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Abstract. We describe new method for energy-energy covariance calculation from the thermal energy up to 20 MeV. It is based on three powerful basic components: (i) Atlas of Neutron Resonances in the resonance region; (ii) the nuclear reaction model code EMPIRE in the unresolved resonance and fast neutron regions, and (iii) the Bayesian code KALMAN for correlations and error propagation. Examples for cross section uncertainties and correlations on ^{90}Zr and ^{193}Ir illustrate this approach in the resonance and fast neutron regions.

1 Introduction

The need for nuclear data covariances (uncertainties and correlations) is becoming increasingly more important for a number of applications, including the development of next generation nuclear power reactors known as ”Gen-IV”, advanced fuel cycles, transmutation and shielding design [1,2]. Recent progress in transport computer codes and improved evaluated nuclear data allow to replace expensive and time consuming measurements on mock-up assemblies with much faster and cheaper numerical simulations. For these simulations to be useful, cross section evaluations have to come with a trusted estimate of uncertainties. Unfortunately, this type of information is very incomplete and often very obsolete, even in the most recent nuclear data libraries. For example, the brand new ENDF/B-VII.0 library [3] contains covariances only for 13 old and 13 newly evaluated materials out of 393.

To answer these needs, we are developing a new methodology for cross section energy-energy covariances from the thermal energy (0.0253 eV) to 20 MeV for nuclides heavier than $A = 20$. Some of our results, for Gd isotopes in the fast neutron region and ^{89}Y, ^{99}Tc and ^{191,193}Ir in the entire energy region, were included in the ENDF/B-VII.0 library.

2 Methodology for Cross Section Covariances

2.1 Basic components

The National Nuclear Data Center, BNL in collaboration with T-16, LANL is developing a methodology for evaluation of cross section covariance data that covers the thermal energy, resolved and unresolved resonance regions as well as the fast neutron region. It is built on the following three major components:

Atlas of Neutron Resonances [4]. This book contains recommended parameters of neutron resonances evaluated on the basis of virtually all pertinent experimental data available in 2005. The Atlas contains evaluated neutron data for all elements and 486 ground and isomeric states of 476 isotopes including uncertainties. The most important quantities for the present project are:

- Thermal cross sections (capture, elastic, fission), with uncertainties,
- Scattering radius, with uncertainties,
- Resonance integrals (capture, fission), calculated or measured, with uncertainties,
- Resonance parameters (radiative, neutron and fission widths), with uncertainties.

Nuclear reaction model code EMPIRE [5]. EMPIRE is a modular system of codes that is well suited for model assisted determination of covariances. A suite of nuclear reaction models includes the spherical optical model, Coupled Channels, Distorted Wave Born Approximation, Multi-step Direct, Multi-step Compound, the exciton model with preequilibrium emission of clusters and gamma rays, and the full featured Hauser-Feshbach (HF) model with multi-particle emission and detailed γ-cascade.

Bayesian code KALMAN [6]. This code, based on the theory of the Kalman filter, allows to estimate covariances by combining experimental uncertainties and correlations with theory predictions. KALMAN calculates cross section covariances P in two steps: (i) the model parameter covariance matrix X is calculated from the experimental covariances V, and (ii) the error propagation is used to calculate cross section covariances P from the model parameter covariances X:

$$\begin{aligned} P &= \left(X^{-1} + C^t V^{-1} C\right)^{-1} \\ &= X - XC^t\left(CXC^t + V\right)^{-1} CX, \end{aligned} \qquad (1)$$

where C is the sensitivity matrix describing response of the model to the perturbation of its parameters.

2.2 Evaluation methods

The above three basic components are combined to two methods, Atlas-KALMAN for thermal and resonance region, and EMPIRE-KALMAN for fast neutron region. The unresolved resonance region can, in principle, be treated by both methods. This overlap constitutes a link between the two approaches, which can be exploited for determining correlations between the resonance and fast neutron regions.

