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Fast Neutron Covariances for Evaluated Data Files

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Abstract

We describe implementation of the KALMAN code in the EMPIRE system and present first covariance data generated for Gd and Ir isotopes. A complete set of covariances, in the full energy range, was produced for the chain of 8 Gadolinium isotopes for total, elastic, capture, total inelastic (MT=4), (n,2n), (n,p) and (n,alpha) reactions. Our correlation matrices, based on combination of model calculations and experimental data, are characterized by positive mid-range and negative long-range correlations. They differ from the model-generated covariances that tend to show strong positive long-range correlations and those determined solely from experimental data that result in nearly diagonal matrices. We have studied shapes of correlation matrices obtained in the calculations and interpreted them in terms of the underlying reaction models. An important result of this study is the prediction of narrow energy ranges with extremely small uncertainties for certain reactions (e.g., total and elastic).

KEYWORDS: Covariances, uncertainties, evaluated nuclear data, model calculations

1. Introduction

Design of new generation of nuclear reactors, such as GEN-IV, and other emerging applications of nuclear technology require reliable estimates of uncertainties associated with evaluated nuclear data in order to predict construction margins involved in the new designs. 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, they have to come with a trusted estimate of the involved uncertainties. The codes, such as SCALE-5, are capable of providing requested uncertainty margins under a condition that relevant information is contained in the underlying evaluated nuclear data files. Unfortunately, this type of information is very incomplete and often very obsolete, even in the most recent nuclear data libraries. For example, a brand new ENDF/B-VII [1] library contains new covariances only for a few materials and actual number of materials with covariance data actually went down due to the removal of the old data incompatible with the current evaluations.

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Need for new covariances has been advocated by the members of the reactor community on many occasions. It was stressed, that even relatively rough approximation would be of enormous help for the development of new concepts - the essential factor being availability of the covariance data for all materials of significant importance. This interest was formalized in the establishment of the WPEC Subgroup 24, dedicated to the development of the covariance generation capabilities in the fast neutron region. In the present contribution we describe such an effort being carried out in US as a collaboration between BNL and LANL with ORNL providing covariances in the resonance region to complete information on data uncertainties.

At present, there are two methods that are being used for evaluation of covariance data in the fast neutron region: (i) Monte-Carlo method proposed by D. Smith in his well-known 'white paper' [2] and (ii) KALMAN-filter coded by Kawano [3] and used in JENDL-3.3 evaluations. Our approach is to use both methods with the BNL nuclear model code EMPIRE [4].

In this contribution we concentrate on covariances in the fast neutron region that can be determined with modern codes for modeling nuclear reactions. However, we fully recognize importance of the covariances in the resonance region. Therefore, we have used the retroactive technique in SAMMY code to produce covariances in the resolved resonance region that are included in our final evaluations.

2. EMPIRE/KALMAN system

EMPIRE [4] is a new generation nuclear reaction code that due to its completeness, flexibility, and simplicity of use is particularly suited for the job. To provide covariance capabilities we have added to EMPIRE an option allowing for sensitivity calculation and included KALMAN code [3] in the system. Following 'EMPIRE philosophy', a series of scripts and utility codes ensure smooth functioning of the system down to the ENDF-6 formatted file, with user's manual intervention reduced to the absolute minimum.

KALMAN implementation was a joint effort of BNL and LANL. Sensitivity calculations were coded in the EMPIRE core. They allow to produce sensitivity matrix 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 produced by KALMAN are ENDF-6 formatted (MF=33, LB=5).

KALMAN approach has a number of very attractive features. First of all, it takes into account experimental data - even a single point can be used to constrain calculated results involving many (say n) model parameters. In is computationally efficient since determination of the sensitivity matrix requires $2n + 1$ calculations, that is usually much less than amount needed to achieve reasonable statistics in the Monte-Carlo method. Generally, most of the CPU time is spent for these sensitivity calculations while actual run of the KALMAN code is very fast. If requested, KALMAN can also produce cross-covariances between different reactions, although we did not pursue this option in the current exercise. Finally, if there is at least one experimental point KALMAN provides also uncertainties for the model parameters and respective correlations (at least for some of them). Actually, KALMAN approach does even more - it adjusts parameters to reproduce experimental data assuming linear dependence given in the sensitivity

matrix. In summary, KALMAN turns out to be a very powerful evaluation tool that might also be used in a large scale calculations aiming in simultaneous global improvement of reaction evaluations and of model parameters.

