Sensitivity and Uncertainty Studies of Average Cross Section parameters with Monte-Carlo sampling

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Abstract

Hauser Feshbach formalism [1] with width fluctuation corrections [2, 3] and some Optical Model recipies are widely used for the calculation of average cross sections. Each model involved in the calculation is parametrized. The parameters can be adjusted to reproduce experimental datasets. As a result, a covariance matrix can be deduced from the fit and used in uncertainty calculation of the group averaged cross sections. Nevertheless, some parameters, such as the mean level spacing, the binding and pairing energy, are not supposed to be adjusted. They have a-priori uncertainties that should be properly taken into account and propagated into the previous adjustement as well as to group averaged cross sections.

In this paper, we propose to use a Monte-Carlo propagation method based on an exact mathematical description to treat these non-adjusted parameters and their effects on the adjusted ones. A full covariance matrix for all the parameters will then be evaluated.

Two isotopes will be treated ^{240}Pu and ^{177}Hf to illustrate the involved methods.

KEYWORDS: Uncertainty, Adjustement, Covariance, HauserFeshbach, Optical Model, Monte Carlo

1. Introduction

In the Unresolved Resonance Range, the modelling of the average cross sections uses several theories. For our application, the level densities are calculated with the Gilbert-Cameron model [4]. The spin cut-off is calculated with the total mean level spacing, D_0 . To calculate the total and shape elastic cross section, we need, for a given orbital momentum l, S_l, the strength function which takes part in the calculation of the average collision matrix $< U_l >$. For partial cross sections, we have to calculate Transmissions for gamma and neutron channels. These transmissions are parametrized as follows :
gamma channel :

$$T_l^{\gamma} = 2\pi \frac{< \Gamma_l^{\gamma} >}{D_l(E,J)} f(E)$$

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neutron channel :

$$T_l^n = 1 - | < U_l > |^2$$

The transmissions are then used to calculate partial cross sections with the HauserFeshbach formulae [1] in conjunction with Width Fluctuations factors [2, 3].

The meta-model is parametrized with other parameters (binding energy, distant levels,...) which are not going to be detailed here. Nevertheless, the method could also be applied to these parameters.

Some of the parameters are adjusted to reproduce experimental datasets. A covariance matrix can be deduced from the fit. Other parameters, not supposed to be adjusted but having a-priori uncertainties should properly be taken into account in the adjustement as well as for the propagation to group averaged cross sections. In this paper we propose to use a Monte-Carlo method to propagate all uncertainties including the non-adjusted parameters. A full covariance matrix for all the parameters will thus be evaluated.

2. Monte Carlo Propagation Method

Let $\overrightarrow{y_i}$ ($i = 1 \dots N_y$) denote some experimentally measured variables, and let $\vec{p}$ and $\vec{x}$ denote the parameters defining the nuclear model employed to calculate these variables theoretically. $\vec{p}$ and $\vec{x}$ have uncertain values, and then, are considered as random vectors. These two parameter vectors are subject to different treatments: $\vec{p}$ is fitted on the observed values $\vec{y}$, while $\vec{x}$ is not fitted. This last parameter vector has an *a priori* uncertainty (with a covariance matrix X) that we have to take into account. In other words, the problem consists to propagate the uncertainties on the parameters $\vec{x}$ during the fitting of the parameters $\vec{p}$?

In this paper, we propose one solution based on the principle of the conditional probabilities.

2.1 Description of the method

Let us suppose that we simulate N sets of parameters $\vec{x}$: $\overrightarrow{x_k}$ ($k = 1 \dots N$). For each one of these simulations, we fit the parameter vector $\vec{p}$. We obtain N sets of fitted parameters called $\overrightarrow{p_k}$ with k the realization number. One recovers also the associated covariance matrix, called P_k, which expresses the uncertainty of $\vec{p}$ around its mean value $\overrightarrow{p_k}$. The parameter vector $\overrightarrow{p_k}$ can be seen as the expectation, in the probabilistic sense, of $\vec{p}$ knowing that $\vec{x}$ is worth $\overrightarrow{x_k}$:

$$\overrightarrow{p_k} = \mathbb{E}(\vec{p}\,|\vec{x} = \overrightarrow{x_k}) \tag{1}$$