Atlas-KALMAN method. One starts with the resonance parameters given in the Atlas. Cross sections are calculated using the multi-level Breit Wigner (or Reich Moore) formalism and converted into a suitable multigroup representation. Uncertainties of resonance parameters (Γ_n, Γ_γ and eventually also Γ_f) and thermal-energy values from the Atlas are propagated with the KALMAN code to obtain uncertainties and correlations for cross sections. Missing uncertainties of resonance parameters are estimated either by extrapolating and interpolating available resonance data or from the neighboring nuclei. When fitting the uncertainty for the thermal capture, the adequate uncertainties are assigned to the resonance parameters of the negative-energy resonance.

EMPIRE-KALMAN method. This method employs a sensitivity matrix produced with the nuclear reaction theory code EMPIRE, and uses it in the Bayesian KALMAN code for determining covariances while taking into account relevant experimental data. To obtain the sensitivity matrix with EMPIRE, about 10-15 of the most relevant model parameters (optical model, level density, preequilibrium strength) are varied independently, typically by ± 5 % around the optimal value, to determine their effect on total, elastic, inelastic, capture, fission, (n,2n), (n,p) and (n,α) cross sections in the full energy range of the evaluation. Sensitivity matrix elements are calculated as a change of a given reaction cross section in response to the change of the particular model parameter. In general, model parameter uncertainties are adjusted to reproduce experimental cross section uncertainties.

3 Results and discussion

3.1 Thermal and Resolved Resonance Region

Cross section uncertainties in the resonance region exhibit complicated structure that can be relatively easily explained in the case of neutron capture. For an isolated neutron resonance, one can use the single-level Breit-Wigner formula for capture cross section, σ_γ, and derive the relative uncertainty due to uncorrelated Γ_γ and Γ_n as:

$$\frac{\partial\sigma_\gamma}{\partial\Gamma_\gamma}/\sigma_\gamma = \left[1 - \frac{2\Gamma_\gamma(\Gamma_\gamma+\Gamma_n)}{(\Gamma_n+\Gamma_\gamma)^2+4(E-E_0)^2}\right]\frac{1}{\Gamma_\gamma}, \qquad (2)$$

$$\frac{\partial\sigma_\gamma}{\partial\Gamma_n}/\sigma_\gamma = \left[1 - \frac{2\Gamma_n(\Gamma_\gamma+\Gamma_n)}{(\Gamma_n+\Gamma_\gamma)^2+4(E-E_0)^2}\right]\frac{1}{\Gamma_n}, \qquad (3)$$

An example of relative cross section uncertainties is given in fig. 1 for ^{90}Zr(n,γ), assuming a single resonance at E_0 = 7.251 keV with Γ_γ = 0.128 eV and Γ_n = 3.0 eV. Since $\Gamma_\gamma/\Gamma_n << 1$, the second term in the right-hand side of eq. (2) is small and the resulting relative uncertainty due to $\Delta\Gamma_\gamma$ is essentially constant. However, the similar term in eq. (3) remains strong, implying complex shape of relative uncertainties around the resonance peak due to $\Delta\Gamma_n$.

In the case of more resonances, with uncorrelated resonances parameters, the capture cross section uncertainty can be expressed as:

$$\Delta\sigma_\gamma^2 = \sum_i \left[\left(\frac{\partial\sigma_\gamma}{\partial\Gamma_{\gamma_i}}\right)^2 \Delta\Gamma_{\gamma_i}^2 + \left(\frac{\partial\sigma_\gamma}{\partial\Gamma_{n_i}}\right)^2 \Delta\Gamma_{n_i}^2\right] \qquad (4)$$

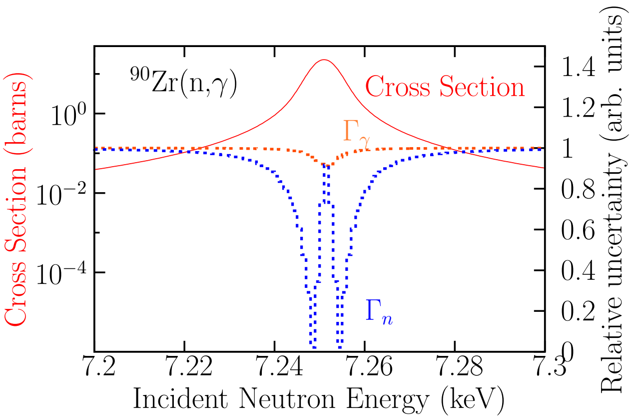

Fig. 1. Relative cross section uncertainties from Γ_γ and Γ_n (right scale) and cross section (left scale) for ^{90}Zr(n,γ) for the single 7.251 keV resonance.

