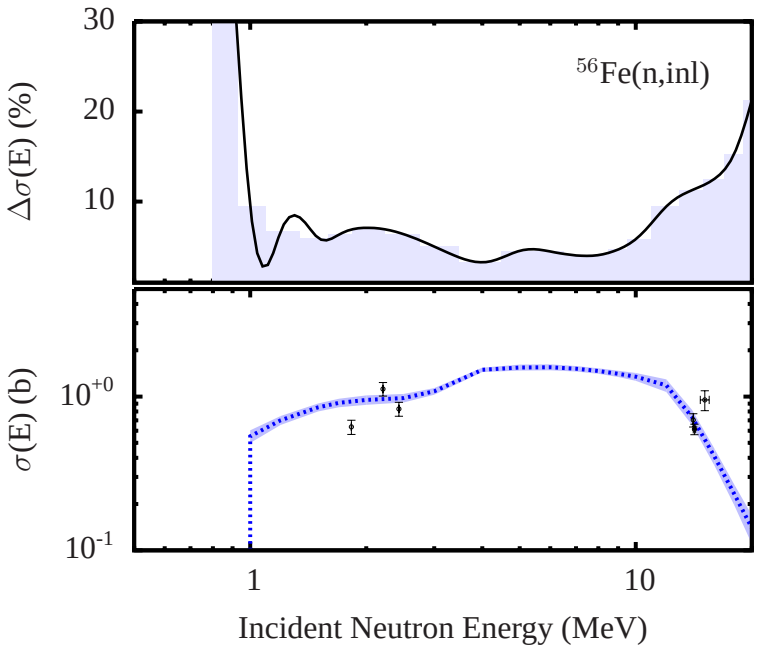

Figure 11: Relative uncertainties of ^{56}Fe(n,n$'$) cross sections obtained with the EMPIRE-KALMAN method. Shown for reference are also cross sections and selected experimental data.

Fig. 13 shows total cross section uncertainties for all 307 nuclei considered in the 'low-fidelity' project. Exceptionally high uncertainties are found for nuclei between Xe and Eu at incident energies below 100 keV. A possible explanation of this effect can be traced to the structure observed in the s- and/or d-wave neutron strength functions. We also note characteristic patterns characterized by regions where the uncertainties are particularly small. Physical origin of these structures is under investigation.

5.2 Individual 'high-fidelity' evaluations

5.2.1 Tungsten

New evaluations for the tungsten isotopes ^{180,182,183,184,186}W in the neutron energy range up to 150 MeV were produced by Capote and Trkov, including the covariance information. The model covariance matrices were generated for all isotopes of tungsten using a Monte Carlo approach (EMPIRE-MC) . A particular feature of the methodology is that it offers a possibility to produce covariances for the P1 component of the elastic and the first inelastic angular distributions in the laboratory system, as well as the covariances for the neutron emission spectra. The model covariance matrix was taken as a prior and was fed into the GANDR system. Selected experimental data from the EXFOR database were processed by the generalized least squares technique to constrain the covariances of the whole system, including cross-correlations. The

