



The Abdus Salam
**International Centre
for Theoretical Physics**



2484-17

ICTP-IAEA Joint Workshop on Nuclear Data for Science and Technology: Medical Applications

30 September - 4 October, 2013

Evaluated data and their uncertainties

A.V. Ignatyuk
*Institute of Physics and Power Engineering
Obninsk
Russia*

Evaluated data and their uncertainties

A.V.Ignatyuk,
Institute of Physics and Power Engineering, Obninsk, Russia

Evaluated data usually mean that some analysis of available experimental data and theoretical model was performed for a definite set of reaction and the optimal recommended data were produced on the basis of the analysis. At present the required evaluations in many cases should include beside the recommended cross sections or other nuclear characteristics also covariance matrices of data uncertainties. Below we shall discuss the main approaches that used for an estimation of both components of evaluated data.

1. FITTING OF DATA

Though a large number of experimental data are available for many cases, such data are not always consistent. In this situation, the evaluation has to be start with a careful analysis and a selection of concordant data. The following step then consisted of fitting the selected data with appropriate analytical functions which represent data in an optimal way at a required energy region.

Of course, the best approach is a fitting of theoretical model parameters. Such an approach is widely used for evaluations of the total neutron cross-sections or the neutron capture cross-sections. It is also the most reasonable method of evaluations in the case of a limited amount of experimental data. However, in the case a large number of data their optimal description can be interesting independently from the theoretical models.

The simplest approach to data description is the spline fit method that based on a piece wise approximation of data at specified important points (knots of the spline) by individual interpolating polynomials for each interval between two knots. These polynomials are matching in such a way that the first and second derivatives are continuous at the knots. The polynomials are usually selected by the 2nd (quadratic interpolation) or the 3rd order (cubic one). Due to the condition of continuous derivatives, one gets a continuous and smooth fit with minimum twisting (oscillating behavior) of the fitting curve. A particular feature of the spline method is that the fit in the selected interval is independent of data in other intervals.

The spline method is well described in Refs. [1, 2] and is widely applied in nuclear data evaluations. Its main problems relate to the following:

- The knots have to be selected by a user, making the fit of a time consuming procedure with partly arbitrary results.
- The cubic splines are not always adequate for complex shapes of curves.
- The calculated uncertainties of the fitted data are not always representative, they look too small at many cases.

The spline-fit codes are available now in many laboratories. In particularly, they were applied successfully by the Chinese group for many evaluations of the charged particle cross-sections interesting for medical radioisotop production [3]. As an example the available experimental data for reaction $^{27}\text{Al}(p,x)^{22}\text{Na}$ are shown in Fig. 1 together with the recommended curve obtained by the spline method.

A more general class of analytical functions is rational functions defined as the ratio of two polynomials. Such approximation was proposed by Padé over hundred years ago [4] and has become one of the most important interpolation techniques of statistical mathematics [5, 6].

A Padé approximant for a function $f(x)$ is defined as the rational function

$$p_L(x) = R_L(x) / Q_L(x) , \quad (1)$$

where R and Q are the polynomials described by L coefficients that match exactly the function $f(x)$ in L points

$$p_L(x_j) = f(x_j) , \quad j = 1, 2, \dots, L . \quad (2)$$

We do not show the degrees of the polynomials R and Q explicitly since the description is based on the recurrent solution where these degrees are defined internally. Until recently, two obstacles hindered an application of the Padé approximation to data processing and analysis: (a) difficulty of realization since rational approximants unlike polynomials lead to complicated nonlinear systems of equations in the least-squares method; (b) a special form of approximant instability - possible real pole-zero pairs (noise doublets).

Both of these two difficulties can be circumvented by undertaking a recursive calculation of many approximants

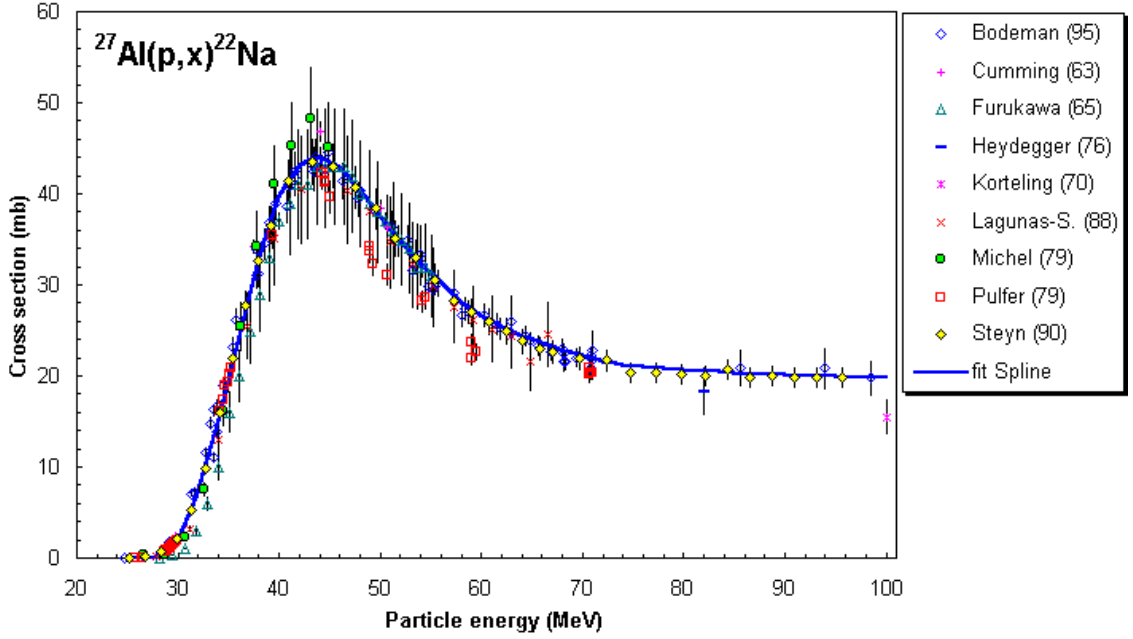


FIG. 1. Experimental data on the $^{27}\text{Al}(p, x)^{22}\text{Na}$ reaction cross-section and their spline fitting.

differing by a choice of interpolation knots along with their statistical optimization by discrete sorting. Eqs. (1) and (2) result in a system of linear equations for coefficients which may be solved using either determinants or recurrent expressions. The simplest recurrent expression is represented by the following equation:

$$p_L(x) = \frac{R_{L-1}(x) + \gamma_L(x - x_{L-1})R_{L-2}}{Q_{L-1}(x) + \gamma_L(x - x_{L-1})Q_{L-2}}, \quad (3)$$

where the coefficient γ_L can be readily determined from the condition

$$p_L(x_L) = f(x_L), \quad (4)$$

and the initial polynomials are constants:

$$R_0(x) = 0, \quad R_1(x) = f(x_1), \quad Q_0(x) = 1, \quad Q_1(x) = 1 \quad (5)$$

Eqs. (3 - 5) satisfy the definition (1) and condition (2).