By using the theorem of the total expectation (see appendix, Eq. 6) and by taking the expectation of the terms of equation (1), it results that :

$$\mathbb{E}(\overrightarrow{p_k}) = \mathbb{E}(\vec{p}) \tag{2}$$

One thus obtains an estimation of the mean values of the parameters $\vec{p}$ thanks to $\mathbb{E}(\overrightarrow{p_k})$, which can be calculated by averaging the N vectors $\overrightarrow{p_k}$ obtained. In a same manner, the covariance matrix P_k is seen as a conditional covariance :

$$P_k = \mathrm{cov}(p_i, p_j\ |\vec{x} = \overrightarrow{x_k}) \tag{3}$$

where p_i and p_j are components of the vector $\vec{p}$ ($i = 1 \dots N_p$, $j = 1 \dots N_p$).

According to the total covariance theorem (see appendix, Eq. 8), we have :

$$\mathrm{cov}(p_i, p_j) = \mathrm{cov}[\mathbb{E}(p_i\ |\vec{x} = \overrightarrow{x_k}), \mathbb{E}(p_j\ |\vec{x} = \overrightarrow{x_k})] + \mathbb{E}[\mathrm{cov}(p_i, p_j\ |\vec{x} = \overrightarrow{x_k})] \tag{4}$$

By using equations (1) and (3), this last expression turns to

$$\mathrm{cov}(p_i, p_j) = \mathrm{cov}(p_{k,i}, p_{k,j}) + \mathbb{E}(P_k) \tag{5}$$

One thus obtains an estimation of the covariance matrix of the parameters $\vec{p}$ by adding two covariance matrices: the first is calculated from the N sets of fitted parameters, the second is the average of the N covariance matrices associated with each fitting.

Monte-Carlo simulations offers the advantage that there is no assumption of linearity on the relation between $\vec{y}$ and $\vec{p}$. In addition, the method does not suppose that the vector $\vec{x}$ has a Gaussian distribution, which is an hypothesis often made by analytical methods. It supposes only that one can simulate $\vec{x}$ according to its joint distribution. For example, the Nataf model consists in defining a marginal distribution (not necessarily Gaussian) for each component of $\vec{x}$, and a matrix of covariance to describe the correlations between components. Some methods exist to simulate the parameter vector in such situations [5].

2.2 Parameter Nomenclatura and Software Tools

In the whole paper the following nomenclatura will be adopted to parameters :

- Constant means that the parameter is not to be varied nor adjusted,
- Sampled means that the parameter is to be varied with Monte Carlo sampling but not adjusted,
- Adjusted means that the parameter is to be adjusted to reproduce a set of experimental results.

The calculation of the cross sections and the propagation of errors using Monte-Carlo sampling are realized with the CONRAD code [6]. The fitting procedure of CONRAD is made *via* an interface with the Minuit2 package, part of the ROOT framework [7].

2.3 Sensitivity calculations : case of the ^{177}Hf capture cross section.

The Table 1 gives the parameters of interest used for the ^{177}Hf capture cross section calculation with their prior values.

Table 1: ^{177}Hf prior average parameters description.

Name	Value	Type	Uncertainty
D_0	2.4	Sampled	0.3(12.5%)
$\Gamma^{\gamma}_{l=0}$(meV)	57	Adjusted	5.7(10%)
$\Gamma^{\gamma}_{l=1}$ (meV)	57	Adjusted	5.7(10%)

The total mean level spacing for incoming s-wave (D_0) will be the only sampled parameter. The adjustement of $\Gamma^{\gamma}_{l=0}$ and $\Gamma^{\gamma}_{l=1}$ on a given experimental data set [8] will therefore be performed for each sample. The involved data set presents very low uncertainties (between 4.1 and 0.8 $\%$). To emphasize on the problem occuring in this balance we also are going to give results with the same set of experimental sections but having slightly different uncertainties (a fixed 10$\%$ value).

The Table 2 summarizes the results by giving the correlations and errors obtained for the three following cases :

- a single adjustement with no Monte Carlo propagation of the D_0 uncertainty (first lines in the table),
- a Monte Carlo propagation with low experimental uncertainties (second lines),
- a Monte Carlo propagation with enhanced experimental uncertainties (last lines).

Table 2: Correlations and errors for the ^{177}Hf cases.

