Nuclear data evaluation: status and perspectives

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Abstract. The knowledge of nuclear reaction data is an important requisite for the development and advances in nuclear technologies, but also for several fields of basic sciences such as nuclear astrophysics, nuclear medicine and material sciences. Nuclear data evaluation aims to reveal the best knowledge of nuclear reactions combining available experimental data, theoretical knowledge and mathematical constraints. A brief introduction into the concept of Bayesian evaluation techniques is given and the importance of proper inclusion of correlations between experiments is discussed. An important aspect is the generation of reliable uncertainty information which is one of the most important demands from the user community. In this context the methods for inclusion of model deficiencies are sketched. Furthermore, the specific problems of evaluations of light nuclear systems are addressed. In the outlook there will be a focus on methods and proposals taking advantage of the availability of increased storage and computational power which enable a more streamlined generation of new and/or updated nuclear data evaluations.

1 Introduction

The availability of reliable nuclear data, in particular reaction data, are an important prerequisite for the development and implementation of novel nuclear technologies such as GenIV reactors, controlled nuclear fusion, closure of the fuel cycle etc. Apart from these energy related fields there also non-energy needs for data, e.g. nuclear medicine, radioprotection, dosimetry and safety, geophysics and environmental research, nuclear astrophysics, space research etc. Nuclear data comprise global quantities (mass, charge, radius, etc.), nuclear structure data (excitations, spin, parity, level densities, etc.) and reaction data (differential and angle-integrated reaction cross sections, polarizations, particle spectra, etc.). In this work we exclusively deal with the evaluation of reaction data, excluding methods used for standards.

Originally, in the second half of the 20^{th} century nuclear data research has been focused on the study of neutron-induced reactions and extended libraries of evaluated nuclear data have been built, primarily of interest for reactor developments. In the meantime novel technologies have been arising on the horizon which require reliable knowledge of γ-, proton-, deuteron- and α-induced reaction data. Corresponding libraries of evaluated data have been set up, but they are still far from the level of completeness compared to the one of neutron-induced reactions.

Nuclear data evaluation is aimed to provide consistent sets of cross sections, spectra, fission yields etc. and represent the best quantitative knowledge of a nuclear reaction process. Due to the original focus on reactor design emphasis was given to angle-integrated cross sections and spectra at incident neutron-energies up to about 20 MeV. Today the range of applications is much wider and requires evaluations in an extended energy range up to about 200 MeV. With increasing energy there is a scarcity of experimental data which must be compensated by the use of nuclear models. Independent of the specific application and scientific interest current nuclear data research should satisfy aspects of economics, optimization and safety/health (see Fig. 1). Nowadays it is expected

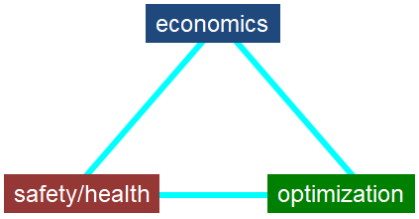

Figure 1. Aspects, independent of a specific application, which must be satisfied by modern nuclear data research.

that nuclear data sets contain besides the mean values also reliable uncertainty estimates which allow optimization of designs satisfying the safety/health regulations without requiring additional cost-intensive experiments. Thus modern evaluations must include reliable information in form of covariance matrices of uncertainties of observables.

After this short introduction the basics of nuclear data evaluation are briefly discussed in Sec.2. In particular the concepts of Bayesian statistics and Information theory are outlined in subsections 2.1 and 2.2, respectively. In Sec.3 the techniques of current nuclear data evaluations are presented starting with a brief overview in subsection 3.1. In subsection 3.2 we present the statistical model widely used

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in most applications. The proper evaluation step and its pitfalls are outlined on the basis of a Generalized Least Square technique in subsection 3.3. The subsection 3.4 is devoted to the impact of model deficiencies on evaluations. Their description via Gaussian processes is discussed in detail. The specific problems of nuclear data evaluation are addressed in subsection 3.5. Future developments are given in Sec. 4 which starts with a sketch of the modified Generalized Least Square technique in subsection 4.1. This technique provides the possibility of extendable nuclear data evaluations, suggested in subsection 4.2 as well as the setup of an evaluation library in subsection 4.3. A summary and concluding remarks are given in Sec.5.

2 Nuclear data evaluation

2.1 Bayesian statistics

As outlined above nuclear data evaluation is aimed to provide best and consistent estimates of reaction data and associated uncertainties compatible with *a-priori* knowledge and satisfying basic principles (e.g. unitarity, sum rules, etc.). A-priori knowledge is provided by nuclear structure information and/or semi-microscopic nuclear reaction models. The latter are of particular importance for evaluations at higher energies because the lack of experimental data must be compensated by model calculations. Bayesian statistics is well suited for the evaluation process because it provides a consistent combination of *a-priori* knowledge and experimental information. In the following we revisit the basics of Bayesian statistics.

The probability is often defined as relative frequency of events in a given infinitely repeatable experiment. This so-called frequentist interpretation is applicable to count rates of detectors, but cannot be applied to parameters of nuclear models. In Bayesian statistics the probability is defined as degree of believe about the truth of a proposition. This interpretation is independent of a given experiment and allows to set up a probability distribution for a given parameter of a nuclear model. Usually a parameter θ of a nuclear model can take uncountable many values in a given interval. For such a random variable we have to define a real valued probability density function (pdf) $\rho(\theta) \in [0, \infty[$ which gives the probability,

$$P(\theta_1 \leq \theta \leq \theta_2) = \int_{\theta_1}^{\theta_2} d\theta\, \rho(\theta)\,, \tag{1}$$

that the parameter θ lies between θ_1 and θ_2. Using $\theta_1 = -\infty$ and $\theta_2 = +\infty$ yields $P(-\infty < \theta < +\infty) = 1$. An extension of the pdf to more than one parameter is straightforward and allows the definition of the *conditional probability density*,

$$\rho(x|y) = \frac{\rho(x,y)}{\rho_Y(y)} \text{ with } \rho_Y(y) = \int_{-\infty}^{+\infty} \rho(x,y)dx\,, \tag{2}$$

where $\rho(x|y)$ denotes the probability density of x if one knows the true value of y. The quantity $\rho_Y(y)$ is the *marginal probability density*.