Fig. 2 shows ^{90}Zr(n,γ) assuming two resonances, at 4.008 keV with $\Delta\Gamma_{\gamma_1}$ = 10 % and at 7.251 keV with $\Delta\Gamma_{\gamma_2}$ = 15.8 %. Only radiative widths are considered. In this case, the capture cross section relative uncertainty reflects the radiative width uncertainties. Close to 4 keV the effect of $\Delta\Gamma_{\gamma_1}$ = 10 % is dominant, while around 7 keV the role of $\Delta\Gamma_{\gamma_2}$ = 15.8 % prevails, with the smooth transition between the two resonances. The dip at 4 keV is caused by the fact that Γ_{γ_1} is comparable to the neutron width of this resonance.

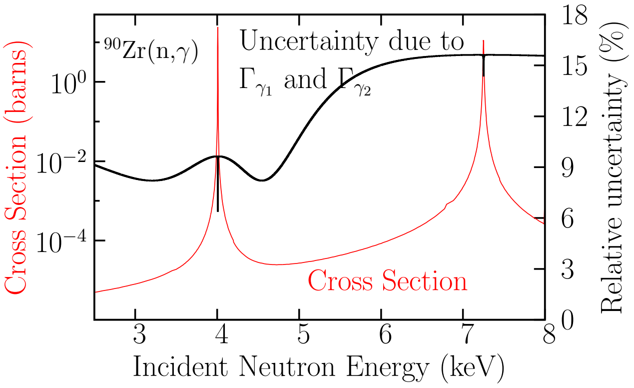

Fig. 2. Relative uncertainties due to radiative widths with two isolated resonances (4.008 and 7.251 keV).

For thermal cross section uncertainty, both the positive and negative energy resonances are considered. The missing uncertainties of the resonance parameters in the Atlas of Neutron Resonance were estimated to be 20% for Γ_γ and 50% for Γ_n. The uncertainties of the bound resonance parameters were adjusted to reproduce the calculated thermal cross section uncertainty given in the Atlas. In table 1 we compare the thermal-energy capture cross section uncertainties obtained in the present work with the values given in the Atlas. One can see that good agreement was obtained for ^{90}Zr and ^{99}Tc. For ^{89}Y and two iridium isotopes, thermal cross section uncertainties can not be matched with the Atlas values due to strong contribution from the positive-energy resonances. In these cases we adopted the conservative approach and our thermal cross sections uncertainties are higher than those given in the Atlas.

Table 1. Thermal-energy capture cross sections uncertainties of the present work compared to the values of the Atlas of Neutron Resonances [4].

Nuclide	Present work	Atlas 2006
^{89}Y	3.1 %	1.6 %
^{90}Zr	23 %	21 %
^{99}Tc	7.9 %	7.9 %
^{191}Ir	1.4 %	1.0 %
^{193}Ir	5.1 %	4.5 %

In table 2 we show capture resonance integrals and their uncertainties. Our results are compared with the values from the Atlas of Neutron Resonances. The resonance integrals are defined as

$$I_\gamma = \int \frac{\sigma_\gamma(E)}{E} dE, \qquad (5)$$

where the integration is done from 0.5 eV up to the end of the resolved resonance region.

Table 2. Capture resonance integrals I_γ and their uncertainties of the present work, compared with the Atlas of Neutron Resonances [4]. The values marked by '$\star$' are calculated, otherwise measured quantities are given in the Atlas.

Nuclide	Present work		Atlas 2006	
^{89}Y	0.96 b	± 2.1 %	0.96 b	± 6.2 %
^{90}Zr	0.17 b	± 5.3 %	0.17 b	± 12 %
^{99}Tc	362 b	± 1.5 %	358 b*	± 5.6 %*
^{191}Ir	3520 b	± 1.8 %	3550 b	± 2.8 %
^{193}Ir	1350 b	± 1.9 %	1350 b	± 7.4 %

In all cases, our resonance integrals agree well with those from the Atlas, but our uncertainties are much smaller, by a factor 2 or more. These discrepancies can be understood as follows.