Correlations			
	D_0	$\Gamma^{\gamma}_{l=0}$	$\Gamma^{\gamma}_{l=1}$
D_0	1	0 0.996 0.930	0 0.96 0.45
$\Gamma^{\gamma}_{l=0}$	-	1	-0.793 0.934 0.22

Uncertainties			
Parameter	Value	Error	Relative Error (%)
D_0	2.4	0.3	12.5
$\Gamma^{\gamma}_{l=0}$(meV)	68.8 68.8 70.2	0.8 8.5 9.9	1.1 12.4 14.2
$\Gamma^{\gamma}_{l=1}$(meV)	64.2 64.2 59.9	2.3 8.4 17.7	3.6 13.4 29.6

With no propagation of errors coming from the D_0 parameter, there is no correlation between the D_0 and Γ^{γ}_{l} parameters and the the last ones exhibit very low uncertainties.

In the case of the Monte Carlo propagation method, to reach a desired level of experimental cross sections, the balance between the D_0 parameter and the Γ^{γ}_{l}'s will create via the Monte-Carlo simulation a correlation close to unity between those parameters corresponding to the first part of the covariance formula of Eq.(5). This is due to the fact that in this energy region, the value of gamma transmission is far lower than the value of neutronic transmission and as a result we have : $\sigma^{n,\gamma}_{l} \propto \frac{T^{\gamma}_{l}}{D(E)}$. The addition of a mean covariance matrix coming from the experimental adjustement (second part of the covariance formula of Eq.(5)) induces a deviation from one. The level of experimental errors is thus of crucial importance.

The major point of this example is to show the extreme dependance of the covariance to the experimental data covariance as well as the functionnal dependancy between parameters for the adjustement than can create big effect via Monte Carlo sampling :

- when experimental errors are of the same order of magnitude than the error related to non-adjusted parameters, an important change in correlation coefficient can be seen : the addition of two very different covariance matrices can create wide effects.

- when experimental errors are far lower than the error related to non-adjusted parameters, the dependancy created by the Monte-Carlo simulation can induce strong correlations between parameters. As a result, one should take care when propagating this new covariance matrix to the cross section because of possible error cancellation and numerical precision problems.

2.4 Uncertainty propagations Principles : application to ^{240}Pu

For the ^{240}Pu case, the parameters of interest are the s-wave mean level spacing, D_0 , the average radiative witdhs Γ_l^γ and the strength functions S_l's. The calculation scheme for the covariance will be the following :

1. adjustement of S_l's on a set of experimental total cross section to obtain a new set of S_l's and a covariance matrix on D_0 and the S_l's : $M_{D,S}$, D and S_l's are not correlated.

2. application of the technique on sampling the D_0 and S_l's with respect to their covariance matrix $M_{D,S}$; and adjustment of the Γ_l^γ's on an experimental capture cross section to obtain a new set of Γ_l^γ's and a covariance matrix on D_0, S_l's and the Γ_l^γ's : $M_{D,S,\Gamma}$.

The final results (correlation matrix and errors on the parameters) are listed in Table 3.

Table 3: Correlations and uncertainties for the adjusted/sampled parameters in ^{240}Pu case.

Correlations

	D_0	$S_{l=0}$	$\Gamma^\gamma_{l=0}$	$S_{l=1}$	$\Gamma^\gamma_{l=1}$	$S_{l=2}$
D_0	1	0	0.49	0	0.26	0
$S_{l=0}$		1	≈ 0	-0.39	≈ 0	0.43
$\Gamma^\gamma_{l=0}$			1	-0.24	-0.39	0.22
$S_{l=1}$				1	≈ 0	-0.90
$\Gamma^\gamma_{l=1}$					1	≈ 0
$S_{l=2}$						1