Using these ingredients one can formulate the *Bayesian Theorem*

$$\rho(x|y) = \frac{\rho(y|x)}{\rho_Y(y)}\rho_X(x) \tag{3}$$

which is the basic formula applied in nuclear data evaluation. Here $\rho_X(x)$ is the *a-priori* pdf, $\rho(y|x)$ is the likelihood, $\rho_Y(y)$ the evidence and $\rho(x|y)$ the *a-posteriori* pdf.

Important quantities for the following discussion are mean values and the covariance matrices. The mean value of an n-dimensional random vector $\vec{X}$ represents its expectation value and is defined by

$$\langle \vec{x} \rangle = \int dx_1 \cdots dx_n\, \vec{x}\rho(\vec{x})\,, \tag{4}$$

where the integration includes all possible values of $\vec{x}$. An uncertainty estimate is frequently provided by a covariance matrix $\mathbf{C}$ given by

$$C_{i,j} = \mathrm{Cov}[X_i, X_j] = \int dx_1 \cdots dx_n (x_i - \langle x_i \rangle)(x_j - \langle x_j \rangle)\rho(\vec{x}) \tag{5}$$

which is symmetric and positive definite. The diagonal elements of $\mathbf{C}$ are always positive valued and are the variances of X_i frequently denoted by $\sigma_i^2 = \mathrm{Var}[X_i] = \mathrm{Cov}[X_i, X_i] = C_{i,i}$.

2.2 Information theory

In general the existing knowledge is not sufficient to define the prior because subjective believe may bias the outcome. This freedom has triggered criticism on Bayesian statistics for a long time. Only in 1957 the problem was solved by Jaynes [1] formulating the *Principle of Maximum Information Entropy* which implies that among all possible probability distributions satisfying a given constraint one should pick out the one with the maximum information entropy. The concept of information entropy H was introduced by Shannon [2]. The information entropy is defined for a countable set of n events $\{E_i\}_{i=1,\cdots,n}$ with probability p_i by the expression.

$$H(p_1, \cdots, p_n) = -K \sum_{i=1}^{n} p_i \log(p_i)\,, \tag{6}$$

where K is a constant.

Considering a problem with the n-dimensional random vector $\vec{x}$ for which the mean value $\langle \vec{x} \rangle$ and the $\mathbf{V}$=Cov$[x_i, x_j]$ is known, the application of the principle of maximum entropy yields the probability density function

$$\rho(\vec{x}) = \frac{1}{\sqrt{(2\pi)^n \|\mathbf{V}\|}} \exp\left[-\frac{1}{2}\left(\vec{x} - \langle \vec{x} \rangle\right)^T \mathbf{V}^{-1} \left(\vec{x} - \langle \vec{x} \rangle\right)\right]. \tag{7}$$

This so-called *multivariate normal distribution* is denoted by $\rho(\vec{x}) = \mathcal{N}(\langle \vec{x} \rangle, \mathbf{V})$ and will be used in the discussion of the evaluation methods.

2.3 Evaluated libraries

The central goal of a nuclear data evaluation is the generation of an evaluated nuclear data file which represents the best knowledge of reactions in a specific system, e.g. neutron-induced reactions of a specific isotope. Besides the metadata describing the system and details of the experimental data sets the evaluated nuclear data file contains the mean values of observables and associated covariance matrices obtained in the evaluation procedure (nowadays mainly from Bayesian update).

Nuclear data files formatted in ENDF [3] contain uncertainty estimates in splitted form, i.e. variances and so-called correlation matrices $\bar{\mathbf{C}}$ for a given reaction,

$$\bar{C}_{i,j} = \mathrm{Cor}[X_i, X_j] = \frac{\mathrm{Cov}[X_i, X_j]}{\sqrt{\mathrm{Var}[X_i]\mathrm{Var}[X_j]}}\,. \tag{8}$$

The matrix elements of the correlation matrix satisfy $-1 \leq \bar{C}_{i,j} \leq +1$, where +1 implies full correlation and -1 full anticorrelation. The diagonal elements of $\bar{\mathbf{C}}$ are always +1. Cross correlations between different reactions are usually not given in the files.

Today evaluated nuclear data files cover available reaction data of almost all accessible isotopes. In the 20^{th} century emphasis was given to neutron-induced reactions, but nowadays with the development of new technologies also evaluated data files for charged-particle induced reactions are generated. Evaluated nuclear data files are formatted in ENDF [3]. Selected by region or application the files are combined into evaluated nuclear data libraries. These libraries are maintained together with other services by International data centers. Without aiming completeness examples of such libraries are JEFF 3.3 [4], ENDF/B-VIII.0 [5], JENDL 5 [6], CENDL 3.2 [7] and many others. In general the libraries show a high level of agreement due to the worldwide accessibility of experimental data sets and international collaboration. However, a comparison of the evaluated libraries exhibits also differences. These differences reflect different evaluation methods as well as different judgements of the quality of experimental data sets by evaluators.