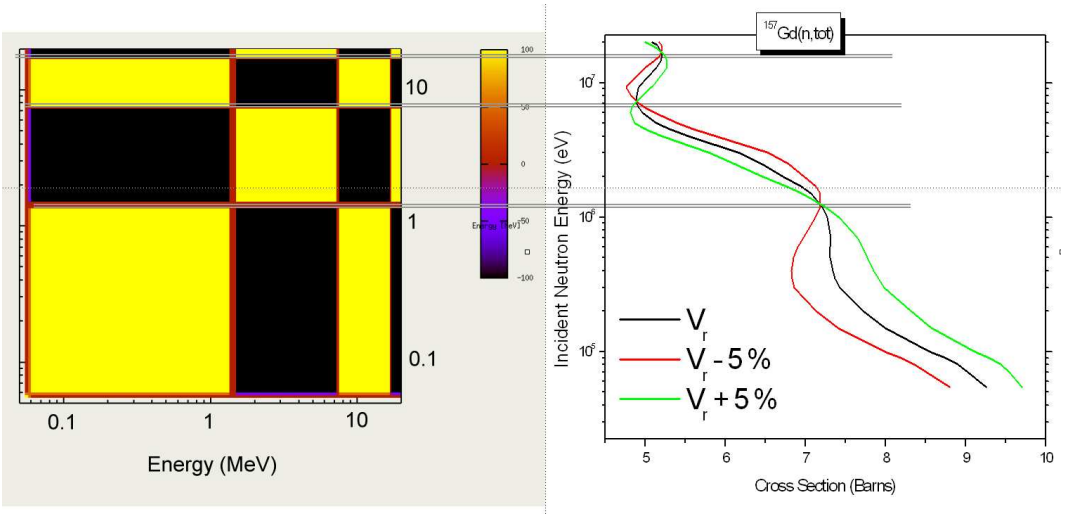
EMPIRE code has also been extended by Capote and Trkov to embrace Monte Carlo method. In this version, the code is run number of times with specified input parameters drawn randomly from the uniform distribution. No parameter correlations are included at this stage. A dedicated codes have been developed to construct covariances and to produce ENDF-6 files.

With the above mentioned extensions, EMPIRE became one of the two (the other one being TALYS [5]) modern tools capable of massive production of covariance data for the evaluated files.

3. Physics and the shape of the correlation matrix

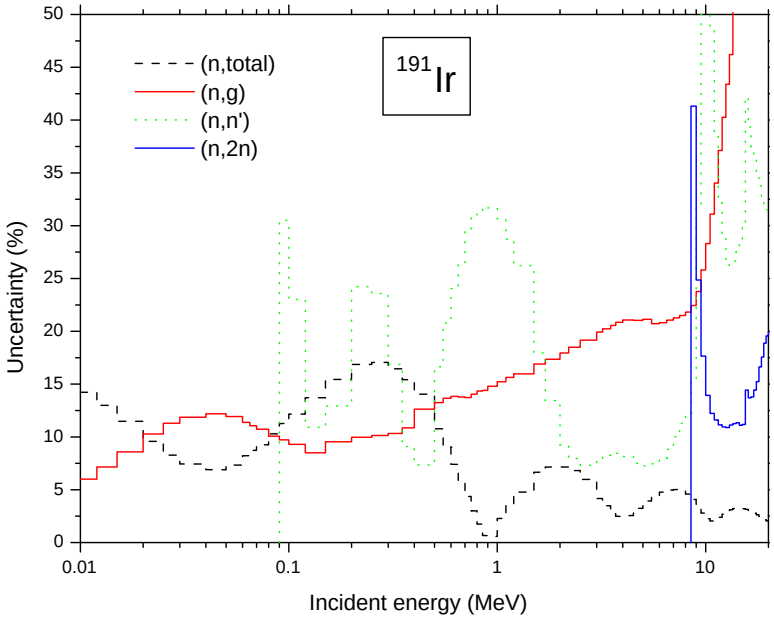
Some plots of model-based correlation matrices reveal very strange, sometimes astonishing structures. In certain cases these structures are of obvious origin, e.g., neutron capture at low incident energies proceeds through the compound nucleus mechanism while above 10 MeV it is dominated by the preequilibrium emission. Since there is no (or very little) correlation among the parameters used in the two nuclear reaction models the two energy regions governed by the respective models are essentially uncorrelated. On the other hand, there are cases, such as total and elastic, were structures in the model-based correlation matrices are intriguing and by no means obvious. In order to understand their origin we investigate role of various parameters on the shape of the correlation matrix. Doing this we were studying correlation matrices produced when individual model parameters were varied separately. Then, we investigated the effect of adding other parameters. This procedure was carried out for a number of the most important parameters. However, because of the well known invariance of the cross sections to the volume integral of the optical model potential and resulting correlation between depth and geometry of the potential we choose to vary only depths while keeping radii and diffuseness constant.

