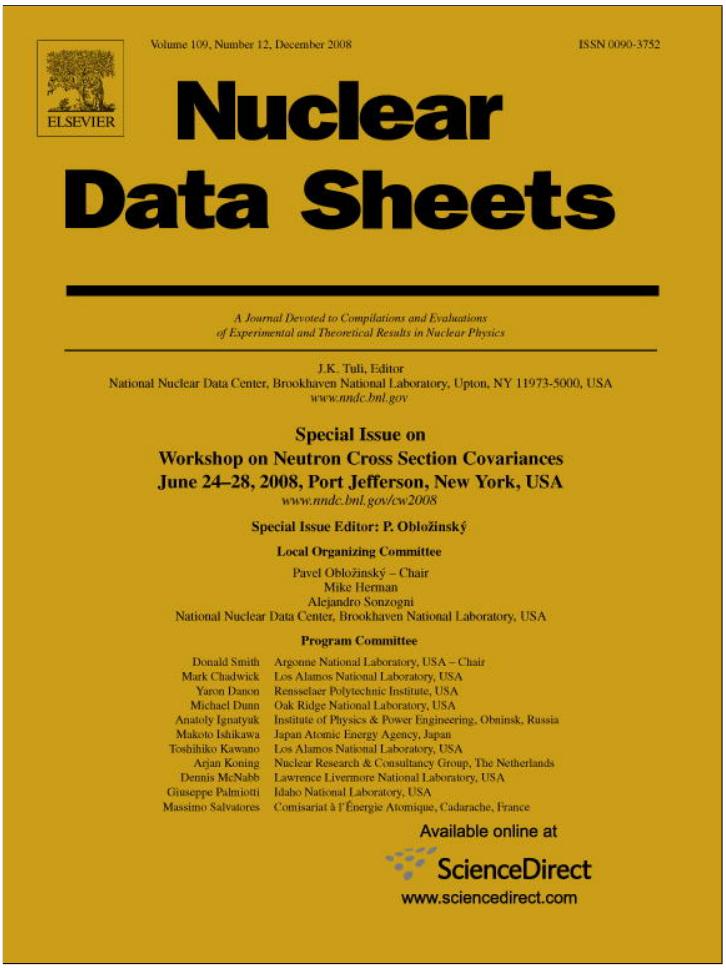

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Consistent Procedure for Nuclear Data Evaluation Based on Modeling

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A complete and consistent procedure to generate evaluated nuclear data files and the associated covariance matrices is presented. The novel procedure is fully based on Bayesian statistics and makes use of the theoretically formulated prior for parameter uncertainties presented by Leeb and Pigni recently. In addition the prior includes also model defects based on a statistical study of the gross structure of experimental data. Furthermore, a so-called correlated Bayesian update approach (CBUA) is proposed in order to account for a realistic treatment of systematic errors in experiments.

I. INTRODUCTION

Evaluated nuclear data files are essential ingredients for the design and construction of nuclear facilities, the radiation safety and the development of novel nuclear technologies. They contain consistent sets of cross section data and spectra, which cover for most isotopes the energy range only up to 20 MeV according to the needs of conventional technology. Associated uncertainty information which is required for the optimization of designs and the estimate of safety margins is available only for few selected isotopes and reactions. Hence, there is an ongoing effort to update the libraries with proper covariance matrices, which provide the relevant information for reliable uncertainty estimates of key quantities.

In addition to this general demand regarding uncertainties, there is also the request for an extension of the energy range up to about 150 MeV driven by the needs of best suited materials in fusion research (IFMIF) as well as the design of novel fission reactors, *e.g.* accelerator driven systems (ADS). The extension of the energy range is not trivial because of the limited set of available experimental data and the increasing number of open reaction channels. Hence, evaluated nuclear data files beyond 20 MeV rely substantially on nuclear model calculations.

Despite the strong and longstanding request from users, the availability of covariance information of evaluated data is not satisfactory. A careful analyses of experimental data has been performed for few isotopes by Vonach and Tagesen [1–4] within the framework of Bayesian statistics. They obtained almost diagonal covariance matrices associated with cross section mean values fluctuating with energy. An alternative approach is the Kalman filter technique [5] which has been used in JENDL and the ENDF-VI evaluations. The method is equivalent to the linearized Bayesian approach. However, unrealistically small uncertainties are frequently reported whose relevance might be questioned.

