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Producing uncertainties and covariance matrix from intermediate data using a Monte-Carlo method.

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Abstract. The necessary improvement of evaluated nuclear data for nuclear applications development is possible through new and high quality experimental measurements. In particular, improving (n, n') cross section evaluations for fast neutrons is a goal of interest for new reactor fuel cycles, such as $^{232}\text{Th}/^{233}\text{U}$ or $^{238}\text{U}/^{239}\text{Pu}$. Our group at CNRS-IPHC developed an experimental program to measure $(n, n'\gamma)$ cross section using prompt γ -ray spectroscopy and neutron energy determination by time-of-flight with a focus on reaching the highest achievable level of accuracy. The collected partial cross sections can then be used to infer the total (n, n') one and contribute to evaluation improvement. The extraction of the exclusive $(n, n'\gamma)$ cross sections from the recorded data involves using many parameters and processing that may introduce uncertainties and correlations. In that case, the usual method for combining and computing uncertainties based on the perturbation theory can be long and complex. It also makes the calculation of covariance hard and the inclusion of some unusual forms of uncertainty even more difficult. To overcome this issue, we developed a process relying on random sampling methods that processes intermediate analysis data to compute cross sections, uncertainties and covariance. As a benchmark, we used this Monte Carlo method on ^{232}Th , ^{233}U and ^{238}U data and reproduced the central values and uncertainties calculated using the analytical method, while also producing covariance matrices for $(n, n'\gamma)$ cross sections. For particular cases, the random sampling method is able to produce uncertainties that better reflect the input data, compared to the analytical method.

1 Introduction

We present this work in the context of studying inelastic neutron scattering cross sections by γ spectroscopy [1–3]. These inelastic reactions are of strong interest for nuclear applications, as they modify the number and the energy of the neutrons in the reactor core. The CNRS-IPHC group is running an experimental program with the GRAPhEME [4, 5] setup installed at the neutron beam facility GELINA [6], operated by the EC-JRC in Geel (Belgium) to measure $(n, xn\gamma)$ reaction cross sections. Data for isotopes such as ^{232}Th [7], ^{235}U [8], ^{238}U [9], $^{182,184,183,186}\text{W}$ [10–12] have been recorded and analyzed. The experimental setup is made up of four High Purity Germanium detectors surrounding the target of interest and a fission

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chamber upstream. The neutron flux is determined using the fission chamber [13]. The energy of the reacting neutrons is calculated from their time of flight. At a given neutron energy, for each γ -ray detector, an angular differential reaction cross section at the corresponding angle is obtained by computing the ratio of specific γ rays (thus selecting the reaction channel) to the number of neutrons, with scaling parameters derived from quantities such as detection efficiency, target mass and density (equation 1). The angle integrated cross section is computed from the different differential ones, using the Gaussian quadrature method [14], as described by equation 2.

The GRAPhEME setup is designed to maximize the precision of measurements. Indeed, it is important to produce cross section values with the lowest achievable uncertainties. In addition, the evaluation of the experimental data requires the production of covariance matrices.

When producing $(n, n'\gamma)$ differential cross sections, one computes the partial cross section at an angle θ with

$$\frac{d\sigma_\gamma(E_n)}{d\Omega}\Big|_\theta = \frac{1}{4\pi} \times \frac{N_\gamma(E_n)_\theta}{\epsilon_\gamma} \times \frac{1}{N_{\text{target}}} \times \frac{\epsilon_{\text{FC}}}{(1 - L_n)N_n(E_n)} \quad (1)$$

Where $N_\gamma(E_n)_\theta$ is the number of detected γ rays at the angle θ for incoming neutrons of energy E_n , ϵ_γ the detection efficiency of the HPGe detector for this γ ray energy, N_{target} the areal density of scattering nuclei in the target, ϵ_{FC} the detection efficiency of the fission chamber, L_n the fraction of neutrons lost between the detecting fission chamber and the studied target, and $N_n(E_n)$ the number of detected neutrons by the fission chamber at energy E_n .

The angle integrated cross section is obtained by summation of two partial cross sections at precise angles:

$$\sigma_\gamma(E_n) = 4\pi \left(w_{110^\circ} \times \frac{d\sigma_\gamma(E_n)}{d\Omega}\Big|_{110^\circ} + w_{150^\circ} \times \frac{d\sigma_\gamma(E_n)}{d\Omega}\Big|_{150^\circ} \right) \quad (2)$$

Where $w_{110^\circ} = 0.6221$ and $w_{150^\circ} = 0.3479$ are the Legendre coefficients at angle 110° and 150° [14].

In our experimental setup, there are four possible couples of 110° and 150° detectors and therefore four different ways to compute the final cross section. In the analytical method, the final value is obtained by averaging first the partial cross sections at an angle together and then computing the angle integrated value. This will have an impact on the uncertainty as the analytical method does not include a way to account for deviation between partial cross sections at the same angle (because different detectors at the same angle have different ranges, thresholds, saturation cut-off).