First, in Ref. [4], only the value for ^{99}Tc is calculated, while the remaining four are measured. Our uncertainties of the resonance integrals are obtained by propagating evaluated uncertainties from both the thermal cross sections (generally pretty accurate) and from the resonance parameters. As such, our uncertainties are based on parameters that are independent from the resonance integral measurements. Therefore, the comparison with experimental uncertainties on I_γ faces a possible discrepancy between microscopic and integral experiments, while comparison with the calculated Atlas uncertainties is only testing the methodology of estimating uncertainties. Second, we neglected certain sources of correlations (*e.g.*, correlation between Γ_γ and Γ_n for each resonance) and these would increase our calculated uncertainties of I_γ.

3.2 Unresolved resonance region

Cross section uncertainties in the unresolved resonance region can be calculated with both the EMPIRE-KALMAN and Atlas-KALMAN methods. Traditionally there is a sharp distinction between the fast neutron energy region and the resonance region as far as evaluation methodology is concerned. Nevertheless, the unresolved resonance region can be estimated either by extending Hauser Feshbach calculations to the very low energy region, or by using average resonance parameters (average neutron and radiative widths) within the single-level Breit Wigner formalism.

In the first case, sensitivities depend only on optical model parameters and on the ã-parameter for the level density of the compound nucleus. It is known that sensitivities to the optical model parameters are increasing as the neutron energy is decreasing. This will directly affect the calculated cross section uncertainties which will smoothly go from a high value at the lower boundary of the unresolved region to a lower value at the upper boundary.

In the second case, only the average resonance width parameters, $< \Gamma_\Gamma >$ and $< \Gamma_n >$, and the scattering radius are considered. In the case of capture cross section, sensitivities to both $< \Gamma_\Gamma >$ and $< \Gamma_n >$ present a smooth and slightly increasing function of the neutron energy. The resulting cross section uncertainty will then be slightly increasing with incident neutron energy.

In conclusion, the two methods predict somewhat different energy dependence for cross section uncertainties, and also somewhat different correlations (one correlated with the fast neutron range, the other one with the resolved neutron range). These differences need further investigation, one should compare the calculated uncertainties with experimental data in order to choose one representation or another.

3.3 Fast Neutron Region

A total of 15 parameters are considered in sensitivity calculations including real and imaginary surface depth of the optical potential for the compound nuclei, particle- and γ-emission widths, level densities, and mean free path in the exciton model. Then, selected experimental data along with sensitivity matrices are used as input for the KALMAN code. Fig. 3 shows our results for the uncertainties of total, (n,2n) and capture cross sections on ^{193}Ir. These results are included in the ENDF/B-VII.0 library.

While the uncertainties on (n,2n) fall below 10 %, near 14 MeV (where many measurements exist), they become much larger at lower energies near the (n,2n) threshold. Likewise, the (n,γ) cross section uncertainty becomes large above a few MeV where data are sparse, and where the cross section is very small. For the (n,tot) cross section, experimental data are considered above 2 MeV. Actually, experimental data in the whole energy constrain model parameters (including crucial depth of the real potential).

Model calculations predict strong correlations in the whole energy range since individual model parameters tend to affect broad energy ranges, while experiment-based covariances are characterized by strong positive correlations aligned along the

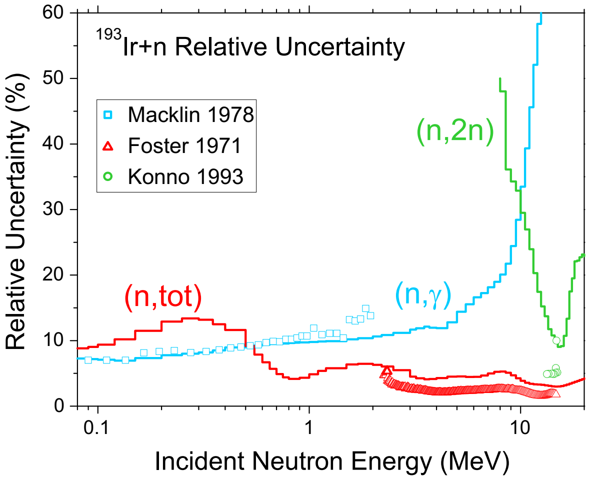

Fig. 3. Relative uncertainties for the total, (n,2n) and capture reactions on ^{193}Ir obtained with the EMPIRE-KALMAN method. Experimental uncertainties considered in the analysis are also presented.