The proper determination of covariance matrices for modelling is still an open question. It was pointed out in Ref. [6] that three sources of uncertainties can be distinguished: (i) parameter uncertainties, (ii) model defects and (iii) numerical errors. The latter are either known or ignored and are not further considered. Most of the studies on covariance matrices deal with the parameter uncertainties, *e.g.* applications of the Kalman filter technique (*e.g.* [5]) and the Monte Carlo simulations with TALYS performed by Koning [7]. A more sophisticated Monte Carlo approach was implemented by Bauge [8] who used the χ^2-hypersurface to extract parameter distributions and correlations. All these methods refer to experimental data assuming that they can be reproduced by the model. Apart from ref. [6] model defects have not been discussed so far. Only recently, Mercatali *et al.* [9] presented a comparison of various criteria for the quality of a model.

In this paper we consider the question of covariance matrices for modelling from a fundamental point of view. Therefore, we give a brief outline of statistics in Sect. II A and discuss the features of the so-called Bayesian update procedure and its linearized version in Sect. II B. In order to account for correlations between experiments and keeping the simple form of an update procedure we propose a correlated Bayesian update approach (CBUA) which is outlined in Sect. II C. In Sect. III we focus on the determination of a well determined *prior* for nuclear data evaluation from modelling. First we summarize in Sect. III A the ideas of ref. [10], which provide covariance matrices associated with uncertainties in nuclear model parameters. In Sect. III B we formulate procedures for

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the determination of model defects. Two methods are proposed, whose covariance matrices are compared at the example of neutron cross sections of ^{16}O. In Sect. IV some concluding remarks are given.

II. BAYESIAN STATISTICS

A. Basic relations

The assignment of uncertainties to scientific data was discussed in detail by Fröhner [11]. It is essentially a problem of statistics and requires the interpretation of probability distributions of the *Subjective School of Thoughts*, *i.e.* as degrees of plausibility [12], which cannot be verified experimentally. Fröhner [11] addressed primarily aspects related to uncertainty estimates of experimental data. Here we will focus on uncertainty estimates of model calculations, which can be used as a prior for nuclear data evaluation. In particular we consider covariance matrices $\langle \Delta\sigma_\rho \Delta\sigma_\eta \rangle$ of integral cross sections σ_ρ and σ_η, where ρ, η characterize both the reaction channel and the energy.

Probability theory is built upon two fundamental relationships for the probability distribution p

$$p(\underline{x}, \underline{\sigma}|M) \; + \; p(\bar{\underline{x}}, \underline{\sigma}|M) = 1\,, \tag{1}$$

$$p(\underline{x}|\underline{\sigma}, M)p(\underline{\sigma}|M) \; = \; p(\underline{\sigma}|\underline{x}, M)p(\underline{x}|M)\,, \tag{2}$$

where Eq. (2) is equivalent to the conditioned probability distribution $p(\underline{x}, \underline{\sigma}|M)$ that the propositions $\underline{x}$ and $\underline{\sigma}$ are *true* under the conditions of the model M. Here we use the propositions relevant in nuclear data evaluation, *i.e.* $\underline{x}$ refers to the set of parameters, $\underline{\sigma}$ to the set of experimental data and M to the nuclear model used. The bar below x and σ indicates that both quantities are vectors, while $\bar{\underline{x}}$ means that the proposition $\underline{x}$ is *'false'*. The product rule, Eq. (2) leads directly to Bayes theorem [13]

$$p(\underline{x}|\underline{\sigma}, M) = \frac{p(\underline{\sigma}|\underline{x}, M)}{p(\underline{\sigma}|M)} p(\underline{x}|M)\,, \tag{3}$$

which allows to update the *prior distribution* $p(\underline{x}|M)$ with the information obtained by measurements expressed in the *likelihood function* $p(\underline{\sigma}|\underline{x}, M)$. Thus the *aposteriori distribution* $p(\underline{x}|\underline{\sigma}, M)$ is the expected probability distribution of the set of parameters taking consistently into account the experimental data and the available knowledge before the experiment.

The likelihood function $p(\underline{\sigma}|\underline{x}, M)$ gives the probability distribution of the data $\underline{\sigma}$ for a model M with parameters $\underline{x}$,

$$p(\underline{\sigma}|\underline{x}, M) = \exp\left[-\frac{1}{2} \left(\underline{\sigma} - \underline{\sigma}^M(\underline{x})\right)^T B^{-1} \left(\underline{\sigma} - \underline{\sigma}^M(\underline{x})\right) \right], \tag{4}$$

where the upper index T denotes transpostion and B is the covariance matrix of the experiment with elements $B_{\rho\eta} = \langle \Delta\sigma_\rho \Delta\sigma_\eta \rangle$ which account for statistical uncertainties and correlated (systematic) errors.