2 Producing covariance and uncertainty

With so many parameters, different kind of uncertainties and correlations, the usual analytic formula derived from perturbation theory ($u_{f(x_1, x_2, \dots, x_i)} = \sum_j \left(\frac{\partial f}{\partial x_j} \right)^2 u_{x_j}^2 + \sum_{j \neq k} 2 \frac{\partial f}{\partial x_j} \frac{\partial f}{\partial x_k} u_{x_j} u_{x_k}$) becomes very complex and may not be enough to take correctly into account all sources of uncertainties in the calculation (for example timing uncertainty will, in that case, mix events from different neutron energies in the same time bins [15]).

We propose here a way to compute the cross section from intermediate quantities (N_γ , ϵ_γ , N_{target} , L_n , N_n and ϵ_{FC}) along with their uncertainties, using them as inputs in a Monte-Carlo code. Each input parameter will be randomly selected according to its distribution law (mostly Gaussian, sometimes uniform distribution around a value, ...). For each realization

of the parameters, the variable values are used to calculate just one value of the final cross section. This is done many times, and, in the end, the series of values are used to compute a central (mean) value with uncertainty (standard deviation of the series) and correlations.

3 Method

This work method is very similar to the one described in chapter 4 of reference [16]. The processing code is written in python 3.6 [17], using numpy [18] and matplotlib [19] as external library for numerical calculations and representation. A Monte Carlo Variable object [20] and a data file reader [21] were also used.

Random variables values are drawn following their distribution law (either normal or uniform) at the start of each iteration, with extra checks to ensure that they stay positive and non-zero when required (for efficiencies, values also cannot be larger than 1). For the number of detected γ rays (N_γ) and neutron events (N_n), a normalization constraint was applied to ensure that the sum of the random values at each energy is compatible with the sum of values given as input (within uncertainties). This is done by drawing random values from the cumulative distribution along randomly shuffled indices, rather than independently using a random variable for each point. The cross section for each detector is then computed using these values, and finally, the angle integrated cross section is calculated for each (110° , 150°) couple. Each couple produces one result. All the calculated results are added to a numpy.array as a new column. In the end, the central values, standard deviation, covariance and correlation matrices is computed.

We note that with this method, the difference between statistical and systematic uncertainties vanishes: all sources of uncertainty are parameters of the code. It is up to the user to correctly define the probability distribution of each variable to reflect their nature and behavior.

3.1 Computing resources cost

The CPU time and memory cost needed to make the calculations was determined using the GNU time tool [22] on a CentOS 7.9 [23] 64-bits machine with sixteen 3.2 GHz CPUs¹ and a total of 32 GB available memory. The memory footprint of the program is proportional to the number of iterations: each iteration adds the same amount of data into the collection of events to process in the end. The software runtime is mostly linear with the number of iterations. There is a small quadratic component due to the increased memory stewardship for any extra iteration, as well as increased processing time for the final step. Typical runtime of the software is just above one minute for 5000 iterations.

3.2 Convergence

To check the convergence of the statistical calculation, we look at the mean and standard deviation of the computed result as the number of iterations increases. After about 1000 iterations, the results converge closer to the final value, with residual variations much smaller than the final uncertainty (see [24]). The uncertainty values converges in the same manner, requiring more iterations (about 2000 to 5000 depending on the processed data set) to keep within a small enough range. Therefore, we decided to keep a minimum of 2000 as the reference number of iterations.

¹Python code is always executed in single thread.

4 Results

Since we are using intermediate files from a full analysis using analytical method, we directly compare our Monte Carlo results to the values obtained with the first method. Figure 1 shows two examples of cross sections computed using both analytical and partial Monte-Carlo methods. Other examples with data for ^{233}U can be seen in [24, 25]. We observe that central values between the two methods are very close to each others, with differences smaller than the uncertainties. The uncertainties are of the same order of magnitude. Differences between uncertainties may be linked to the correlated random sampling described above that maintains the normalization of the reference distribution (within uncertainties), leading to larger spread for points with the smallest yields, as well as the differences between methods, that we will discuss below.