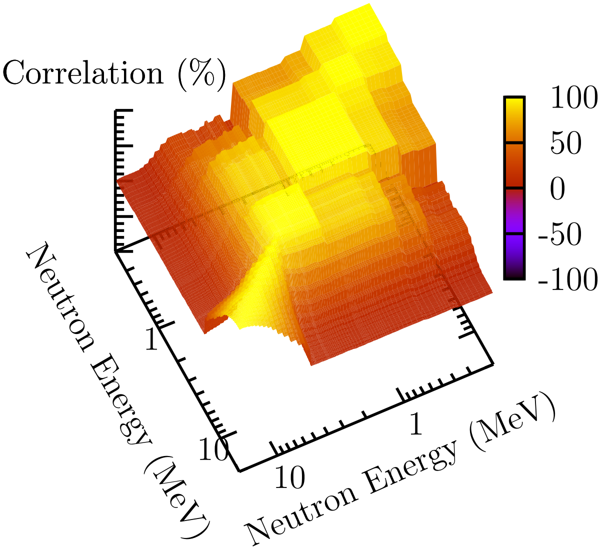

Fig. 4. Correlation matrix for the ^{90}Zr neutron capture cross sections in the fast neutron region obtained with the EMPIRE-KALMAN method without experimental data.

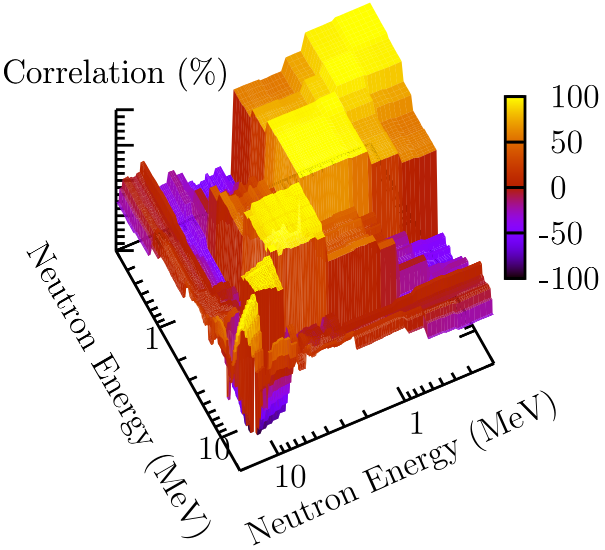

Fig. 5. Same as fig. 4, with experimental data.

diagonal and zero outside (short-range correlations). This is because measurements are believed to be quite independent from each other, *i.e.*, long-range correlations (systematic errors) are assumed to be relatively weak. Figs. 4 and 5 show the calculated correlation matrices for the capture cross section on ^{90}Zr, with and without experimental data.

One observes that essentially flat and positively correlated shape obtained in the model-based calculations is severely affected by the inclusion of experimental results. Correlation matrix with experimental data reveals more complicated structure with strong correlations aligned within a relatively narrow band along the diagonal. The positive long-range correlations, typical for model predictions, are annihilated or turned into anticorrelations leaving only short- and medium-range positive correlations. Thus, we get a picture that is intermediate between long-range correlations (model calculations) and short-range correlations (experiment).

4 Conclusion

We are developping a methodology to calculate cross section covariance from thermal energy up to 20 MeV, combining the features of the Atlas of Neutron Resonances, the nuclear code EMPIRE and the Bayesian code KALMAN. In the resolved and unresolved resonance region, the information on the resonance parameters and thermal cross sections from the Atlas are used to calculate cross section uncertainties and correlations, assuming, for the time being, no parameter correlation. The EMPIRE-KALMAN approach is used in the fast neutron region and as well as in the unresolved resonance region.

In future, we plan to study the effect of resonance parameter correlations in the resolved and unresolved resonance regions, and correlation between the resonance region and fast neutron region.

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