B. Linearized Bayesian update

Knowing the prior distribution, Bayes theorem (3) can easily be implemented via Monte Carlo techniques. However, almost all applications in nuclear data evaluation make use of a linearized version of Bayes theorem, which assumes normal distributions of the prior,

$$p(\underline{x}|M) = N \exp\left[-\frac{1}{2} (\underline{x} - \underline{x}_0)^T A_0^{-1} (\underline{x} - \underline{x}_0) \right], \tag{5}$$

where $\underline{x}_0$ is the apriori mean value of the parameter vector $\underline{x}$, A_0 the apriori covariance matrix of the parameters and N is an appropriate normalisation factor. Together with the likelihood function (4) one obtains via Bayes theorem the aposteriori distribution (3), which in this case reduces to an exponentional function

$$\begin{aligned} p(\underline{x}|\underline{\sigma}, M) \; = \; & \tilde{N} \exp\left[-\frac{1}{2} (\underline{x} - \underline{x}_0)^T A_0^{-1} (\underline{x} - \underline{x}_0) \right. \\ & \left. -\frac{1}{2} \left(\underline{\sigma} - \underline{\sigma}^M(\underline{x})\right)^T B^{-1} \left(\underline{\sigma} - \underline{\sigma}^M(\underline{x})\right) \right]. \end{aligned} \tag{6}$$

Introducing the sensitivity matrix S with matrix elements

$$S_{\eta,m} = \frac{\partial \sigma_\eta^M}{\partial x_m} \tag{7}$$

allows via linearisation to extract from the exponent of (6) the aposteriori mean value $\underline{x}_1$ and the aposteriori covariance matrix A_1 of the parameters,

$$\underline{x}_1 \; = \; \underline{x}_0 + A_0 S^T (Q + B)^{-1} (\underline{\sigma} - \underline{\sigma}^M(\underline{x}_0))\,, \tag{8}$$

$$A_1 \; = \; A_0 - A_0 S^T (Q + B)^{-1} S A_0 \tag{9}$$

with

$$Q = S A_0 S^T\,. \tag{10}$$

The implementation of the linearized version becomes particularly simple if the dimension of the inverted matrix, *i.e.* $Q + B$ is small. Therefore it is used to perform a sequential process and to include one experiment after the other. Thus in the n-th step the data of the n-th experiment are included leading from $\underline{x}_{n-1}$ and A_{n-1} to $\underline{x}_n$ and A_n. This linearized update procedure is applied to nuclear data evaluations by Vonach and Tagesen [1, 2] and is also used in the SAMMY code. In principle also the Kalman filter technique employed by [5] corresponds to such a linearized Bayesian update procedure.

We considered a schematic example to study the differences between the Bayesian update procedure and the application of (8,9) in one step. Especially we assume an observable $f(x) = a + bx + cx^2$ with simulated experimental data given by

$$\tilde{f}(y) = (a + by + cy^2)(1 + d * r) + \Delta\tau(y)\,, \tag{11}$$

where a, b and c are parameters, $r \in [-1, +1]$ is a uniform random variable, d is the width of the random interval

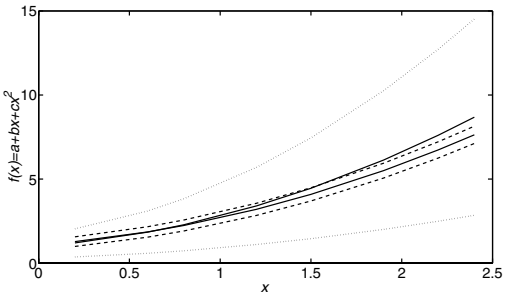

FIG. 1: The mean value (thick solid) and the error bands (long dashed) of the function $f(y)$ obtained from 400 sets of simulated experimental data assuming $d = 0.2$ and $\Delta\tau(y) = 0.2$. For comparison the mean value (thin solid line) and the error band (dotted line) of the prior are shown.