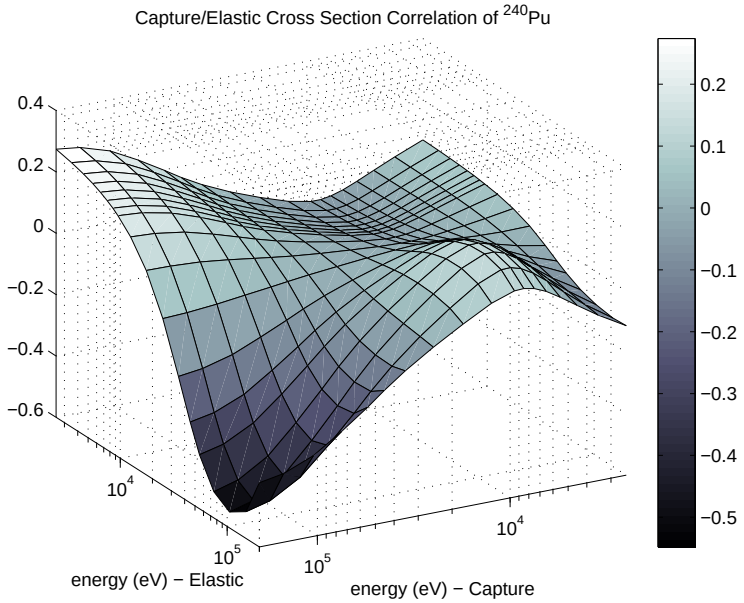
Uncertainties

Parameter	Value	Error	Relative Error (%)
D_0	13.43	0.7	5.2
$S_{l=0}(10^{-4})$	1.15	0.06	5.1
$\Gamma^\gamma_{l=0}$(meV)	19.9	2.1	10.7
$S_{l=1}(10^{-4})$	1.54	0.09	5.8
$\Gamma^\gamma_{l=1}$(meV)	15.4	3.1	19.9
$S_{l=2}(10^{-4})$	2.1	0.3	15.3

One can see that a complicated structure emerges from the Monte Carlo propagation for the covariance matrix. An interesting aspect here is the relative independence of the average radiative width with the strength functions. This is due to the fact that in our energy region, the indirect effects of strength function via neutron transmission values are negligible for the first orbital momenta because $T_n \gg T_\gamma$. A further development on this case could be done by going to higher energy values where higher orbital momenta contributions as well as inelastic scattering can produce non-negligible effects.

Using the preceeding covariance matrices, we realize a Monte-Carlo simulation of the correlated parameters and look at cross sections distributions. The Figure 1 shows the correlation obtained between Capture/Elastic cross sections as a function of energy for the [2.5 keV ; 200 keV] interval.

Figure 1: ^{240}Pu Capture/Elastic cross section correlations with Conrad



Negative correlations between capture and elastic cross sections appear at higher energies : at these energies, transmission coefficients for higher orbital momenta for the gamma neutron channel are comparable and they can compete in the HauserFeshbach formalism. Another example of cross section correlations is given in Figure 2.

2.5 Generalization

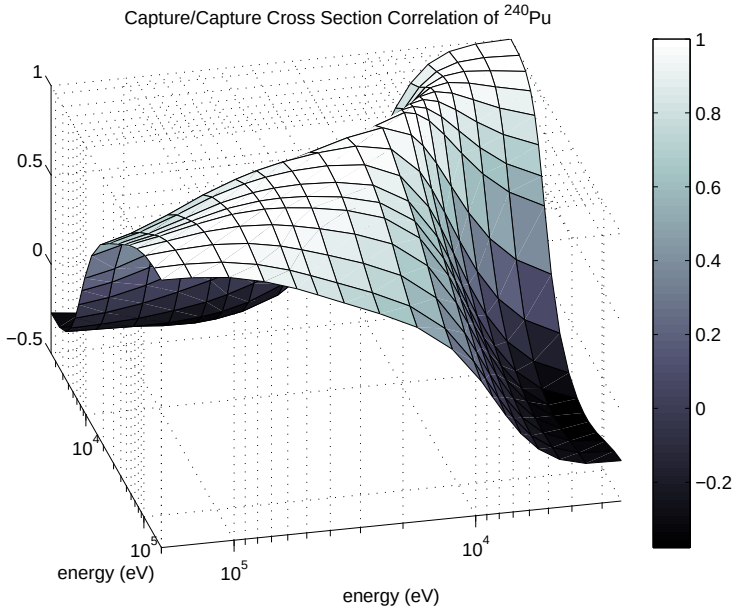
A general method of uncertainty propagation even with several kinds of data sets can be settled using the same kind of arguments previously exposed. Treating experimental data sets corresponding to cross section which exhibits different dependencies in the general parameter phase space is then possible without any ”fake” adjustment of low sensitive parameters. For the time beeing, the only assumption made is that all parameters have Gaussian distribution. As a result, the general calculation scheme is a sequential one:

1. adjust a set of parameter on a given experimental data set to obtain a first covariance matrix ;

2. apply the technique on sampling the covariance matrix using a Cholesky decomposition and for each sample adjust another set of parameters to obtain a growing covariance matrix ;

3. go to the second step if necessary.