As a rational function, the Padé approximant can be expressed by a set of polynomial coefficients or by a set of coefficients of the pole expansion. The last expansion is based on the analytical properties of the rational functions in the complex plane. One uses a complex variable $z = x + iy$ and replaces $p_L(x)$ by $p_L(z)$ which can be defined as the following:

$$p_L(z) = c + \sum_l \frac{a_l}{z - \eta_l} + \sum_k \frac{\alpha_k(z - \varepsilon_k) + \beta_k}{(z - \varepsilon_k)^2 + \gamma_k^2}. \quad (6)$$

This equation can also be called the resonance expansion, in which ε_k and γ_k are the energy and the total half-width of the k -th resonance, while α_k and β_k are the partial widths and interference parameters. The first sum corresponds to the real poles, while the second sum relates to the complex poles.

A prominent disturbing feature of the numerically generated rational approximants is the appearance of real poles (zero denominators) inside the approximation interval which is physically meaningless and makes the approximant unusable. These poles are closely accompanied by real zeros of the numerator, constituting noise doublets that prevented wide use of Padé approximants in data fitting.

The noise doublets are not only neutralized but become useful, corresponding to the terms with $z \approx \eta_l$ inside the interval of approximation with relatively small coefficients a_l in the first sum of Eq. (6). These terms are

cancelled in the present method and eliminated from the sum, and the regularization generates satisfactory results. Normally, the noise doublets appear with increasing L at the final stages of the approximation and indicate, together with statistical criteria, that the analytical information is exhausted.

The situation may be different if some points in the input experimental data deviate abnormally from the general trend. Under such circumstances, the noise doublets appear at relatively low L near such ‘bad’ points, describing them by local singularities rather than by smooth components. When the singularities are eliminated, the resulting regularized curve ignores the particularly bad points – this approach identifies points with aberrations automatically. From the point of view of statistical mathematics, the method of discrete optimization is equivalent to the least-squares technique, and therefore the experimental data set must be statistically consistent. When there are several sets of experimental data and discrepancies between different sets are significantly larger than their declared uncertainties, the statistical processing of the data is possible only after data selection by an expert.

The Padé codes construct the approximating rational function and calculate the coefficients of the pole expansion for each resonance Eq. (6). Thus, we have an analytical expression that can be easily calculated at any energy point. Effective codes for practical applications of the Pade approximation were developed by the Obninsk group [7]. The simplest version of codes permits to analyze up to 500 experimental points with a number of parameters $L \leq 40$ and with the ratio limit of analyzed functions up to $F^{max} / F^{min} \leq 10^6$. A more detailed description of the method can be found in Ref. [7] and some important questions of its application are presented in Refs. [8, 9]. The Pade approximation is also very convenient for calculations of the data uncertainties and the corresponding covariance matrices.

The fitting procedure is always connected with a minimization of the deviation functional

$$\chi^2 = (N - L)^{-1} \sum_{j=1}^N (p_L(x_j) - f_j)^2 / \sigma_j^2 \quad . \quad (7)$$

Such minimization is carried out by iterations using the discrete optimization (sorting) approach. The minimal deviation for a given L are computed by looking through a possible choice of L points from the available N points and the construction of corresponding approximants (3). Once this process is completed, L is changed and the iteration is repeated until an overall minimum is found from all discrete possibilities available.

One of the advantages of the discrete optimization technique as compared to the continuous least-squares method (LSM) is the possibility of using manifold functionals. Theoretical estimates show that the mean quadratic deviation of the approximant found by the discrete optimization from the continuous LSM solution is about $(N/L)^{1/2}$ times less than the average error corridor of analyzed data. Thus, the approximant is statistically equivalent to the LSM solution.

As an example the experimental data for reaction $^{103}\text{Rh}(p,n)^{103}\text{Pd}$ are shown in Fig. 1 together with the results of the model calculations, considered at the previous lecture, and the recommended curve obtained by the Pade approximation. It is obvious, that the fitted curve much better describes the measured cross-section than the theoretical models and a very big job is needed to achieve a comparable quality of description by the fitting of the theoretical model parameters. The Pade approximants were widely used to prepare the recommended data for the charge particle production of therapeutic radionuclides [10].

A fit of the theoretical model parameters is more reasonable for the neutron capture cross-sections. For the capture a small adjustment of the radiative strength function can be enough to describe the available experimental data at the wide energy region. In Fig. 3 the experimental data are shown for the $^{197}\text{Au}(n,g)$ reaction together with the theoretical model description and the evaluated curve adopted as one of the neutron standard cross-sections. The standard cross sections were obtained on the basis of the consistent fitting of the most precise neutron data and their good agreement with the model calculations confirm the high accuracy of the compound reaction theory. At the energy region below several MeV there is no space for many uncertainties connected with the pre-equilibrium processes.