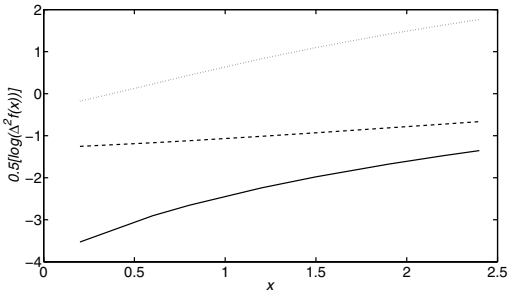

FIG. 2: Square root of the variance of the $f(y)$-values obtained by Bayesian update (solid line), full Bayesian procedure in one step (dashed line) and the prior (dotted line).

and $\Delta\tau(y)$ is a systematic error. The statistical variance $\Delta^2\sigma(y)$ and the systematic error are of the form

$$\Delta^2\sigma(y) = \frac{4}{3}d^2 f^2(y)\,, \tag{12}$$

$$\Delta\tau(y) = e + f\sqrt{(}y) \tag{13}$$

and are used to construct the covariance matrix of the simulated experiment

$$B_{i,j} = \Delta\tau(y_i)\Delta\tau(y_j) + \delta_{i,j}\Delta^2\sigma(y_i)\,. \tag{14}$$

We constructed 400 sets of *experiments*, each consisting of 8 $\tilde{f}(y_i)$-values with $a = 1, b = -1, c = 1$, where $y_i \in [0.2, 2.4]$ are 8 different but fixed argument values. In Fig. 1 we show the mean values and the error band obtained by a full Bayesian calculation in one step. Using the same *experimental data* in a Bayesian update procedure leads to a slightly different mean value, but also to a different error band. A comparison of the variances is given in Fig. 2, which indicates that the Bayesian update procedure tends to too small uncertainties. It can easily be shown that the origin for the difference between Bayesian update and the full Bayesian calculation in one step is the neglect of correlations between experiments in the update procedure. This defect of the Bayesian update procedure may also explain in part the unrealistically small uncertainties found in determinations of covariance matrices based on modelling.

C. Correlated Bayesian update approach

The standard Bayesian update procedure is a simple and efficient procedure to include new experimental data into the evaluation. We therefore aimed at the formulation of a similar approach which includes the correlations between experiments in first order. Our starting point is the consideration of two experiments of equivalent dimension, which should be included into the evaluation. For these two data sets we performed in closed form the standard Bayesian update procedure and the full Bayesian calculation. Comparison of the two results allows to extract the terms due to correlations between experiments. Thus we obtain a modified Bayesian update formula

$$\begin{aligned} A_i &= A_{i-1} - A_{i-1}S^T(SA_{i-1}S^T + B_i)^{-1}SA_{i-1} \\ &+ A_0 S^T\left[E_{cor} + F_{cor} + G_{cor} + G_{cor}^T\right]SA_0\,, \end{aligned} \tag{15}$$

where the first two terms of Eq. (15) correspond to the standard update procedure and $E_{cor}, F_{cor}, G_{cor}$ are contributions due to the correlations C between experiment '1' and '2'. The terms are all of similar form. As an example we give here E_{cor}

$$\begin{aligned} E_{cor} &= \left[(Q + B_1) - (Q + C^T)(Q + B_2)^{-1}(Q + C)\right]^{-1} \\ &- \left[(Q + B_1) - Q(Q + B_2)^{-1}Q\right]^{-1}. \end{aligned} \tag{16}$$

In an update procedure we do not want to keep the whole history of the evaluation process. Hence B_1 will not be available and we use in the correlation term for this matrix the covariance matrix B_2 of the experiment which is included in the current step.

In order to show the feasibility of the *Correlated Bayesian Update Approach* we have applied it on the previous example. Since we do not know the correlations between experiments we have multiplied the block matrices describing the correlations between different experiments with an over all factor q. In Fig. 3 the variances for different q-values are shown. Although there is still place for refinement of the CBUA this first example shows that the variances show a saturation which in case of $q = 1$ is the size of the smallest systematic error.