Figure 1: Model-based correlation matrix for total cross sections on ^{157}Gd (left panel) and total cross sections calculated for three values of the real depth in optical potential (right panel). The horizontal lines trace structure in the correlation matrix to the 'crossing points' in the calculated cross sections.



In Fig. 1 we present self-correlation matrix for total cross section obtained when only real depth of the optical potential is ascribed 10% uncertainty while all other parameters used in the calculation are assumed to be exactly known, i.e., do not contribute to the covariance. A striking feature seen in Fig. 1 is a sort of tartan pattern - in which square, strongly positive-correlated regions, border with similar, but anti-correlated, regions. The transition between these regions is very sharp. This noticeable pattern is due to the well know feature of the optical model - change in the depth of the real volume potential causes a sort of a shift in energy of the total and elastic cross sections. This shift makes the shape resonance bump to move leading to the crossing points as depicted schematically in Fig. 1. Change of the real potential depth results in the increase of the cross section on one side of the crossing point and decrease on the other. Therefore, we get perfect anti-correlation of the energy regions on both sides of the crossing point. It turns out that including other optical model parameters does not modify the essence of this picture. The only effect of other parameters is to smooth the transition boundaries but the general shape remains unchanged. We note, that this structure of the covariance matrix has an important impact on model-based uncertainties. At the crossing points uncertainties become very small since model calculations at these points are nearly insensitive to any reasonable variations of the model parameters.

Figure 2: Uncertainties on evaluated cross section calculated with the EMPIRE-KALMAN method for ^{191}Ir total, inelastic, capture and (n,2n) cross section



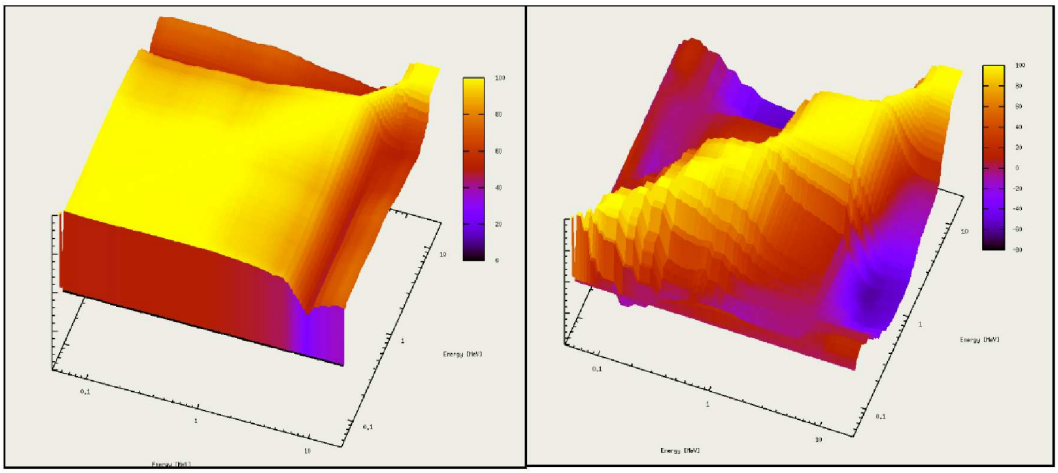
Adding experimental data, as discussed in the following section, generally has a dramatic effect on the correlations matrix. In the case of total and elastic, however, model-generated effect is so strong that it is still recognizable even if many experimental points are included in the analysis. In Fig. 2 we show uncertainties for several cross sections on ^{191}Ir. One observes the expected structure in the total cross section uncertainty - a very pronounced minimum