2. COVARIANCE MATRICIES OF UNCERTAINTIES

During the past decade, there has been a dramatic increase in the demand for evaluated nuclear data that are comprehensive in scope with respect to both materials and reaction processes included, and that provide some

specification of estimated uncertainties in the results. This demand has come about because of a renewed interest in the nuclear power option as a means to satisfy the energy needs of society while at the same time limiting the emission of gaseous carbon compounds that may contribute significantly to global warming. The concern about data uncertainties is related to the need to ensure that nuclear power will be safe, reliable and

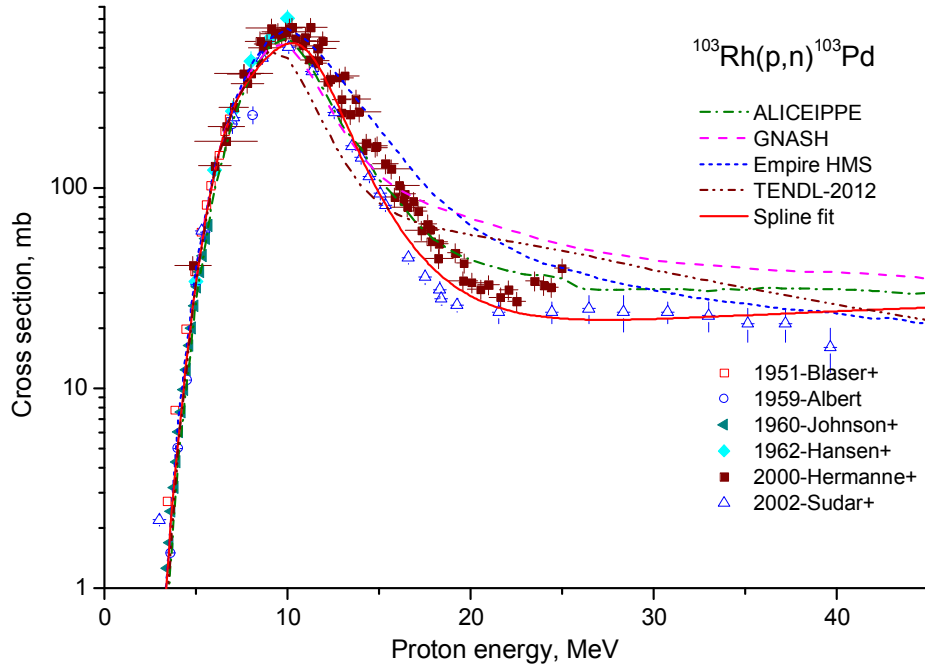


Fig. 2. Experimental data for the $^{103}\text{Rh}(p, n)^{103}\text{Pd}$ reaction cross-section in comparison with the theoretical model calculations and the Pade fitting for $L=13$.

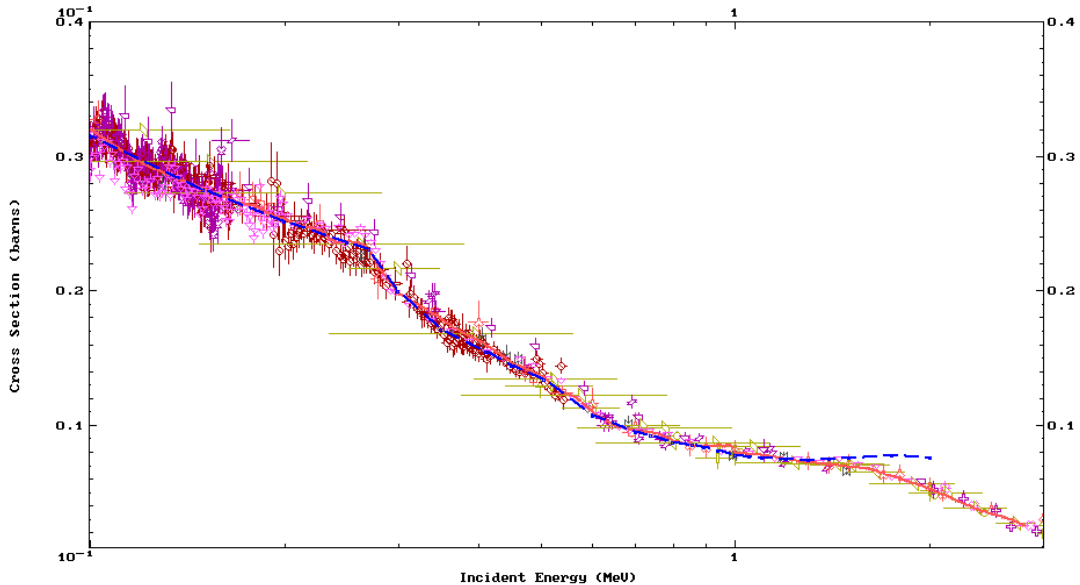


Fig. 3. Experimental data for the $^{197}\text{Au}(n, g)$ cross section in comparison with the theoretical model calculations and the recommended curve obtained by the GMA method.

economically competitive with other alternative energy options (e.g. wind, solar, geothermal, etc.). Similar words can be said concerning all other applications of nuclear data. Modern nuclear systems analysis procedures are now able to accommodate nuclear data uncertainties thereby providing further stimulus for their provision.

When we are talking about uncertainties of some set of data, it is necessary to define not only the possible uncertainty (the error) of each point, but also the available connections between the errors of all point. Such set of data is usually named the covariance matrix of uncertainties. A case of the independent error of each point corresponds to the diagonal form of covariance matrices.

Covariances of nuclear data, in principle, can be obtained by sole analysis of experimental data if there are enough measurements to adequately define all reactions of interest in their respective energy ranges. Such analyses can be reinforced using some additional information provided by the model calculations. The presently used methods of covariance evaluations can be classified in three categories: *i)* deterministic approach closely related to the Generalised Least Square Method (GLSM)]; *ii)* stochastic ones that involve Monte Carlo calculations using random set of model parameters; *iii)* hybrid approaches that combine features of the deterministic and stochastic treatments. All these methods have their advantages and drawbacks. The most impressive examples of method applications are discussed in Ref. [11], which summarizes the practical achievements of various approaches. We will concentrate below on the deterministic approach that seems most convenient for medical applications, in which the cross section of definite reaction is evaluated mainly independent from other competitive reactions.

The least-squares fitting, considered above (7), corresponds to uncorrelated data. The fitted data are independent of each other, and their uncertainties are used as weight of each data point. To take into account correlations the procedure should be extended to the generalized least-squares technique in which the weight is expressed by the inverse of a covariance matrix of the data.