III. PRIOR DETERMINATION

The choice of the proper prior is of great importance for nuclear data evaluations, which suffer from a scarcity of experimental data. Thus the evaluation is essentially given by the model prior providing mean values and associated covariance matrices. Following [6] there are three sources of uncertainties in model calculations. Thus the total covariance matrix is a sum of three terms, *i.e.* (1)

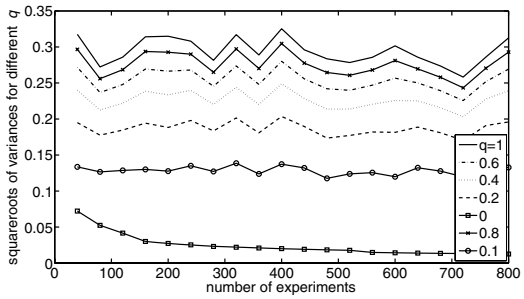

FIG. 3: Square root of the variance of the $f(y)$-values obtained by the Correlated Bayesian Update Approach assuming different strength of the correlations.

the covariance matrix due to parameter uncertainties, (2) the covariance matrix associated with numerical errors and (3) the so-called model defects. In this paper we outline the procedure developed in [10, 14] to account for parameter uncertainties. The numerical errors can usually be controlled and are not discussed here. The major part of this section is devoted to the formulation of model defects, for which no systematic treatment is available at present.

A. Parameter uncertainties

Based on the concepts of maximum information entropy and invariant measures Jaynes [15] formulated an unambiguous criterion for the apriori distribution. These ideas have been adapted and applied for nuclear data evaluation in Refs. [10] and [14]. The basic idea is maximizing the information entropy S under constraints stemming from apriori knowledge,

$$\delta \quad \left\{ -\int dx_1 \cdots \int dx_n p(\underline{x}) \ln \frac{p(\underline{x})}{m(\underline{x})} + \sum_{k=1}^{K} \lambda_k G_k[p(\underline{x})] \right. \\ \left. -\lambda_0 \left[\int dx_1 \cdots \int dx_n p(\underline{x}) - 1 \right] \right\} = 0 \,, \qquad (17)$$

where $\lambda_i, i = 1, \ldots, K$ are Lagrange parameters and G_k are functionals, which contain apriori knowledge, *e.g.* mean values and correlations of parameters. The function $m(\underline{x})$ is an *invariant measure* ensuring the form invariance under change of variables. In the presented version we have formulated the models with scaling parameters for which the invariant measure is known to be $1/x$. Furthermore we did not solve the full variation principle, but consider the uncorrelated eigenparameters $\underline{\xi}$ for which the probability is of simple product form. Assuming the knowledge of the mean values the corresponding apriori distribution is then given for each eigenparameter

$$p(\xi_\ell) = \frac{m(\xi_\ell)}{Z(\lambda_\ell)} \exp\left[-\lambda_\ell \xi_\ell)\right] \qquad (18)$$

with the partition function

$$Z(\lambda_\ell) = \int d\xi_\ell m(\xi_\ell) \exp\left[-\lambda_\ell \xi_\ell\right] \,. \qquad (19)$$

An important step in this procedure is the determination of the admissible range of the parameters and their correlations. In Ref. [14] several physics constraints have been worked out especially for optical model parameters.

With the knowledge of the apriori distribution it is straightforward to determine the covariance matrices associated with parameter uncertainties.

B. Model defects

The collision of a nucleon with a nucleus represents a quantum mechanical many-body problem for which no rigorous ab-initio calculations starting from the nucleon-nucleon interaction are feasible at present. In order to overcome this problem, nuclear models have been formulated, which describe various aspects of the collision. Usually these models contain effective parameters simulating specific features of the many-body problem, but obviously they cannot account for all pecularities of the reaction processes. Especially it may happen that variation of the model parameters over the whole domain does not match the actual value of the observable. This so-called *model defect* has to be taken into account in an evaluation of nuclear data based on modelling.

Estimates of the model defects and the associated covariance matrices are difficult because the failures are of non-statistical nature and cannot be determined via theoretical considerations. In order to quantify model defects one must take recourse to experimental data. However, one must avoid double counting using *e.g.* only data from neighbouring nuclei in the same energy range, which are not used in a subsequent evaluation.

At present there exists no established method to determine model defects. In the following we propose two procedures: (i) the *scaling procedure* which defines for each isotope energy independent scaling factors for each reaction channel and (ii) *remodelling* which defines an energy dependent scaling factor for each reaction channel.