around 1 MeV and a number of lesser minima. Actually, experimental data in the whole energy constrain model parameters (including crucial depth of the real potential) leading to further improvement of the precision at the crossing points. Since general validity of the optical model in not questionable, we believe that the reduction of uncertainty at the crossing points is real. Therefore, in each total cross section we may expect at least 3 energy points with very small uncertainty. Experimentalist could take advantage of this feature whenever reference cross section is needed for normalization of an experiment.

4. Experimental data and model generated covariances

Model-based covariances, in most cases, assume that the reaction model itself is perfect, applicable, and sufficient to describe the investigated observable. Thus, the only source of uncertainties in the model-based covariances are the uncertainties of model parameters while direct measurements of the observable are totally ignored. Koning has compared model-based covariances that he obtained using Monte Carlo method implemented in the TALYS code [5] with the covariances resulting from analysis of experimental data as obtained by Tagesen and Vonach [6] for some well measured cross sections on ^{56}Fe. This comparison demonstrates a striking difference between the two approaches. 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 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. We should expect, that bringing both sources of knowledge (model calculations and experiment) together should produce intermediate result for the correlation matrix and... lower uncertainties.

Figure 3: Model-based self-correlations for neutron capture on ^{157}Gd (left panel) compared to self-correlations when experimental data are included in EMPIRE/KALMAN analysis (right panel).

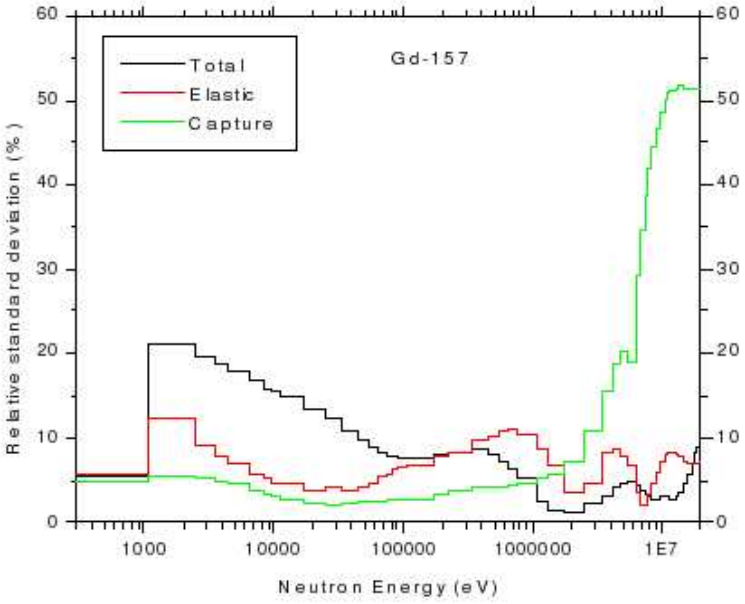


This expectation is confirmed by KALMAN/EMPIRE calculations that naturally include both model-based prior and experimental data. In Fig. 3 we compare self-correlations for neutron capture cross sections on ^{157}Gd obtained under two scenarios: (i) pure model calculations and (ii) model calculations together with experimental data for neutron capture. One observes that

essentially flat and highly correlated shape obtained in the model-based calculations is severely affected by inclusion of experimental results. The correlation matrix 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).

While experimental data are naturally included in the KALMAN approach they are not necessarily intrinsic to other methods and their inclusion seems to be essential for producing realistic covariances. Recently, Monte Carlo EMPIRE calculations were coupled to the GANDER system to account for the experimental data and applied for the determination of the covariance data for the new ^{232}Th evaluation. The preliminary results [7] are very encouraging and put into evidence role of correlations between different experiments. Including these correlations avoids unphysically small cross section uncertainties.