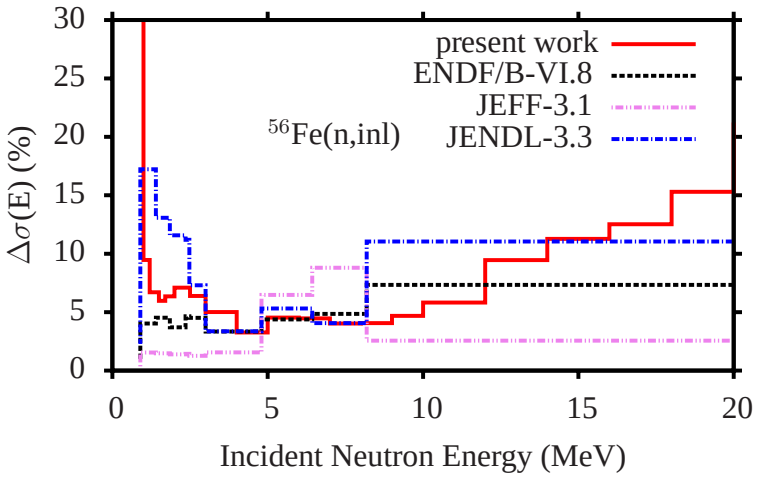

Figure 12: Relative uncertainties of ^{56}Fe(n,n′) cross sections compared to three major nuclear data libraries. The 'low-fidelity' results (denoted 'present work' on the figure) are in the point-wise form, while the other data are in the 44-energy group representation.

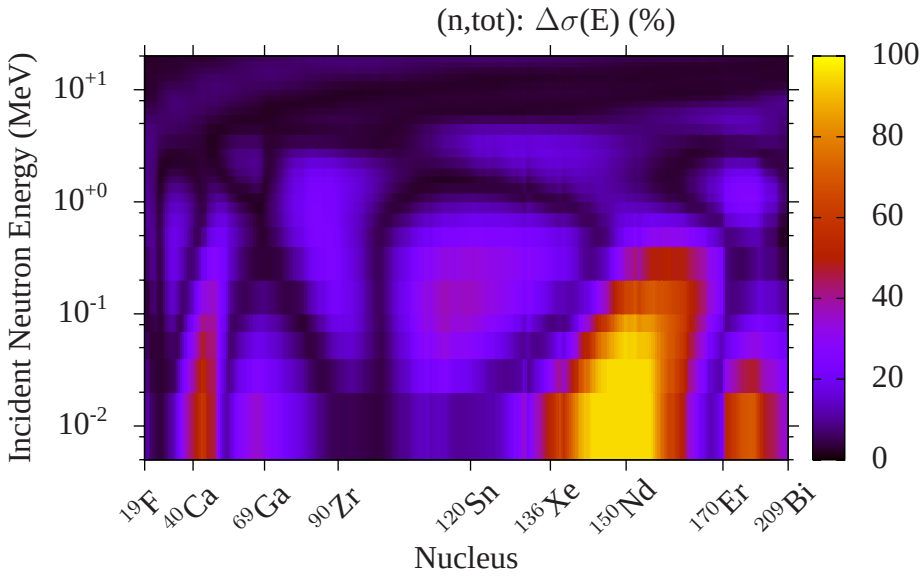

Figure 13: Relative uncertainties for the total cross sections on 307 materials obtained with the EMPIRE-KALMAN method in the fast neutron energy region.

resulting adjusted cross sections and the covariance matrix were transferred to the final evaluated data files for the tungsten isotopes. The evaluated files were tested on selected fusion neutronics benchmarks and fast reactor benchmarks. The next step in data validation will be the application of the covariance information to determine the uncertainties in the calculated integral parameters due to nuclear data.

5.2.2 Lead

At NRG, Koning and Rochman use a Monte Carlo method to generate covariance data for the fast neutron range. All covariances basically come from uncertainties of the nuclear model calculations. However, the final uncertainties are guided by the existing experimental data uncertainties. Instead of a Bayesian updating method a combination of Monte Carlo, maximum-likelihood estimation and binary reject/accept method is used to obtain the covariance matrix for both nuclear model parameters and the final nuclear data.

For all Pb isotopes, the initial, "best", set of results was produced by a TALYS calculation with an input parameter set which led to the JEFF-3.1 evaluation, see Ref. [10] for a description of these optimal parameter sets. Next, for each isotope 3000 TALYS runs were performed with random nuclear model parameters, producing uncertainty bands which can be used in figures and a full covariance matrix for the ENDF data file. An example for the first inelastic level of ^{208}Pb is given in the Fig. 14.