First let us define the common framework. We assume that we use data from N neighbouring isotopes, from which we believe that the applied model describes the reaction channel of interest, c, equally well as for the isotope actually considered. The energy region is divided into M bins with energy $E_m, m = 1, \cdots, M$ at the center of the m-th bin. We assume that for the reaction considered there exist for most of the neighboring isotopes experimental data for each energy bin. Thus we can introduce an index set $Ebin(m,n)$ to classify the experimental data for the n-th isotope in the m-th energy bin. We introduce the bin quantities

$$\langle D_n^{(c)}(E_m) \rangle = \sum_{j \in Ebin(m,n)} w_j^{(c,m,n)} \frac{\sigma_{ex}^{(c)}(E_j)}{\sigma_{th}^{(c)}(E_j)} \,, \qquad (20)$$

$$\langle \left(D_n^{(c)}(E_m) \right)^2 \rangle = \sum_{j \in Ebin(m,n)} w_j^{(c,m,n)} \left(\frac{\sigma_{ex}^{(c)}(E_j)}{\sigma_{th}^{(c)}(E_j)} \right)^2 , \tag{21}$$

where $w_j^{(c,m,n)}$ is the chosen weight, E_j is the energy of the j-th experimental point and *ex* and *th* refer to experimental and model cross section, respectively. In this contribution we choose

$$w_j^{(c,m,n)} = \frac{\sigma_{th}^{(c)}(E_j)}{\sum_{j' \in Ebin(m,n)} \sigma_{th}^{(c)}(E_{j'})}, \tag{22}$$

which emphasizes the scaling factors at the highest values of the cross section. These definitions allow a compact formulation of the two proposals for a covariance matrix associated with model defects.

1. Model defects from scaling procedure

In this procedure one defines first an overall scaling factor $D^{(c)}$ via averaging over all neigboring isotopes,

$$D^{(c)} = \frac{1}{N} \sum_{n=1}^{N} \langle D_n^{(c)} \rangle , \tag{23}$$

with

$$\langle D_n^{(c)} \rangle = \sum_{m=1}^{M} w_m^{(c,n)} \langle D_n^{(c)}(E_m) \rangle . \tag{24}$$

The weights $w_m^{(c,n)}$ should be in correspondence with those for the averages over the energy bins of Eqs. (20) and (21). The covariance matrix for the reaction channel of the considered isotope is then introduced via

$$\begin{aligned} \langle \ \Delta\sigma^{(c)}(E_m) \Delta\sigma^{(c)}(E_{m'}) \rangle &= \sigma_{th}^{(c)}(E_m) \sigma_{th}^{(c)}(E_{m'}) \\ \times \ \frac{1}{N} \sum_{n=1}^{N} & \left[\left(\langle D_n^{(c)}(E_m) \rangle - D^{(c)} \right) \left(\langle D_n^{(c)}(E_{m'}) \rangle - D^{(c)} \right) \right. \\ + \ \delta_{m,m'} & \left. \left(\langle \left(D_n^{(c)}(E_m) \right)^2 \rangle - \left(\langle D_n^{(c)}(E_m) \rangle \right)^2 \right) \right] . \end{aligned} \tag{25}$$

The first term of Eq. (25) is due to the defect of the model, while the second term reflects the uncertainty in the scaling factor due to the limited accuracy of the experimental data. However, it must be remarked that this covariance matrix is not fully of statistical nature.

2. Model defects associated with remodelling

The formulation of an energy-dependent scaling factor

$$D^{(c)}(E_m) = \frac{1}{N} \sum_{n=1}^{N} \langle D_n^{(c)}(E_m) \rangle \tag{26}$$

changes the inherent features of the original model (*e.g.* the energy dependence) and we denote this procedure as

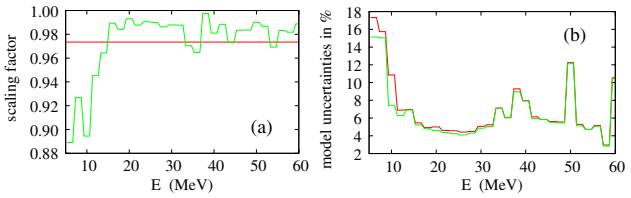

FIG. 4: (a) The scaling factor and (b) the square root of the variances in % of the model cross section for n-^{16}O total cross sections for both methods. The results of the scaling method are denoted in red and those of remodelling in green.