Figure 4: Uncertainties for the total, elastic and capture on ^{157}Gd obtained in the analysis with the EMPIRE/KALMAN system.



Another interesting method, called backward-forward Monte-Carlo, has been reported by E. Bauge at the WPEC-2006 meeting in Paris. This method determines the model parameter covariance matrix from the Monte-Carlo (MC) sampling combined with a χ^2 approach (backward MC), and then propagates the covariance of the model parameters to obtain the cross section covariance matrix by MC sampling (forward MC). It will be interesting to see practical applications of this method.

5. Results

A complete set of covariances was generated for the full chain of 8 Gadolinium isotopes [8] using KALMAN method and EMPIRE code in the fast and unresolved resonance regions. The retroactive method in the SAMMY code was used in the resolved resonance region. These evaluations make part of the ENDF/B-VIIb2 release and are accessible at [1]. In addition, we have also generated fast neutron covariances for ^{191,193}Ir.

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 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%). These calculations have been extended throughout the unresolved resonance region. Fig. 4 shows total, elastic and capture uncertainties obtained for ^{157}Gd. A similar set of observables is presented in Fig. 2 for the case of ^{191}Ir. All files were successfully processed through ERRORJ to produce group-wise covariance data. Fig. 5 shows an example of correlation matrix and associated uncertainties in group-wise form in the case of neutron capture on ^{157}Gd.

6. Challenges and future developments

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

- determination of model parameter uncertainties - is essential for predicting covariances, especially but not only, for reactions lacking any experimental data. A considerable effort will have to be undertaken to achieve this goal.

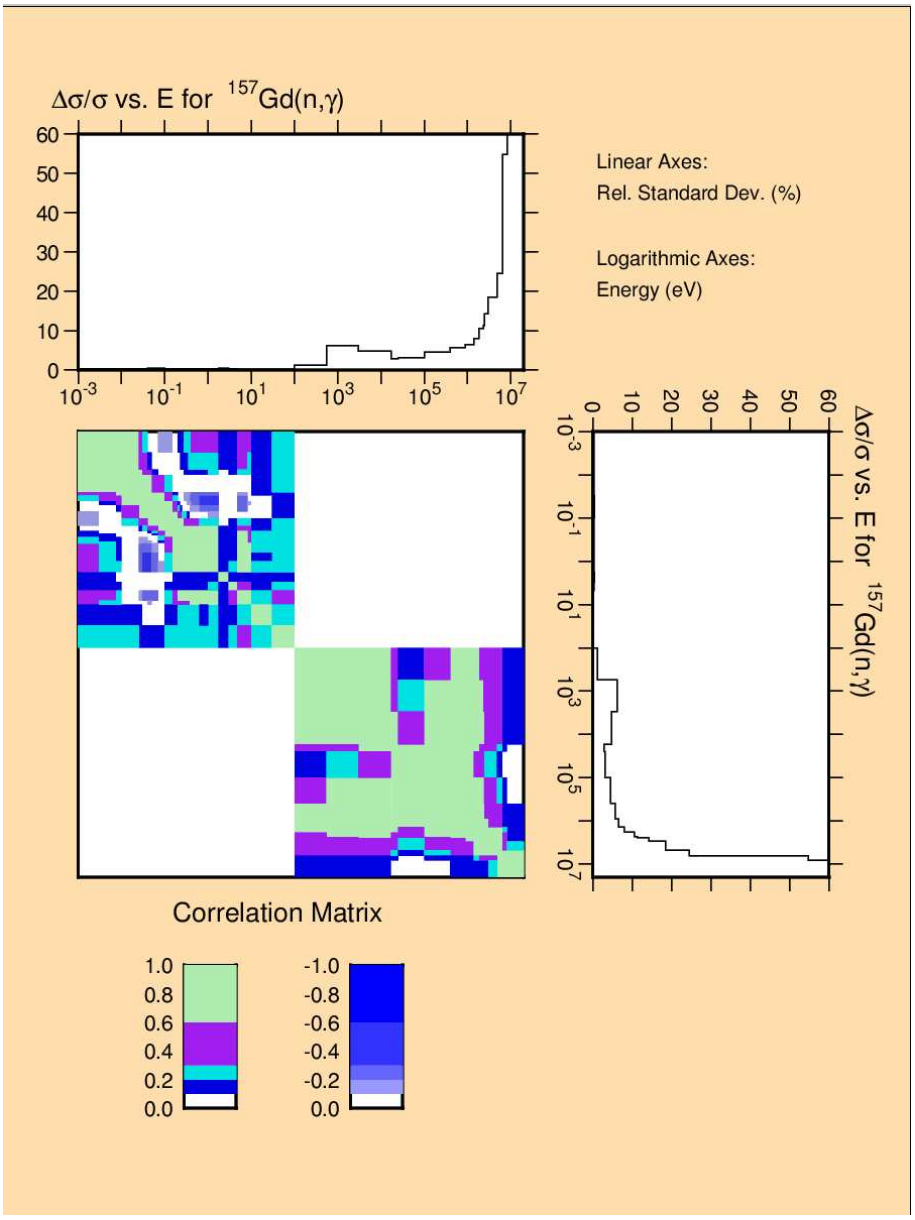
- understanding of the effect of correlations among experimental points and different measurements - it is a general tendency that Bayesian methods, helped by the reaction model constrains, tend to produce unrealistically small uncertainties if many experimental points are involved (e.g., total cross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