3 Implementations of Nuclear Data Evaluations

3.1 Methods of Nuclear Data Evaluation

At present most evaluation techniques follow the guidelines of Bayesian statistics, presented in subsection 2.1. However, there are technical differences between the methods regarding (1) the choice of prior and likelihood and (2) the method to determine mean values and uncertainties, i.e. either by Monte Carlo procedures or generalised least square techniques. Among the Monte Carlo procedures we distinguish between Bayesian Monte Carlo (BMC) [8], Unified Monte Carlo-G [9], Unified Monte Carlo-B [10] and others. The second group of methods make use of various forms of least square techniques. A concise overview of different methods, including a hybrid one, is given in Ref. [11]. The advantage of Monte Carlo procedures is their statistical nature which yields probability distribution functions (pdf) of observables and allows a full statistical analysis. Least square methods are based on multivariate probability distributions of the parameters and yield only the point of highest probability and the corresponding error matrix. Comparisons of different techniques indicate that the least square technique works well if the actual probability distribution functions are almost symmetric. With increasing asymmetry of the actual pdf the mean values of the least square method deviate from the true ones. For a simplified discussion of characteristic features of evaluations we consider only least square methods in the following. However, most concepts can also be transferred to Monte Carlo type procedures.

Apart from these technical differences, nuclear data evaluations can be performed either in the space of observables or in the space of model parameters and may lead to different results. In the following the discussions are limited to methods in the space of observables.

3.2 Statistical Model of Evaluation

The basis of every nuclear data evaluation is the definition of the statistical model. In general the statistical model is given by

$$\vec{\sigma}_{exp} = \mathcal{M}(\vec{p}) + \vec{\epsilon}_{exp}\,, \tag{9}$$

where $\vec{\sigma}_{exp}$ is a vector built of M_{exp} measured values of different observables $\sigma_i, i = 1, \cdots, M_{exp}$ and $\vec{\epsilon}_{exp}$ is the vector of the corresponding experimental uncertainties $\epsilon_i, i = 1, \cdots, M_{exp}$. Usually it is assumed that $\vec{\epsilon}_{exp}$ is a random variable with multivariate probability distribution $\vec{\epsilon}_{exp} \approx \mathcal{N}(\vec{0}, \mathbf{B})$. The vector $\vec{p}$ is built of the parameters $p_i, i = 1, \cdot, N_{mod}$ of the theoretical model(s) $\mathcal{M}(\vec{p})$ for the calculation of observables. Restricting to multivariate probability distributions of the prior $\pi(\vec{p})$ and the likelihood $\ell(\vec{\sigma}|\vec{p})$

$$\pi(\vec{p}) \approx \mathcal{N}(\vec{p}_0, \mathbf{A}_0)\,, \tag{10}$$

$$\ell(\vec{\sigma}_{exp}|\vec{p}) \approx \mathcal{N}(\mathcal{M}(\vec{p}), \mathbf{B})\,. \tag{11}$$

Here, $\vec{p}_0$ is the best set of model parameters, $\mathbf{A}_0$ is the a-priori covariance matrix of parameters. The present information is sufficient to apply Bayes theorem, Eq.(3), and to determine the *a-posterior* values of the parameters $\vec{p}_1$ and their covariance matrix $\mathbf{A}_1$.

An important step is the determination of the *prior* $\pi(\vec{p}_0|\mathbf{A}_0)$. For a multivariate distribution the mean value $\langle\vec{p}\rangle$ is equivalent to $\vec{p}_0$ and assuming reasonable error bands of p_i the covariance matrix $\mathbf{A}_0 = \mathrm{Var}[\vec{p}_0]$ is frequently obtained by Monte Carlo sampling. Apart from the Backward-Forward Monte Carlo (BFMC) method [12] uncorrelated parameters are assumed.

The determination of the likelihood requires the determination of many observables from nuclear models. In general the calculations of nuclear models are rather involved and time consuming. A linearization of the model, e.g.

$$\mathcal{M}(\vec{p}) = \vec{\sigma}_{ref} + \mathbf{S}\left(\vec{p} - \vec{p}_{ref}\right) \text{ with } S_{ij} = \left.\frac{\partial\sigma_i(\vec{p})}{\partial p_j}\right|_{\vec{p}_{ref}}\,, \tag{12}$$

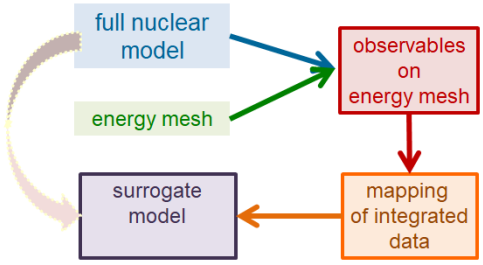

Figure 2. Scheme for the generation of the surrogate model for angle-integrated reaction cross sections.

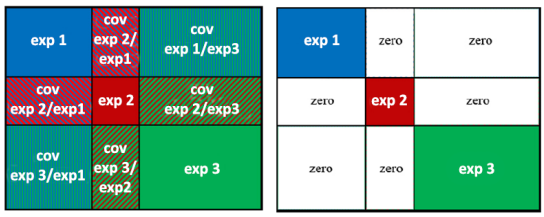

Figure 3. Typical forms of **B**: (a) all correlations included; (b) correlations between experiments ignored.

would accelerate calculations, but is of limited use because of highly non-linear relationships between parameters and observables in many nuclear models. Preferable is a switch to a surrogate model on the level of observables using dense meshes in energy and/or angles (see Fig. 2). The surrogate model is defined by the center value $\vec{\sigma}_0 = \mathcal{M}(\vec{p}_0)$ and the associated prior covariance matrix $\tilde{\mathbf{A}}_0$=Var$[\mathcal{M}(\vec{p})]\big|_{\vec{p}=\vec{p}_0}$. Both are obtained either by Monte Carlo sampling or via least square techniques. In general the determination of the prior requires multiple calculations of observables from nuclear models and is very time consuming.