We can denote experimental data by an dimensional vector $\mathbf{y} = (\sigma(\varepsilon_1), \sigma(\varepsilon_2), \dots, \sigma(\varepsilon_n))^t$, where n is the number of experimental points and the symbol t means the transposed matrix, while the evaluated cross sections are expressed by a vector $\mathbf{x} = (\sigma(E_1), \sigma(E_2), \dots, \sigma(E_m))^t$. In order to determine the least-squares solution uniquely, n must be larger than m . The relation of these vectors is, in the linear regression model,

$$\bar{\mathbf{y}} = \begin{pmatrix} \sigma(\varepsilon_1) \\ \cdot \\ \cdot \\ \sigma(\varepsilon_n) \end{pmatrix} = \begin{pmatrix} c_{11} \dots c_{1m} \\ \cdot \\ \cdot \\ c_{n1} \dots c_{nm} \end{pmatrix} \begin{pmatrix} \sigma(E_1) \\ \cdot \\ \cdot \\ \sigma(E_m) \end{pmatrix} + \begin{pmatrix} u_1 \\ \cdot \\ \cdot \\ u_n \end{pmatrix} = \hat{\mathbf{C}}\bar{\mathbf{x}} + \bar{\mathbf{u}} \quad (8)$$

where $\mathbf{u} = (u_1, u_2, \dots, u_n)$ is a vector of uncertainties, and \mathbf{C} is the design matrix, which is defined as $c_{ij} = \partial y_i / \partial x_j$ and gives an appropriate spline-interpolation of the evaluated cross sections. For case of a simple linear interpolation, the elements of the matrix \mathbf{C} can be written as

$$c_{ij} = \begin{cases} (\varepsilon_i - E_{j-1}) / (E_j - E_{j-1}) & E_{j-1} \leq \varepsilon_i < E_j \\ (\varepsilon_i - E_{j+1}) / (E_j - E_{j+1}) & \text{for } E_j \leq \varepsilon_i < E_{j+1} \\ 0 & \text{otherwise.} \end{cases} \quad (9)$$

The least-squares solution for \mathbf{x} is given by the equations:

$$\bar{\mathbf{x}} = \hat{\mathbf{X}}\hat{\mathbf{C}}^t\hat{\mathbf{V}}^{-1}\bar{\mathbf{y}} \quad , \quad (10)$$

$$\hat{\mathbf{X}} = (\hat{\mathbf{C}}^t\hat{\mathbf{V}}^{-1}\hat{\mathbf{C}})^{-1} \quad , \quad (11)$$

where \mathbf{V} is the covariance of the experimental data and \mathbf{X} is the covariance of the evaluated cross sections. The covariance \mathbf{X} obtained must be multiplied by the deviation per degree-of-freedom

$$\chi^2 = \frac{(\bar{\mathbf{y}} - \hat{\mathbf{C}}\bar{\mathbf{x}})^t\hat{\mathbf{V}}^{-1}(\bar{\mathbf{y}} - \hat{\mathbf{C}}\bar{\mathbf{x}})}{n - m} \quad . \quad (12)$$

The above algorithm was realized in the SOK code by Kawano [12] and was used successfully for evaluations of various cross sections in the case when an amount of experimental data is large enough. Main problems of code applications relate to an estimation of the data correlation matrices. For the most of data measurements the

diagonal uncertainties are given only and rather great efforts are required to obtain the correlation matrix for a full set of data.

The more general minimization approach (GMA) is required in the case of an analysis of several various functionals, for example, in a simultaneous description of the cross sections and cross-section ratios. For such tasks the GMA code was written by Poenitz [13] and it is widely used for evaluation of the neutron cross-section standards [14]. The recommended curve for the $^{197}\text{Au}(n,\gamma)$ reaction, shown in Fig. 3, was obtained on the basis of consistent analysis of the complete data-base for the standard reactions, and the corresponding uncertainties and the correlation matrix for this reaction are presented in Fig. 4. The uncertainties for the whole energy region fluctuate between 1 and 2 %, and the correlations for neighboring intervals achieve 40-50 %, but they reduce to 20-15 % for more distant intervals and drop to 2-5 % for the strongly remote intervals.

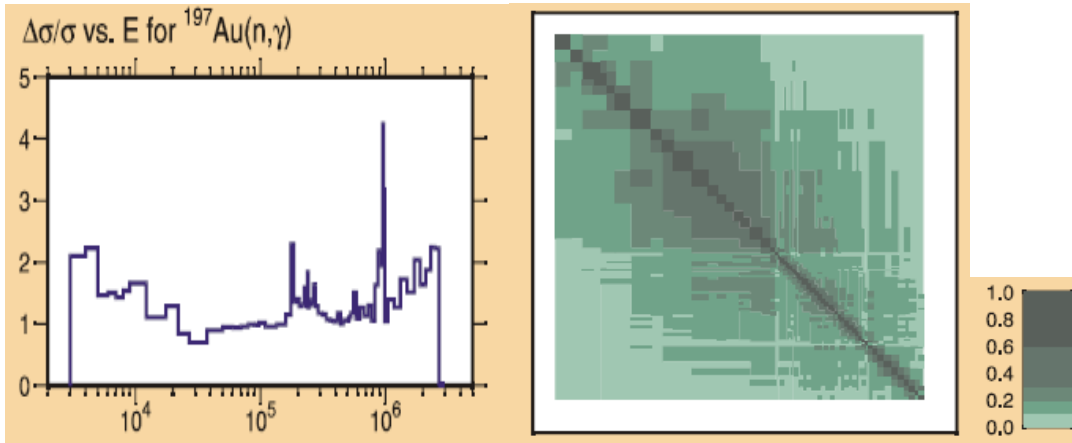


Fig. 4. Correlation matrix for the $^{197}\text{Au}(n,g)$ reaction. The ordinate scale is the relative deviations (%) and abscissa scales are the energies (eV).

In the case of a limited amount of experimental data we are induced to combine the available data with some model description. Then, the final cross-section covariances are calculated from the updated covariances for model parameters. This procedure consistently accounts for the experimental uncertainties and the uncertainties of the model parameters ensuring that the final cross-section uncertainties are at least as good as the smaller of the two.