- effect of uncertainties intrinsic to the model itself - this effect is very 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).

7. Correlations among resolved, unresolved and fast neutron regions

Traditionally, there is a sharp distinction between the resonance and the fast energy region as far as evaluation methodology is concerned. This division stems from the fact that nuclear

Figure 5: Self-correlation matrix and related uncertainties for neutron capture on ^{157}Gd obtained with the EMPIRE/KALMAN system (unresolved resonance and fast neutron regions) and SAMMY (resolved resonance region). The results were processed into multi-group structure through NJOY-99.125 and ERRORJ. Note lack of correlations between the resolved resonance region and the remaining two regions



reaction models can only be used above the resonance region. The division is naturally propagated also on the covariance data. Resolved resonance, unresolved resonance, and fast neutron regions are always assumed to be uncorrelated that results in correlations matrices partitioned into three isolated squares along the diagonal.

Different experimental methods and inability of any model calculations to treat simultaneously resolved resonance and fast neutron regions seem to justify such an assumption. In reality, however, there are good reasons why all three regions should be correlated. First of all, parameters used in the unresolved regions are often extrapolation of those in the resolved region so the correlation is obvious and pretty strong. On the other hand, model calculations in the fast neutron region use certain parameters, such as level densities, that are obtained from the analysis of neutron resonances. This brings direct correlation between the fast neutron and the resolved resonance regions and indirect correlation of the fast region with the unresolved one. These, so far neglected, correlations might actually be quite significant in practical applications. While physics of these correlations is pretty clear no methods have been developed to quantify them. In the present contribution, we do not address these issues but note that correlations among the three distinct energy regions need to be taken into account once techniques for determining covariance data within the regions are fully mastered.

8. Conclusions

We have described implementation of the KALMAN code into the EMPIRE system and presented first covariance data obtained for Gd and Ir isotopes. The system has essentially been developed for treatment of the fast neutron region but is also capable of predicting covariances in the unresolved resonance region. The latter one can also be treated with the SAMMY code and this overlap will, in our future work, be used to compare the two, basically very different, methods.

We have studied complicated shapes of correlation matrices obtained in the calculations and found out that they can be understood in terms of the underlying reaction models. Importantly, we predict that for certain reactions (e.g., total and elastic) there are narrow energy ranges with extremely small uncertainties.

We have shown that model generated covariances tend to show very strong long-range correlations while those determined solely from experimental data tend to account only for a short-range correlations leading to the nearly diagonal matrix. Both sources of information must be included to produce covariances that reflect 'full knowledge' of the problem.

We have set up the basic tool for generation of fast neutron covariances for evaluated nuclear data files. However, there is still a number of issues that have to be solved before mass productions of reliable covariance data can be carried out. First of all, we badly need resonable estimates for the uncertainties of the model parameters, next we have to address the problem of how good our models are.

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