3.3 Bayesian Update

The evaluation step, i.e. the Bayesian update, benefits from the surrogate model, which uses the values of the observables $\vec{\sigma}_0$ on a chosen energy and/or angular mesh as parameters. Using a high density of mesh points a linear interpolation (or bilinear interpolation of differential data) provides reliable values for the observables at any intermediate energy and/or angle. A benefit of the linear interpolation is the conservation of sums at any energy and/or angle. Using the surrogate model in the least square technique the Bayesian update is given by

$$\vec{\sigma}_1 = \vec{\sigma}_0 + \tilde{\mathbf{A}}_0\mathbf{S}^T\left(\mathbf{S}\tilde{\mathbf{A}}_0\mathbf{S}^T + \mathbf{B}\right)^{-1}\left(\vec{\sigma}_{exp} - \mathbf{S}\,\vec{\sigma}_0\right), \quad (13)$$

$$\tilde{\mathbf{A}}_1 = \tilde{\mathbf{A}}_0 - \tilde{\mathbf{A}}_0\mathbf{S}^T\left(\mathbf{S}\tilde{\mathbf{A}}_0\mathbf{S}^T + \mathbf{B}\right)^{-1}\mathbf{S}\tilde{\mathbf{A}}_0\,. \quad (14)$$

Here, $\vec{\sigma}_{exp}$ is the vector built of experimental data and **B** is the covariance matrix of experimental uncertainties. The matrix **S** performs the interpolation of the observables from the model grid to the energies/angles of the mesh of experimental data. At first glance one might believe that this Bayesian update procedure considering the parameters of the surrogate model as random variables leads to complete freedom. But this is not true because the covariance matrix $\tilde{\mathbf{A}}_0$ of the prior contains the essential features of the involved nuclear models. The information is contained in few eigenvectors associated with the largest eigenvalues of $\tilde{\mathbf{A}}_0$, while the impact of those associated with small eigenvalues is negligible.

The Bayesian update Eqs. (13,14) is straightforward but contains some pitfalls. The procedure provides reasonable *a-posterior* mean values $\vec{\sigma}_1$ but the variances of observables extracted from $\tilde{\mathbf{A}}_1$ are frequently too small. One reason for this phenomenon is the use of an incomplete covariance matrix **B** of experimental data. Usually the determination of the experimental uncertainties is focussed on a single experiment or a series of experiments of the same group which lead to a block form of the total **B**-matrix displayed in Fig. 3b. Thus correlations between different experiments are frequently ignored. Effectively the same block form of **B** occurs if experiments are included in the evaluation via a series of Bayesian updates. This sequential inclusion is also problematic with regard to systematic errors which are treated statistically although they are not of statistical nature. Consequently it is preferred to include all experimental data in one Bayesian update. If this is not possible one should group experimental data according to their experimental technique, e.g. transmission experiments, experiments in scattering chambers etc. Because of the essential differences in the techniques, the correlations between these groups will be rather small.

3.4 Model Deficiences

The statistical model defined in Eq. (9) assumes perfect nuclear models. Therefore, differences between model values and experimental data are only due to measurement uncertainties. This assumption is not realistic and does not account for the actual limitations of microscopic descriptions of nuclear systems. Actually one must take recourse to modelling which excellently describes some features of the considered system but not all its facets. Therefore, nuclear models are not perfect and part of the differences between model values and experiment may be due to model deficiencies.

The impact of model deficiencies on *a-posteriori*-values can easily be grasped from the principal component analysis [13] of the prior covariance matrix $\tilde{\mathbf{A}}_0$. As mentioned in subsection 3.3 the eigenvectors associated with the largest eigenvalues contain the features of the nuclear models. If the experimental data favor a description by a superposition of eigenvectors associated with small eigenvalues of $\tilde{\mathbf{A}}_0$ the resulting $\tilde{\mathbf{A}}_1$ will lead to too small experimental uncertainties. This concept is quite general and explains the impact of model deficiencies on evaluations, i.e. to underestimate the actual uncertainties.

In the past different approaches for the inclusion of model deficiencies have been worked out, e.g. [14–16]. Among these the phenomenlogical approach [14] which can be considered as an Ornstein-Uhlenbeck procedure or

the pseudostatistical estimate of covariance matrices via comparison with experimental data by Leeb et al. [15]. These first approaches do not satisfy inherently sum rules and in addition their statistical basis is partly questionable.

In 2015 Schnabel presented a statistically consistent formulation for the inclusion of model deficiencies [17]. Key point of the formalism is an extended statistical model

$$\vec{\sigma} = \mathcal{M}(\vec{p}) + \vec{\epsilon}_{mod} + \vec{\epsilon}_{exp}\,, \tag{15}$$

where $\vec{\epsilon}_{mod}$ represents the model deficiencies which are described via Gaussian processes. A Gaussian process is not a fixed functional form, but an ensemble of functions which satisfies a given mean value and covariance function. For example one makes for evaluations in the intermediate energy range the assumptions

$$\langle \vec{\epsilon}_{mod} \rangle = 0, \tag{16}$$

$$K_0(\epsilon_i, \epsilon_j) = \delta^2 \exp\left[-\frac{1}{2\lambda}(E - E')^2\right], \tag{17}$$

where δ and λ are so-called hyper-parameters describing the strength and the period of the oscillations in energy. Frequently one has an idea about a reasonable choice of these hyper-parameters. If not, proper values can be determined via maximization of the marginal likelihood with regard to the hyper-parameters,

$$(\delta, \lambda) = \arg\max \left\{ \rho\left(\vec{\sigma}_{exp} | \delta, \lambda\right) \right\} \tag{18}$$

with

$$\rho\left(\vec{\sigma}_{exp} | \delta, \lambda\right) = \int d^d p_i \int d^M \epsilon_j \, \ell\left(\vec{\sigma}_{exp} | \vec{p}, \vec{\epsilon}_{mod}\right) \times \pi(\vec{p}) \;\; \pi(\vec{\epsilon}_{exp} | \delta, \lambda)\,. \tag{19}$$