Figure 2: ^{240}Pu Capture/Capture cross section correlations with Conrad



3. Conclusion

The method employed in this paper makes an extensive use of Monte Carlo sampling and can be of interest :

- for propagating uncertainties of non-adjusted parameters, which can be model parameters but also parameters coming from experimental setup such as normalization, etc ...,
- for the treatment of different experimental data sets to find the general covariance matrix on all the parameters.

Several lessons can be taken from this first study :

- the evaluation of primer experimental uncertainties is fundamental for this method (as well as any kind of methods) and therefore should be done properly,
- the model parameters for the calculation of average cross section in the unresolved resonance energy range are strongly tied by the functional form.

One can notice that the generalization of this method is possible in the parameter estimation process of nuclear models for cross sections in the resolved resonance energy range. Furthermore, the method can be generalized with a much more complicated Monte Carlo engine to treat non-gaussian parameters. The last important thing is that the software tool CONRAD by using an open object-oriented architecture allows an easy use of Monte Carlo sampling to propagate uncertainties.

Appendix : the total covariance theorem

Let Z_1, Z_2 and Z_3 denote three continuous random variables. First of all, let us write the following classical equality, called the total expectation theorem:

$$\mathbb{E}[\mathbb{E}(Z_1 \,|Z_2)] = \mathbb{E}(Z_1) \tag{6}$$

This formula can be shown using the Fubini's theorem and the Bayes formula [9]. A more theoretical demonstration is given in Ref. [10]. This theorem is a very powerful tool to calculate the expectation of a complex probability law but whose conditional probability laws are simple.

Another formula, called the total variance theorem, consists in decomposing the variance of a random variable with its conditional variance and its conditional expectation:

$$\mathrm{var}(Z_1) = \mathbb{E}[\mathrm{var}(Z_1 \,|Z_2)] + \mathrm{var}[\mathbb{E}(Z_1 \,|Z_2)] \tag{7}$$

In this paper, we use a covariance decomposition thanks to its conditional covariance and conditional expectation. By analogy with the formula (7), we called it the total covariance theorem:

$$\mathrm{cov}(Z_1, Z_2) = \mathbb{E}[\mathrm{cov}(Z_1, Z_2 \,|Z_3)] + \mathrm{cov}[\mathbb{E}(Z_1 \,|Z_3), \mathbb{E}(Z_2 \,|Z_3)] \tag{8}$$

The demonstration of this formula is similar to that of the total variance theorem. We thus give only the demonstration of the total covariance theorem:

$$\begin{aligned}
\mathbb{E}[\mathrm{cov}(Z_1, Z_2 \,|Z_3)] &= \mathbb{E}[\mathbb{E}(Z_1 Z_2 \,|Z_3) - \mathbb{E}(Z_1 \,|Z_3)\mathbb{E}(Z_2 \,|Z_3)] \\
&= \mathbb{E}[\mathbb{E}(Z_1 Z_2 \,|Z_3)] - \mathbb{E}(Z_1)\mathbb{E}(Z_2) \\
&+ \quad \mathbb{E}(Z_1)\mathbb{E}(Z_2) - \mathbb{E}[\mathbb{E}(Z_1 \,|Z_3)\mathbb{E}(Z_2 \,|Z_3)] \\
&= \mathbb{E}(Z_1 Z_2) - \mathbb{E}(Z_1)\mathbb{E}(Z_2) \\
&+ \quad \mathbb{E}[\mathbb{E}(Z_1 \,|Z_3)]\mathbb{E}[\mathbb{E}(Z_2 \,|Z_3)] - \mathbb{E}[\mathbb{E}(Z_1 \,|Z_3)\mathbb{E}(Z_2 \,|Z_3)] \\
&= \mathrm{cov}(Z_1, Z_2) - \mathrm{cov}[\mathbb{E}(Z_1 \,|Z_3), \mathbb{E}(Z_2 \,|Z_3)]
\end{aligned}$$

This last equation is equivalent to Eq. (8).

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