The key ingredient of the method is the sensitivity matrix, which represents complex model calculations. If we denote the combination of models as an operator \mathbf{M} that transforms the vector of model parameters \mathbf{p} into a vector of cross-sections $\sigma(\mathbf{p})$ for a specific reaction channel, then the sensitivity matrix \mathbf{S} can be interpreted as the linear term in the expansion of the operator \mathbf{M} :

$$\hat{\mathbf{M}}\vec{p} = \sigma(\vec{p}) \quad (13)$$

$$\hat{\mathbf{M}}(\vec{p} + \delta\vec{p}) = \sigma(\vec{p}) + \hat{\mathbf{S}}\delta\vec{p}$$

In practice, the elements s_{ij} of the sensitivity matrix are calculated numerically as partial derivatives of the cross sections at the energy E_i with respect to the parameter p_j :

$$s_{ij} = \frac{\partial \sigma(E_i, \vec{p})}{\partial p_j} \quad (14)$$

In case of covariance determination, the initial values of the parameters, \mathbf{p}_0 , are already determined by the model description of the analyzed cross-sections. Their covariance matrix \mathbf{P}_0 is assumed to be diagonal while the uncertainties of the parameters are estimated using systematics, independent measurements or educated guesses. The model-based covariance matrix (prior) for the cross sections, \mathbf{C}_0 , can be obtained through a simple error propagation formula:

$$\mathbf{C}_0 = \mathbf{S}\mathbf{P}_0\mathbf{S}^t \quad (15)$$

The experimental data, if available, are included through a sequential update of the parameter vector \mathbf{p} and the related covariance matrix \mathbf{P} as:

$$\begin{aligned}\bar{p}_{n+1} &= \bar{p}_n + \hat{P}_n \hat{S}^t (\hat{C}_n + \hat{C}_{\text{exp}})^{-1} (\bar{\sigma}_{\text{exp}} - \sigma(\bar{p}_n)) \quad , \\ \hat{P}_{n+1} &= \hat{P}_n + \hat{P}_n \hat{S}^t (\hat{C}_n + \hat{C}_{\text{exp}})^{-1} \hat{S} \hat{P}_n \quad ,\end{aligned}\tag{16}$$

where n -index relates to a number of iterations.

The updating procedure described above is often called Bayesian, although Eqs. (16) are the usual definition of iteration approach. An important technical issue, which has to be addressed in most of the covariance methods, is ensuring that the energy grid, E_i , for the model calculations and experimental data is the same to enable matrix operations in Eqs. (16). In practical codes this is achieved by bi-spline interpolation of model cross-sections and sensitivity matrices.

The above approach was adapted to the EMPIRE code complex and has been effectively used for the covariance evaluations included in the ENDF/B-VII neutron library. With different theoretical models this approach was used also for the evaluations of the JENDL-4.0 library. As in the case of evaluations based on the experimental data only, the main problem of the combined approach remains an estimation of experimental data correlations. Construction of covariances is usually confronted by two principal difficulties. The first relates to a disagreement between the uncertainty distribution based on the error estimations declared by authors and the reasonable statistical laws for uncertainties. Attempts to improve the distribution by rejection of some outlying data introduce badly controlled uncertainties in results and thwart the proper estimation of systematic uncertainties, which are crucial for a complete uncertainty evaluation of all available data.

The second difficulty of the covariance construction is connected with the essential differences of matrices obtained with various approximating functions even if the resulting descriptions are practically indistinguishable. As a rule, the local uncertainties corresponding to the diagonal matrix elements increase for a large number of approximating parameters, but the off-diagonal elements responsible for correlations decrease. As a result, the uncertainty of any integral function averaged over a broad energy spectrum depends on the local uncertainties in a rather complex way and is very sensitive to evaluations of long-range systematic uncertainties.

The analysis of uncertainties for Russian evaluations is carried out now on the basis of the unrecognized error-estimation method [15]. Along with a consistent consideration of statistical errors of experimental data the method allows to determine some systematic data-uncertainties usually underestimated by their authors and to establish also some implicit correlations of data. This approach has been used successfully for evaluations of the standard neutron cross sections [14] and is currently being applied routinely to construct the uncertainties and corresponding covariance matrices for the BROND-3 library.

The method of the unrecognized error estimation is based on a priori equal reliability of all available experimental data, of course excluding proved erroneous results. However, the systematic and statistic uncertainties of each experimental work are determined in accordance with the observed distribution of data. Some initial description of data is required at the beginning and deviations from it can be considered as the selective values of uncertainties. The averaged deviation of experimental data from the approximating function is regarded for each analyzed work as its systematic error and the deviations of experimental points from the approximant shifted on the systematic error are regarded as the statistical errors. An optimal description of all data is achieved by the traditional iteration procedure minimizing mean squares deviations with the obtained statistical and systematic errors. The rational functions of an optimal order are used for the corresponding approximants (the Pade approximation) and the problem of small uncertainties (the Peel paradox) is taken into consideration under the minimization process and a construction of the resulting covariance matrices for the approximating function. More details of the method can be found in Ref. [15].

To display the main features of our approach the results of the fission cross-section analysis of ^{235}U can be used [16]. In accordance with the EXFOR library this cross section was measured for the neutron energies from 2 keV up to 20 MeV at 107 experiments and the available data include more than 10 thousand points. After averaging over the intermediate resonance fluctuations and a rejection of some old low-accuracy measurements 84 experiments with 2311 points were conserved in the analysis. The results of 32 experiments, which contain one or two points only, were then combined and considered as one measurement. The obtained distribution of the systematic and averaged statistical uncertainties for the selected experiment is shown in Fig. 5.