Assuming the a-posteriori pdf including model deficiencies is given by

$$\pi\left(\vec{p}, \vec{\epsilon}_{comb} | \vec{\sigma}_{exp}\right) = \tilde{C} \cdot \ell\left(\vec{\sigma}_{exp} | \vec{p}, \vec{\epsilon}_{mod}\right) \cdot \pi\left(\vec{p}\right) \cdot \pi\left(\vec{\epsilon}_{comb}\right)\,, \tag{20}$$

where we assume multivariate normal distributions for the a-priori parameters $\pi(\vec{p}) = \mathcal{N}(\vec{p}_0, \mathbf{A}_0)$, the experimental error $\vec{\epsilon}_{exp} = \mathcal{N}(\vec{0}, \mathbf{B})$ and the likelihood $\ell(\vec{\sigma}_{exp} | \vec{p}, \vec{\epsilon}_{mod}) = \mathcal{N}(\mathcal{M}(\vec{p}) + \vec{\epsilon}_{mod}, \mathbf{B})$. The model deficiencies $\vec{\epsilon}_{mod}$ are defined by a Gaussian process Eqs. (16,17) on the grid of experimental data. With the model deficiencies on the grid of interest $\vec{\epsilon}_{pred}$ one can build $\vec{\epsilon}^{\,T}_{comb} = (\vec{\epsilon}^{\,T}_{pred}, \vec{\epsilon}^{\,T}_{mod})$ with $\pi(\vec{\epsilon}_{comb}) = \mathcal{N}(\vec{0}, \mathbf{K}_0)$. In addition no correlation between model parameters $\vec{p}$ and model deficiencies is assumed, i.e. $\pi(\vec{p} \mid \vec{\epsilon}_{mod}) = \pi(\vec{p})$.

The introduction of model deficiencies lead to a conceptional modification of the true values of the observables which are given by

$$\vec{\sigma}_{true} = \vec{\sigma}_{mod} + \vec{\epsilon}_{mod}\,. \tag{21}$$

The best value of the observables as well as the posterior covariance matrix which enters into nuclear data files have been worked out in [17]

$$\vec{\sigma}^{\,best}_{true} = \int d\vec{p}\, d\vec{\epsilon}_{comb}\, \vec{\sigma}_{true}(\vec{p}, \vec{\epsilon}_{pred})\, \pi(\vec{p}, \vec{\epsilon}_{comb} | \vec{\sigma}_{exp})\,. \tag{22}$$

$$\mathbf{A}^{best}_{true} = \int d\vec{p}\, d\vec{\epsilon}_{comb}\, \pi(\vec{p}, \vec{\epsilon}_{comb} | \vec{\sigma}_{exp}) (\vec{\Delta}^{best}_{true})(\vec{\Delta}^{best}_{true})^T \tag{23}$$

with

$$\vec{\Delta}^{best}_{true} = (\vec{\sigma}_{true}(\vec{p}, \vec{\epsilon}_{pred}) - \vec{\sigma}^{\,best}_{true})\,. \tag{24}$$

In order to simplify actual calculations it is useful, analogously to subsection 3.2, to introduce a linearized model. Thus one obtains Bayesian update formulas in closed form. Because of the conceptional change due to the introduction of model deficiencies, Eq. (21), the equations are more involved and have been worked out by Schnabel [17]. A first application evaluating the total neutron-^{181}Ta cross section shows the impact of model deficiencies (Fig. 4)

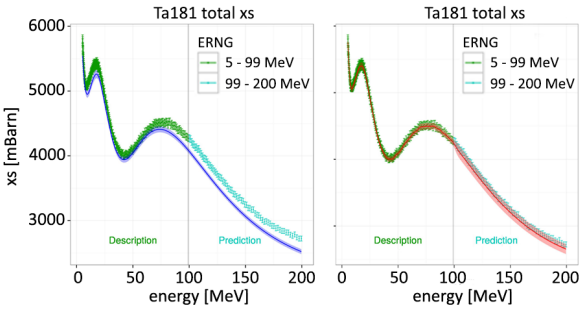

Figure 4. Impact of inclusion of model deficiencies on the evaluation of the total neutron-^{181}Ta cross section [17]. Only experimental data up to E_n =100 MeV are included in the evaluation, (a) model deficiencies ignored; (b) model deficiencies included.

3.5 Evaluation of light nuclear systems

The evaluation of reaction data of light nuclear systems ($A \leq 20$) requires a different treatment. Because of the small number of nucleons involved, the number of levels of the compound nucleus at low energies is rather small. Consequently, the reaction cross sections exhibit resonant behaviour up to rather high energies. Available microscopic models are very involved, but nevertheless limited with regard to quantitative reliability. Therefore, phenomenological R-matrix analyses [18] are performed for the description of reactions in the resonant energy range. Several standard R-matrix codes are used for these analyses, e.g. SAMMY [19], REFIT [20], AZUR [21] etc. With increasing energy the number of open channels increase and so the number of R-matrix parameters. Therefore, R-matrix analyses in an extended energy range up 30 MeV and higher are problematic not only for the high number of parameters, but also due to scarcity of available experimental data. Therefore, R-matrix analyses are limited in energy.

In general evaluations of reaction data of light nuclear systems are not based on Bayesian statistics. Either they are based exclusively on available experimental data or on a combination of R-matrix analysis at low energies with a fit of available experimental data at higher energies. Uncertainties are usually generated from the Hessian of the χ^2-fit and are frequently too small.