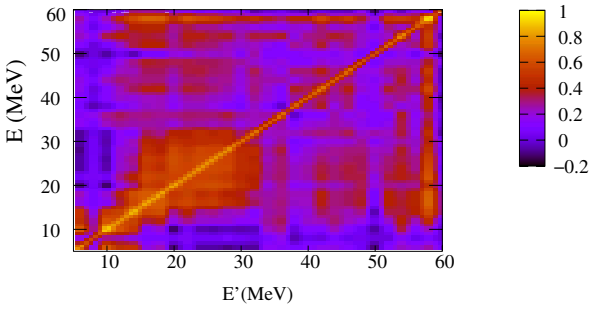

FIG. 5: Correlation matrix of the model defects in the total cross sections of oxygen using the scaling procedure of subsection III B. The model calculations are performed with the TALYS code with adapted optical potential.

remodelling. A reasonable covariance matrix is given by

$$\begin{aligned} \langle \ \Delta\sigma^{(c)}(E_m) \Delta\sigma^{(c)}(E_{m'}) \rangle &= \sigma_{th}^{(c)}(E_m) \sigma_{th}^{(c)}(E_{m'}) \\ \times \ \frac{1}{N} \sum_{n=1}^{N} & \left[\Delta D_n^{(c)}(E_m) \Delta D_n^{(c)}(E_{m'}) \right. \\ + \ \delta_{m,m'} & \left. \left(\langle \left(D_n^{(c)}(E_m) \right)^2 \rangle - \left(\langle D_n^{(c)}(E_m) \rangle \right)^2 \right) \right] \end{aligned} \tag{27}$$

with

$$\Delta D_n^{(c)}(E_m) = \langle D_n^{(c)}(E_m) \rangle - D^{(c)}(E_m) . \tag{28}$$

3. Example

The procedures defined in this section allow the estimate of the model defects, comprising the corrections of the mean value and the associated covariance matrix for the relevant reactions. In order to show the feasibility we apply the procedure to neutron-induced reactions of oxygen in the energy range between 5 and 60 MeV. Apart from a slightly adapted neutron-oxygen optical potential we use the code TALYS with default parameters as nuclear model description. We tested both procedures using total cross section data from the EXFOR library of the neighbouring nuclei ^{12}C, ^{14}N, ^{19}F, ^{23}Na and ^{24}Mg. In Fig. 4a the scaling factor $D^{(c)} = 0.9735$ as well as the energy-dependent remodelling factor $D^{(c)}(E_m)$ are displayed. The latter exhibits only a small energy dependence beyond 20 MeV resulting in similar uncertainties

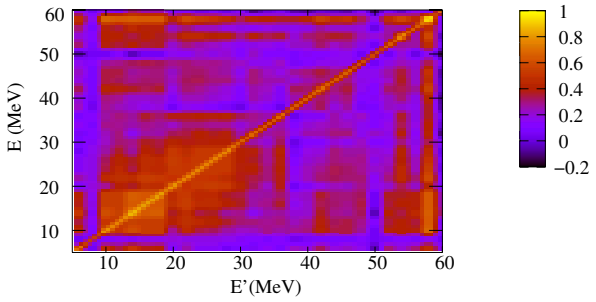

FIG. 6: Correlation matrix of the model defects in the total cross sections of oxygen using the remodelling procedure.

of the model defects for both methods (Fig. 4b). In Fig. 5 we show the correlation matrix due to model defects for the total cross section obtained by the scaling method of subsect. III B.

For comparison we show in Fig. 6 the corresponding correlation matrix obtained via the remodelling procedure of subsection III B. Both procedures yield a similar gross structure of the correlations, which reflects the fact that the scaling procedure is a fair approach for the total cross section beyond 20 MeV.

IV. SUMMARY

We have outlined a consistent procedure for nuclear data evaluations which rely heavily on modelling. The considerations are based on Bayesian statistics and provides a theoretically well defined prior associated with parameter uncertainties. In addition, it contains two proposals for a proper formulation of model defects. These procedures use available experimental information from neighboring nuclei, but depending on the nature of the nuclear model they can be extended to other projectiles.

An essential outcome of this contribution is the importance of the proper treatment of systematic errors. Applying Bayes theorem via an update procedure ignores correlations between experiments and assumes a statistical distribution of systematic errors, which may result in unphysically small uncertainties of the evaluation. In order to maintain the advantages of the update procedure we have suggested a so-called *Correlated Bayesian Update Approach* (CBUA), which contains essentials of the correlations between experiments.

In summary, we have presented a complete and consistent method to set up nuclear data evaluations including covariance information for systems with scarce experimental information. At present this method is particularly useful for nuclear data evaluations beyond 20 MeV, where limited experimental data are available.

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