Because the final approximated function for the fission cross section of ^{235}U is very close to the well-known evaluation recommended recently as the neutron standard [14], the plots of the cross sections can be omitted and only the uncertainties will be discussed. The uncertainties presented in different libraries are shown in Fig. 6. The uncertainties for ABBN-93 and CEA-2004 were obtained on the basis of the expert estimations, while the uncertainties for neutron standard cross sections

were evaluated by means of the careful statistical analysis of all available data with a thorough estimation of experimental uncertainties and correlations of various measurements [14]. A rather good agreement between our evaluations of the uncertainties and the standards recommended above 100 keV only can be considered as an additional justification of our approach. Of course, a priori evaluation of systematic uncertainties and data correlations made for the standards is more correct than a posteriori statistical estimation of unrecognized errors. However, in a majority of practical tasks we have not enough information for the rigorous estimation of systematic uncertainties and the statistical estimation of uncertainties and correlations of available data becomes quite reasonable or even the only possible approach.

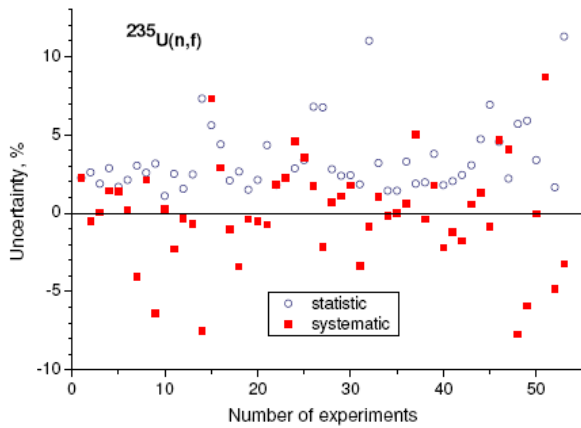


Fig. 5. Distribution of relative uncertainties for the fission cross-section data of ^{235}U in accordance with the unrecognized error-estimation method.

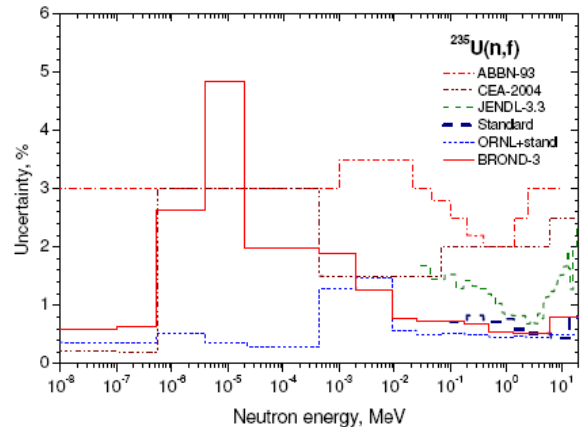


Fig. 6. Relative uncertainties of the fission cross-section evaluations for ^{235}U adopted in different libraries.

Fig. 6 also includes estimations of the cross section uncertainties for the resolved resonance region (< 2 keV). Below the first resonance with the energy $E_r = 0.271$ eV the uncertainty is determined by the current accuracy of the thermal fission cross section and equals about 0.2 % [14]. In the recent ENDF/B-VII evaluation the thermal cross section was shifted a little to improve agreement with some benchmark data and in accordance with that the uncertainty for the epithermal region was increased about two times. Above 1 eV several resonances contribute to the wide-group uncertainties. Accuracies of the resonance width estimations are about 10 % or worse. The wide-group uncertainties due to averaging over resonances should be several times lower. Such values are indeed obtained in the ABBN-93, CEA-2004 and our evaluations for the entire resonance region. Too small uncertainties obtained in the ORNL analysis look strongly underestimated.

It will be useful to compare several other examples of uncertainties evaluations. In Fig. 7 the available experimental data for the $^{56}\text{Fe}(n,p)$ reaction are compared with some recent evaluations. The differences between the evaluated cross sections are rather small, but the split of the estimated uncertainties is quite essential. The uncertainties of JENDL-4.0 are about 5 % for the energy region above 5.5 MeV and they increase up to 45 % at the energies below 3.5 MeV. The uncertainties of the international dosimetry file IRDF-2002 are much lower: 8.5 % at the near-threshold region, about 1 % at the energies around 15 MeV and increase to 4 % for 20 MeV. The BROND-3 evaluation with some additional experimental data gives practically the same cross section as IRDF-2002, but the uncertainties are decreased to 5 % at the near-threshold region and to 1.0 – 1.5 % for the energies above 15 MeV. The correlation matrix of BROND-3 is very similar to IRDF-2002.

The evaluations of the $^{56}\text{Fe}(n,\alpha)$ reaction are shown in Fig. 8. There is only one experimental point for this reaction, but nobody relates too seriously to its accuracy. So, all evaluations are based on the theoretical models. Discrepancies between the evaluated cross sections are rather moderate, but a disagreement in the uncertainty estimations is much larger. The uncertainties of JENDL-4.0 are about 60 % at the energy region below 8 MeV and they decrease to 10 % for the energies above 12 MeV. The uncertainties of JEFF-3.1 are above 80 % at the near-threshold region, about 5 -6 % at the energy interval between 6 and 16 MeV, and they increase to 40 % at the energies about 20 MeV. In the ENDF/B-VII.1 file the uncertainties are taken about 20 % for the whole