The concept of Bayesian evaluation techniques is not directly applicable to light nuclear systems, because R-matrix theory is not a predictive microscopic model, but requires experimental data for the determination of its parameters. Hence we must assume complete ignorance, i.e. a uniform distribution of the parameters as prior, which implies a simple least-square fit without *a-priori* knowledge.

The question arises whether there is really no *a-priori* knowledge. Considering standard R-matrix analyses of light nuclear systems one recognizes that the poles at low energies are associated with the levels of the compound nucleus. It is well known that the energies of the R-matrix poles are shifted with respect to the resonances, but the sequence of J^π-values frequently coincides. From previous R-matrix analyses we know that the form of resonances are sensitive to the J^π-values. Furthermore we know a-priori also the thresholds of reactions. These points altogether constitute *a-priori* information almost independent from previously performed R-matrix analyses. Therefore, we suggested the generation of an R-matrix based prior [22] via Monte Carlo sampling, varying the pole energies (±0.5 MeV), the matching radius (±0.2 fm) and the γ-width amplitudes min(±0.25,Turchin criterion[23]). With this information a prior for neutron-induced reactions of ^{9}Be was generated and used in a Bayesian update including four channels, i.e. ^{9}Be(n,n)^{9}Be, ^{9}Be(n,α)^{6}He, ^{9}Be(n,n$_2$)^{9}Be* and ^{9}Be(n,2nα)^{4}He. In Fig. 5 the prior and the a-posterior description of elastic neutron-^{9}Be scattering is displayed. The prior contains the gross features due to the levels but contains almost no information from the performed R-matrix fit.

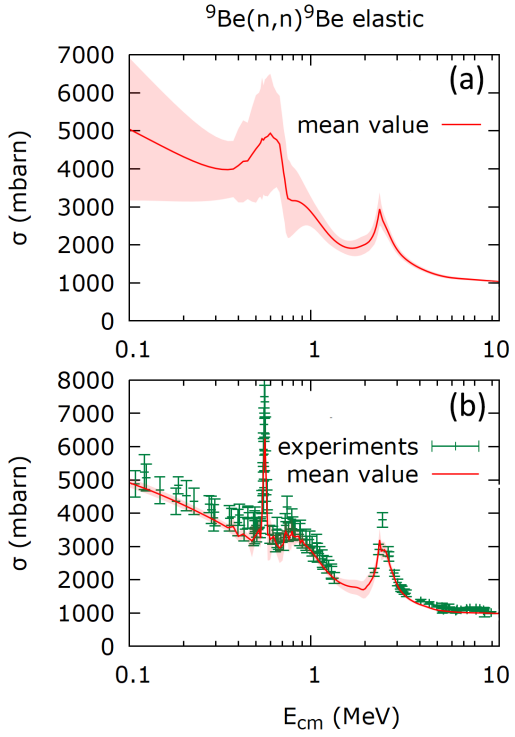

Figure 5. Elastic neutron-^{9}Be cross section; top - R-matrix based prior; bottom - after Bayesian update. Results taken from [22].

4 Perspectives

4.1 The modified Generalized Least-Square method

The increasing computer power enables large scale calculations not possible in the past. Specifically, we discussed in subsection 3.3 the advantage of linear interpolations which lead to matrices with large dimensions. In 2017 Schnabel and Leeb [24] proposed a Generalized Least Square technique which is faster and best suited for large scale calculations. The key of the method is a reformulation of the Bayesian update which avoids the determination of the prior covariance matrix. An important element is the generation of the **U** built of N_{MC} Monte Carlo vectors $\sigma(\vec{p}_i)$ of observables at the fixed energies/angles of the model grid calculated by the model with randomly varied sets of parameters $\vec{p}_i$. The matrix $\mathbf{U} = (\vec{u}_1, \cdot, \vec{u}_N)$ with

$$\vec{u}_i = \vec{\sigma}_i - \vec{\sigma}_0 \quad \text{and} \quad \vec{\sigma}_0 = \frac{1}{N}\sum_{i=1}^{N_{MC}} \vec{\sigma}_i \,. \tag{25}$$

If $\vec{\sigma}$ contains L values of observables the dimension of **U** is $L \times N_{MC}$. Analogously a matrix $\mathbf{V} = (\vec{v}_1, \cdots, \vec{v}_{N_{MC}})$ is introduced with $\vec{v}_i = \mathbf{S}\vec{u}_i$, where **S** is a matrix mediating the interpolation between the model grid of dimension L and the grid of experimental data points of dimension M_{exp}.

With these definitions a reformulation of the Bayesian update is obtained

$$\vec{\sigma}_k = \vec{\sigma}_0 + \frac{1}{N_{MC}}\mathbf{U}\vec{w}_k \quad \text{and} \quad \mathbf{A}_k = \frac{1}{N_{MC}}\mathbf{U}\mathbf{W}_k\mathbf{U}^T \tag{26}$$

with $k = 1, 2, \cdots$ and

$$\vec{w}_{k+1} = \vec{w}_k + \mathbf{W}_k\mathbf{V}^T\mathbf{X}\left(\vec{\sigma}_{exp} - \mathbf{S}\vec{\sigma}_0 - \frac{1}{N_{MC}}\mathbf{V}\vec{w}_k\right), \tag{27}$$

$$\mathbf{W}_{k+1} = \mathbf{W}_k - \frac{1}{N_{MC}}\mathbf{W}_k\mathbf{V}^T\mathbf{X}_k\mathbf{V}\mathbf{W}_k \tag{28}$$

with $\vec{w}_0 = \vec{0}$ and $\mathbf{W}_0 = \mathbf{1}$. For a concise formulation we introduced

$$\mathbf{X}_k = \left(\mathbf{S}\mathbf{A}_k\mathbf{S}^T - \mathbf{B}_k\right)^{-1} . \tag{29}$$

In this formulation of the Bayesian update the necessary storage for $L >> N_{MC}$ is drastically reduced because neither $\mathbf{A}_0$ nor $\mathbf{A}_k$ (both of dimension $L \times L$) must be calculated. The whole information is contained in the vectors $\vec{\sigma}_0$, $\vec{w}_k$ and the matrices **U**, $\mathbf{W}_k$. The covariance matrix for any channel can be extracted from these quantities. In Fig. 6 the scheme of an evaluation and the storage requirements are displayed.