As an example, we give the resulting uncertainties of some of the most important nuclear model parameters for $n + ^{206}$Pb in Table 1. The parameter uncertainties for the other isotopes considered are similar. The procedure starts with a set of "global" parameter uncertainties, which gives credible uncertainty bands throughout the periodic table, which apply for reaction channels for which no experimental data exist. Considering the available experimental data in the binary reject/accept method, the values of Table 1 are obtained. A full parameter correlation matrix is available, but we feel that an extensive discussion of that is outside the scope of this report. A full discussion is given in [11]

Table 1: Uncertainties of some nuclear model parameters for ^{206}Pb, given as fraction (%) of the absolute value. Consult Ref. [10] for a detailed description of these parameters.

Parameter	Uncertainty (%)	Parameter	Uncertainty (%)	Parameter	Uncertainty (%)
r_V	1.5	d_1^n	9.4	Γ_γ	50.
a_V	2.0	d_2^n	10.	a (^{207}Pb)	4.5
v_1^n	1.9	d_3^n	9.4	a (^{206}Pb)	6.5
v_2^n	3.0	r_{SO}	9.7	a (^{205}Pb)	6.5
v_3^n	3.1	a_{SO}	10.	σ^2	19.
v_4^n	5.0	v_{so1}^n	5.0	g_π (^{207}Pb)	6.5
w_1^n	9.7	v_{so2}^n	10.	g_ν (^{207}Pb)	6.5
w_2^n	10.	w_{so1}^n	20.		
r_D	3.5	w_{so2}^n	20.		
a_D	4.0	$M2$	21.		

5.2.3 Manganese and zirconium

Work is in progress at NNDC (Pigni, Herman, Obložinský) to produce cross section covariances for the ENDF/B-VII.0 files for ^{90}Zr and ^{55}Mn. EMPIRE calculations are used to produce sensitivity matrices to the relevant model parameters. Then the KALMAN code will be used to determine covariances accounting for the selected set of experimental data. The first results are expected by end of June 2008.

5.3 Future work - GNEP

The NNDC and LANL are cooperating in preparation of covariances for the ENDF/B-VII.0 data adjustment within the GNEP project. This activity involves about 100 materials, i.e., about 25% of those addressed in