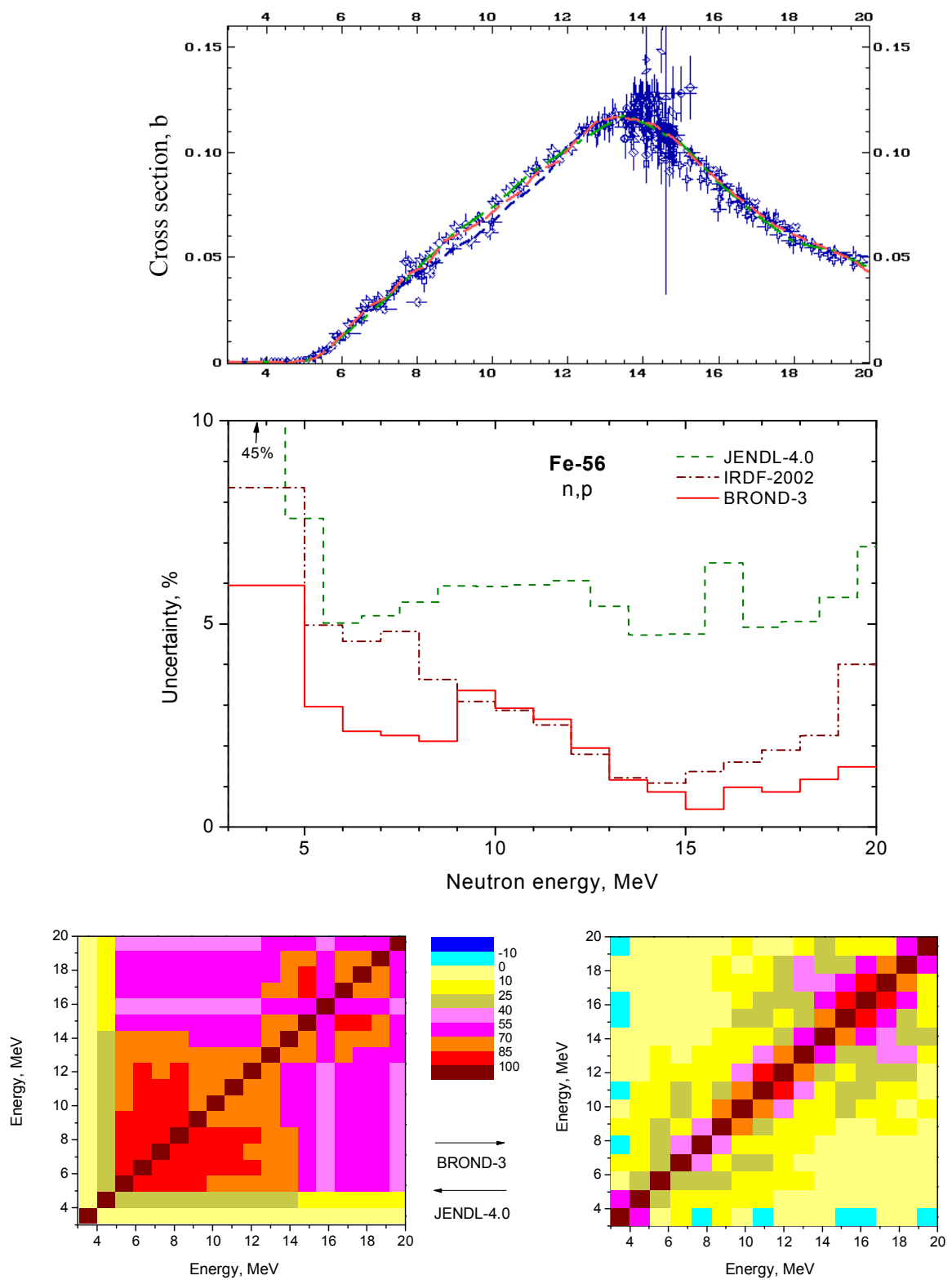


Fig. 7. Evaluated cross sections of the $^{56}\text{Fe}(n,p)$ reaction (overhead), the corresponding uncertainties (in middle) and the correlation matrices (below).

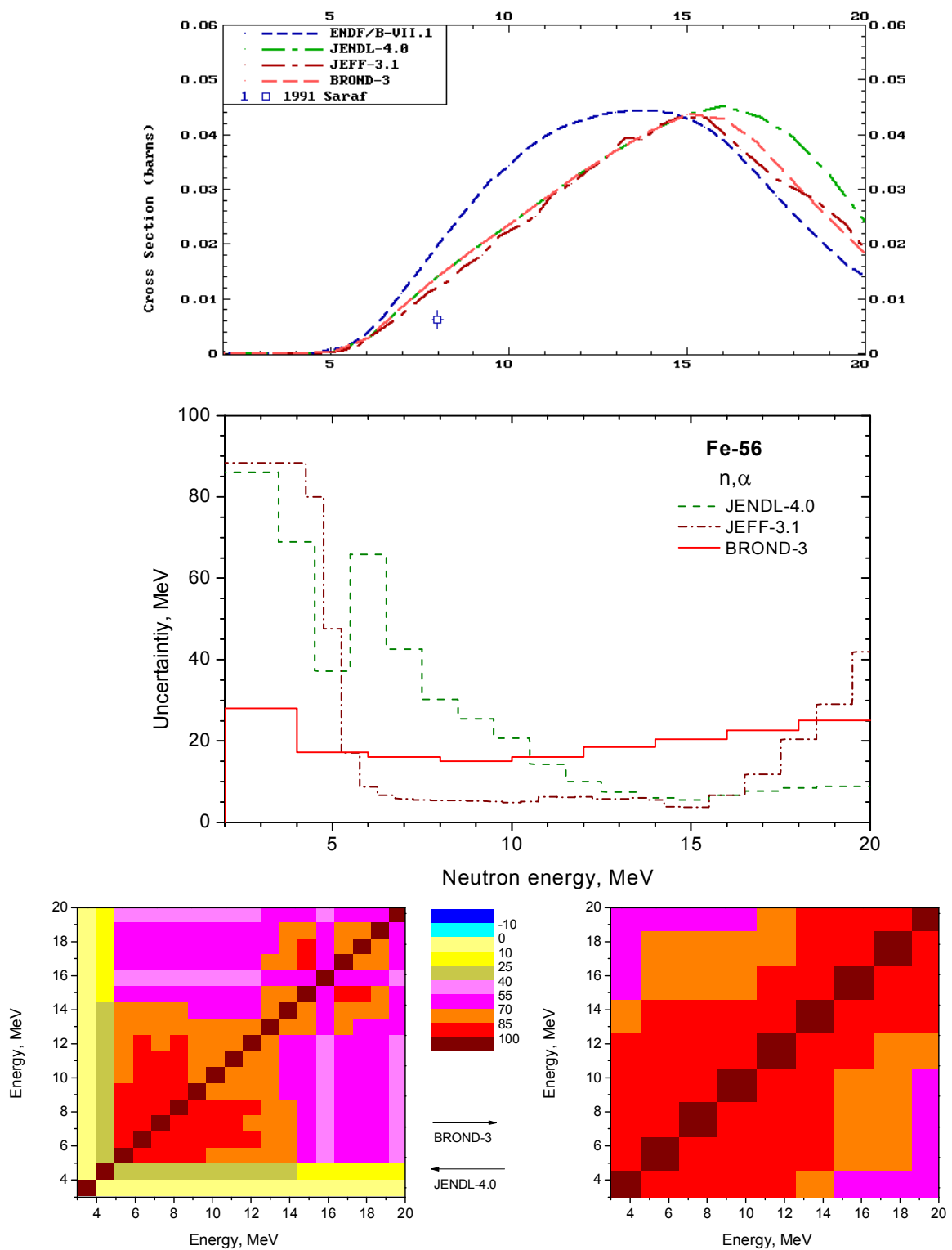


Fig. 8. Evaluated cross sections of the $^{56}\text{Fe}(n,\alpha)$ reaction (overhead), the corresponding uncertainties (in middle) and the correlation matrices (below).