4.2 Extendable nuclear data evaluations

The modified Generalized Least-Square method introduced in the previous subsections provides a possibility

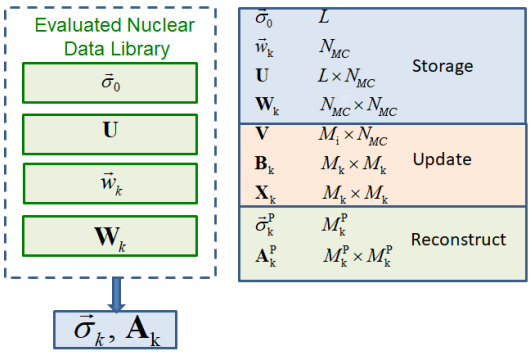

Figure 6. Scheme of the modified Generalized Least-Square method left - key quantities of an evaluation; right - storage requirement of various processes. Here L is the number of mesh points on the model grid, N_{MC} is the number of Monte Carlo samplings and M_k is number of experimental points in the $(k-1)^{th}$ step.

to extend the evaluation including additional experimental data. Because the complete information is contained in the left box of Fig. 7. For the inclusion of a further

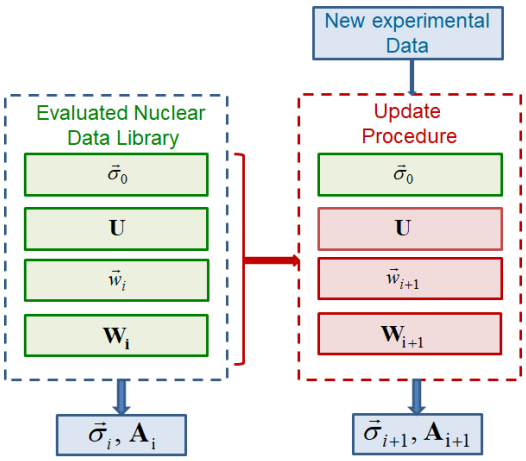

Figure 7. Schematic visualisation of the extension of an existing evaluation with new experimental data.

experimental data set it is not required to repeat the evaluation because the complete information about the evaluation is already contained in the stored quantities. Only correlations between the new experiment and the already included ones cannot be taken into account in this process. Despite this drawback the option of extension could be very valuable for the planning of dedicated experiments and their impact on evaluations.

4.3 Evaluation data library

The generation of an evaluated nuclear data file is an important piece of work and requires expertise, manpower and significant time. Because of the decreasing number of evaluators the time gaps between measurement of data and inclusion into evaluations are rather long. Another aspect is the difficulty to repeat a specific evaluation because decisions of the evaluator are hidden in extended documentation and their recovery is tedious and time-consuming. Therefore evaluations usually start from the very beginning thus doubling part of the work already invested. The formulation of the modified Generalized Least-Square method allows a compact storage of an evaluation. This feature can be used to combine all important data of an evaluation together with data bank moduls for experimental data sets, corresponding data modifications, and standards for input and output of evaluations. In Fig. 8 a first draft of such an Evaluation Library is sketched. The

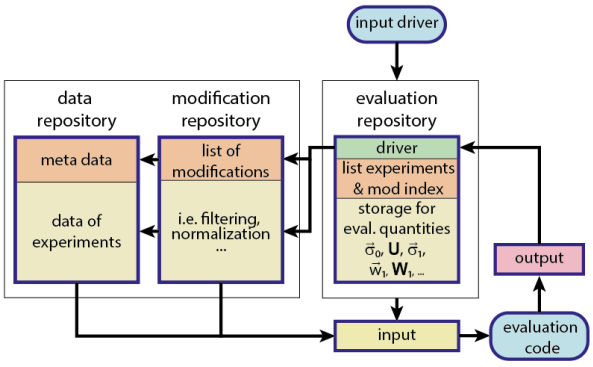

Figure 8. First draft of the components of an Evaluation Library.

availability of an *Evaluation Library* would increase the efficiency of evaluators significantly. It would also allow to repeat a given evaluation from scratch but with additional experimental data.

5 Summary and concluding remarks

In this paper a concise review of the concepts and the basic techniques of nuclear data evaluation are given. Typical problems are addressed which impact the uncertainty estimates and thus the reliability of nuclear data evaluations. In this context model deficiencies are discussed and their statistically consistent inclusion in evaluations is described. The special problems of nuclear data evaluations of light nuclear systems are addressed and a possibility for the implementation of a quasi-Bayesian evaluation is shown. Finally, a perspective of nuclear data evaluations is given. These are guided by the fact of decreasing men power which had to be compensated by increased automatisation. Developments based on the modified General Least Square method are suggested, i.e. (i) the concept of extendable nuclear data evaluations and (ii) the generation of an evaluation data library. The latter will avoid the doubling of work and significantly reduce the efforts of reproduction, modification, improvement and further developments of evaluated files.