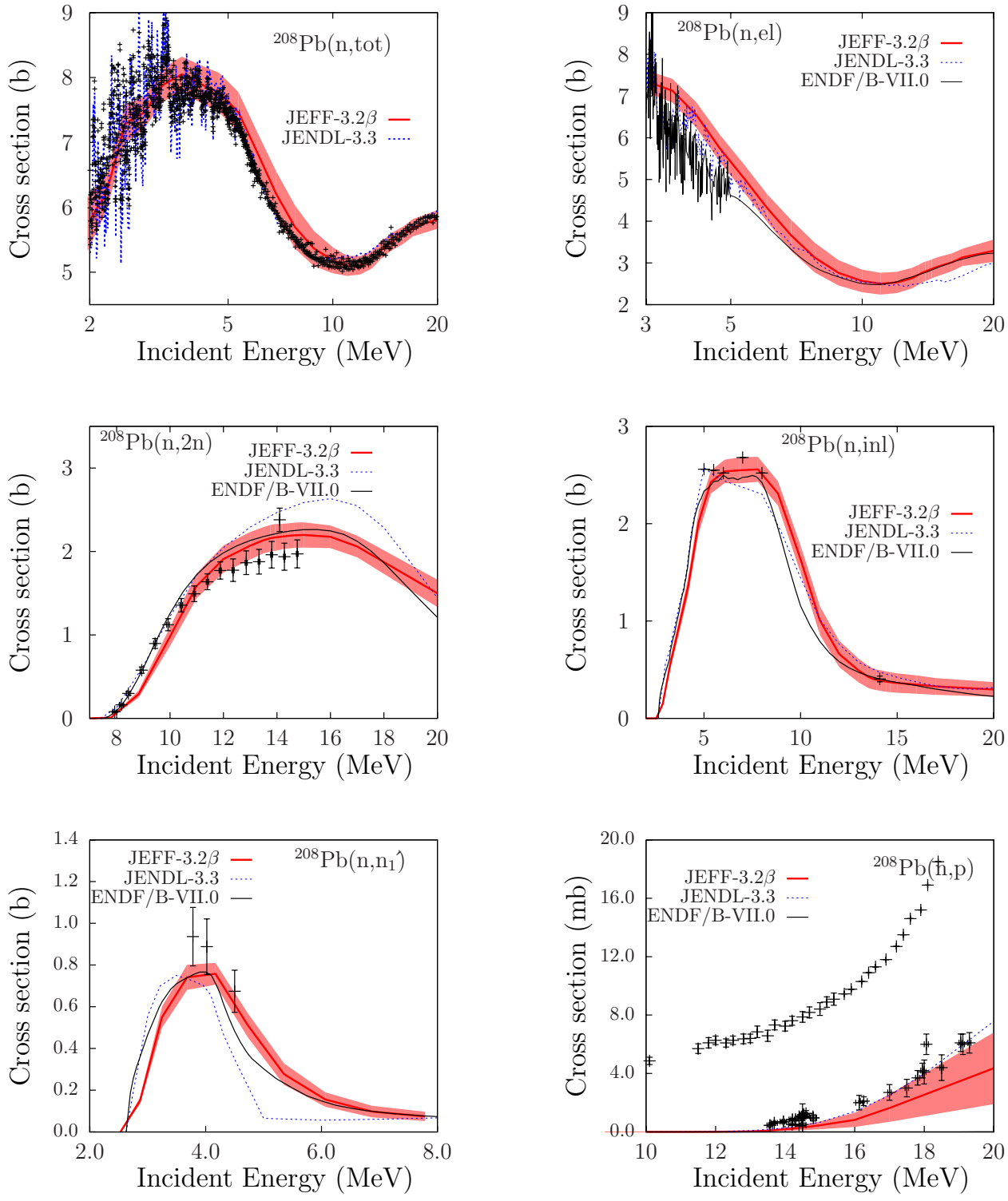

Figure 14: Cross section uncertainties in the fast neutron range for some neutron-induced reactions on ^{208}Pb.

the 'low-fidelity' exercise. The quality requirements, however, go beyond the 'low-fidelity' level. Therefore, the experimental data will have to be taken into account, at least for the priority materials. The project has started in 2008 and is scheduled for 3 years

Los Alamos will be working on assessing uncertainties in the prompt neutrons spectrum using a Monte Carlo technique to describe the evaporation of the neutrons from excited fission fragments. This approach will go a step further than the currently used Los Alamos (or Madland-Nix) model for predicting prompt fission neutrons. It will also make use of recently acquired data at LANSCE (Haight et al.).

6 Conclusions

SG24 has been making progress 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 is being enlarged to include fission neutron spectra, neutron multiplicities and mu-bars. Recent efforts concentrated on comparing different approaches to covariance determination and implementation of the Unified Monte Carlo approach. Although there has been a substantial progress in understanding differences among different methods the methodology is not yet fully mature and several issues have not yet been resolved. In spite of these, there have been a pressing request from the users community 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. Further studies are needed, however, to resolve ambiguities encountered in the current implementations. The most pressing are: the treatment of the experimental data in MC methods, understanding reasons for low uncertainties in KALMAN (in presence of very many experimental data), and finding ways of avoiding such unrealistic uncertainties. Practical implementation of the new UMC concept appears to be a major task. Although UMC seems to be computationally intensive it still might be the most adequate approach in cases involving measurement ratios and strong non-linearities in general.

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. This issue is addressed with the International Atomic Energy Agency (IAEA) coordinated research project RIPL-3. Finally, there is urgent need to clean the Exchange Format (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. This important activity is being carried out within the WPEC Subgroup 30.

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