energy region the BROND-3 evaluation are rather close to ENDF/B-VII.1. For lack of experimental data it is difficultly to believe in the uncertainty estimations about 5 %. The uncertainties of ENDF/B-VII.1 and BROND-3 look more reasonable. Off-diagonal elements of the uncertainty correlation matrices are moderate for JENDL-4.0 and much larger for BROND-3. The strong correlations of matrix elements are quite typical for evaluations based merely on theoretical models.

CONCLUSION

An activity of covariance evaluations has strongly increased during the last ten years. As a result, covariance capabilities have been developed in all major nuclear reaction codes used for nuclear data analysis. Several large-scale projects have been undertaken to produce a vast amount of covariances for the existing neutron data libraries. However, disagreements in the uncertainty estimations are still large in many cases. The main reason of discrepancies is limited information about the correlation of input experimental data. As a rule, the statistical uncertainties of such data are defined quite reasonable, but the systematics uncertainties are not given for many experiments. A consistent estimation of such uncertainties should be considered as the first order task for the removing contradictions between the available evaluations of nuclear data recommended for practical applications.

It is clear that further investigations of the evaluation methods should be continued to better identify their individual strengths and weaknesses as well as ranges of applicability. Efforts should be made to eliminate to the extent possible instances where evaluations by the different methods using similar input lead to uncertainties that do not adequately cover observed dispersions between the evaluated central values.

REFERENCES

1. De Boor, C., *A Practical Guide to Splines*, Springer-Verlag, Berlin (1978) 129–143.
2. Schumaker, L.L., *Spline Function: Basic Theory*, J. Wiley, New York (1981) 108–118.
3. Gul, K., Hermanne, A., Mustafa, M.G., Nortier, F.M., Obložinský, P., Qaim, S.M., Scholten, B., Shubin, Y., Takács, S., Tárkányi, F.T., Zhuang, Y., *Charged Particle Cross-section Database for Medical Radioisotope Production: Diagnostic Radioisotopes and Monitor Reactions*, Tecdoc-1211, IAEA, Vienna, 2001.
4. Padé, H.E., *Sur la Représentation d'une Fonction par des Fractions Rationnelles*, *Ann. L'école Norm.* **9/3** (1892) 3–93.
5. Graves-Morris, P.R. (Ed.), *Padé Approximants and their Applications*, Academic Press, New York (1973).
6. Baker Jr., G.A., *Essentials Of Padé Approximants*, Academic Press, New York (1975).
7. Vinogradov, V.N., Gai, E.V., Rabotnov, N.S., *Analytical Approximation of Data in Nuclear and Neutron Physics*, Energoatomizdat, Moscow (1987) In Russian.
8. BADIKOV, S.A., GAI, E.V., GUSEINOV, M.A., RABOTNOV, N.S., “Padé Approximants in Curve Fitting and Resonance Analysis”, *Proc. 3rd IMSL User Group Europe Conf.*, Bologna, Italy, 26 – 28 March 1990, p. B11.
9. Gai, E.V. *Some Algorithms for the Nuclear Data Evolution and Construction of the Uncertainty Covariance Matrices*, *Voprosy Atomnoy Nauki i Techniki*, ser. Nuclear Constants, 2007, iss. 1-2, pp. 56-65.
10. Bětak, E., Caldeira, A.D., Capote, R., Carlson, B.V., Choi, H.D., Guimaraes, F.B., Ignatyuk, A.V., Kim, S.K., Kiraly, B., Kovalev, S.F., Menapace, E., Nichols, Nortier, M., Pompeia, P., Qaim, S.M., Scholten, B., Shubin, Sublet, J.-Ch., Tárkányi, F.T., *Charged Particle Cross-section Database for Medical Radioisotope Production: Diagnostic Radioisotopes and Monitor Reactions*, Tecdoc-1211, IAEA, Vienna, 2001.
11. *Covariance Data in the Fast Neutron Region*, International Evaluation Co-operation, v.24, NEA/WPEC-24, OECD, Paris, 2011.
12. Kawano, T., *Evaluation of Fission Cross Sections and Covariances for U233, U235, U238, Pu239, Pu240, and Pu241*, Report JAERI-Research 2000-004, Takai-mura, 2000.
13. Poenitz, W.P., *Evaluation Methods for Neutron Cross Section Standards*, *Proc. Conf. on Nuclear Data Evaluation Methods and Procedures*, Report BNL-NCS-51363, Vol. 1 (1981), pp. 249-290.

14. A.D. Carlson, V.G. Pronyaev, D.L. Smith, N.M. Larson, Chen Zhenpeng, G.M. Hale, F.-J. Hamsch, E.V. Gai, Soo-Youl Oh, S.A. Badikov, T. Kawano, H.M. Hofmann, H. Vonach, S. Tagesen, International Evaluation of Neutron Cross Section Standards, Nuclear Data Sheets, 110 (2009) 3215-3324.
15. Gai, E.V., Some Algorithms for the Nuclear Data Evaluation and the Covariance Matrix Construction, Voprosy Atomnoi Nauki i Tekhniki, ser. Nuclear Constants, 2007, iss. 1, p. 56.
16. Gai, E.V., Ignatyuk A.V., Uncertainties and Covariances of the Fission Cross Sections and the Fission Neutron Multiplicities for Actinides, Nuclear Data Sheets, 109 (2008) 2890–2893.