Despite the worldwide efforts in developing reliable nuclear data evaluations there are still open questions of high importance, i.e. (i) the interpretation of uncertainty estimates, (ii) a unique evaluation from low to high energies and (iii) large scale evaluations of a series of isotopes including their intercorrelations. These problems should

be tackled in future exploiting the increasing computing capabilities, enhanced use of machine learning and methods of artificial intelligence. But independent of fast technical progress, the expertise of evaluators will be central for the quality of the final evaluated file.

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References

[1] E.T. Jaynes, Information theory and statistical mechanics, Phys. Rev. **106**, 620 (1957). 10.1103/PhysRev.106.620

[2] C. Shannon, A mathematical theory of communication, Bell System Technical Journal **3**, 379-423 (1948). 10.1002/j.1538-7305.1948.tb01338.x

[3] Ed. M. Herman, A. Trkov, ENDF-6 Manual, Report BNL-90365-2009 Rev.1 (2009). https://www.oecd-nea.org/dbdata/data/manual-endf/endf102.pdf

[4] A.J.M. Plompen et al., The joint evaluated fission and fusion nuclear data library, JEFF-3.3, Eur. Phys. J. A **56**, 181 (2020). 10.1140/epja/s10050-020-00141-9

[5] D.A. Brown et al., ENDF/B-VIII.0: The 8^{th} Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data, Nucl. Data Sheets **148**, 1-142 (2018). 10.1016/j.nds.2018.02.001

[6] Osamu Iwamoto et al., Japanese evaluated nuclear data library version 5: JENDL-5, J.Nucl Science and Technology **60**, 1-60 (2022). 10.1080/00223131.2022.2141903

[7] Zhigang Ge et al., CENDL-3.2: The new version of Chinese general purpose evaluated nuclear data library, EPJ Web of Conferences **239**, 09001 (2020). /10.1051/epjconf/202023909001

[8] A. Koning, Bayesian Monte Carlo Method for Nuclear Data Evaluation, Nucl. Data Sheets **123**, 207-213 (2015). 10.1016/j.nds.2014.12.036

[9] D.L. Smith, *Unified Monte Carlo Approach to Fast Neutron Cross Section Data Evaluation*, in Proc. of the 8th International Topical Mtg. on Nucl. Applics. and Util. of Accelerators, Pocatello, July 29 – August 2, p. 736 (2007).

[10] R. Capote, D.L. Smith, A. Trkov, M. Meghzifene, A New Formulation of the Unified Monte Carlo Approach (UMC-B) and Cross-Section Evaluation for the Dosimetry Reaction ^{55}Mn(n,γ)^{56}Mn, J. ASTM International **9**, JAI104115JAI, 179-196 (2012). 10.1520/JAI104115

[11] R. Capote, D.L. Smith, A. Trkov, Nuclear data evaluation methodology including estimates of covariances EPJ Web of Conferences **8**, 04001 (2010). 10.1051/epjconf/20100804001

[12] E. Bauge, Full Model Nuclear Data and Covariance Evaluation Process Using TALYS, Total Monte Carlo and Backward-forward Monte Carlo, Nucl. Data Sheets **123**, 201-206 (2015). 10.1016/j.nds.2014.12.035

[13] K. Pearson, On lines and planes of closest fit to systems of points in space, Philosophical Magazine **2**, 559 (1901). 10.1080/14786440109462720

[14] M.T. Pigni, H. Leeb, *Uncertainty estimates of evaluated ^{56}Fe cross sections based on extensive modelling at energies beyond 20 MeV* in: Proc. Int. Workshop on Nuclear Data for the Transmutation of Nuclear Waste (GSI Darmstadt, Darmstadt, 2003) PO21.

[15] H. Leeb, D. Neudecker, Th. Srdinko, Consistent Procedure for Nuclear Data Evaluation Based on Modeling, Nucl. Data Sheets **109**, 2762 (2009). 10.1016/j.nds.2008.11.006

[16] D. Neudecker, R. Capote, H. Leeb, Impact of model defect and experimental uncertainties on evaluated output, Nucl. Instr. Meth. A **723**, 163 (2013). 10.1016/j.nima.2013.05.005

[17] G. Schnabel, *Large Scale Bayesian Nuclear Data Evaluation with Consistent Model Defects*, PhD Thesis, TU Wien (2015).

[18] A.M. Lane, R.G. Thomas, R-matrix theory of nuclear reactions, Rev. Mod. Phys. **30**, 257 (1958). 10.1103/RevModPhys.30.257

[19] N.M. Larson, *Updated Users Guide for SAMMY: Multilevel R-Matrix Fits to Neutron Data Using Bayes Equations, ORNL/TM-9179/R8 ENDF-364/2* (October 2008).

[20] M.C. Moxon, T.C. Ware, C.J. Dean, *REFIT2009: A Least-Square Program for Resonance Analysis of Neutron Transmission, Capture and Scattering Data, Users Guide for REFIT-2009-10* (April 2010). https://databank.io.oecd-nea.org/codes/refit/

[21] R.E. Azuma, E. Uberseder, E.C. Simpson, C.R. Brune, H. Constantini, R.J. de Boer, J. Gönnes, M. Heil, P.J. LeBlanc, C. Ugalde, M. Wiescher, Phys. Rev. C **81**, 045805 (2010). 10.1103/PhysRevC.81.045805

[22] H. Leeb, T. Srdinko, Towards a Bayesian evaluation technique for light nuclear systems, EPJ web of Conferences **294**, 04006 (2024). 10.1051/epjconf/202429404006

[23] V.F. Turchin, V.P. Kozlov, M.S. Malkevich, Usp. Fiz. Nauk. **102**, 345 (1970) [Sov. Phys. Usp. **13**, 681 (1971)].

[24] G. Schnabel, H. Leeb, A modified Generalized Least Squares method for large scale nuclear data evaluation, Nucl. Instr.. Meth. A **841**, 87 (2017). 10.1016/j.nima.2016.10.006