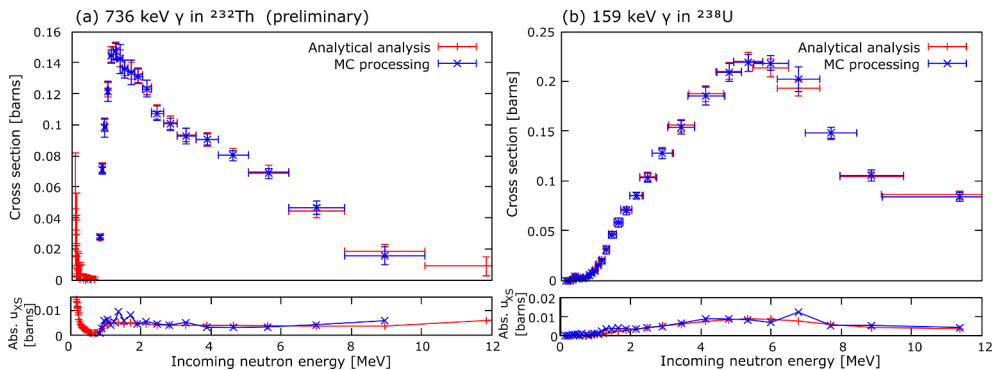


Figure 1. Comparison of $(n, n' \gamma)$ cross sections computed using the analytical method (red) and partial Monte Carlo method (as described in this paper) (blue) for (a) the 736 keV γ -ray in ^{232}Th (preliminary results) and (b) the 159 keV γ -ray in ^{238}U [1]. The smaller bottom panels show the absolute uncertainties in barns.

4.1 Taking into account complex sources of uncertainties

In the case of the 159 keV γ -ray in ^{238}U (panel (b) of figure 1), we observe a structure in the uncertainty, around 6-8 MeV, that does not appear in the analytical treatment. It is unexpected, particularly in regards to the overall agreement between central values and uncertainties at other energies and for other transitions. Upon inspection of the input given to the Monte Carlo processing, this structure actually reflects variations in the differential cross sections computed for different detectors used in the weighted summation to compute the angle integrated cross section. Figure 2 shows the four differential cross sections used. The difference between the blue and gray line (corresponding to two detectors at 110°) in particular is due to correction for timing uncertainty. It leads to a spread in the calculated cross section depending on which one of these two detectors is used when summing. That will automatically increase the standard deviation of points at 6.7 MeV in particular. That explains the high value point for the uncertainty at this energy. (The timing uncertainty at the source of this could be accounted for in a total Monte Carlo method, but not with an analytical or partially Monte Carlo one.) When combining the detectors to produce the angle integrated cross section, the analytical method *averages out* the spread and the computed uncertainty misses this particular feature. In the end, for such cases, the uncertainty from the Monte-

Carlo method may be larger, but reflects better the reality of the data than with the analytical method that underestimates the uncertainty.

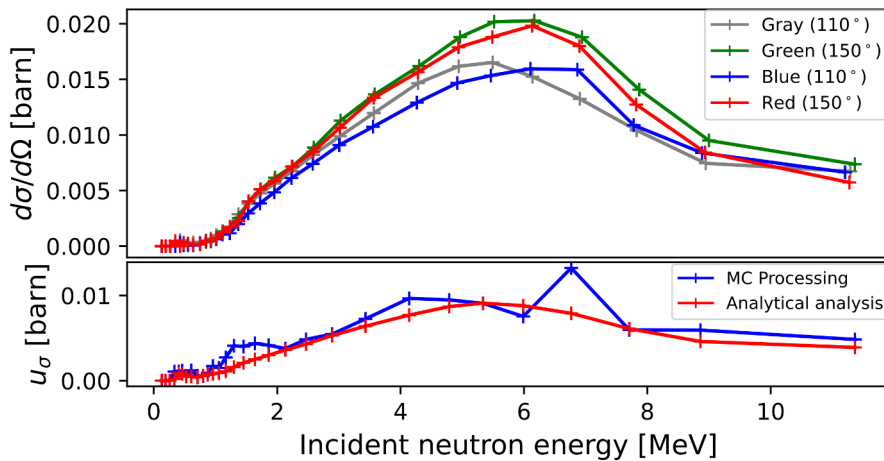


Figure 2. Differential cross sections for the 159 keV γ -ray in ^{238}U calculated with the analytical method [1]. The bottom panel shows the computed uncertainty on the angle integrated cross section using the Monte Carlo method (blue) and analytical method (red).

4.2 Covariance matrix

Since the analytical method does not produce covariance, it is not possible to compare the matrices produced with the Monte-Carlo method to a reference (Figure 3). However, from the expected shape of the data, and the knowledge of the experimental setup, we have certain expectations. The number of scattering centers in the target is the dominant uncertainty in our analysis and a shared parameter between all points, so the mostly positive correlation is expected. Structures in the 159 keV γ -ray in ^{238}U correlation matrix (Figure 3, right) reflects the observed spread of data in the differential cross section at 110° discussed earlier in part 4.1. As the Th data is preliminary, we do not comment on it at this time.

In the end, we believe that the differences in final values and uncertainties are not larger than what it would be between two independent analysis using different toolkits. The interest of the method is that it produces covariance data without implementing a long and complex mathematical formula, and it checks for possible sources of uncertainty not properly taken into account.

5 Conclusion and perspective

The Monte Carlo method on intermediate analysis files works and gives similar values to the one that are computed with the analytical method. The final values are compatible between the two methods, and the uncertainties are within a 10 % range of each other, which is a reasonable level of divergence between the two analysis strategies. In addition, we determined that some deviations between the Monte-Carlo and analytical methods may be a consequence of a source of uncertainties or correlations that are not implemented in the analytical method.

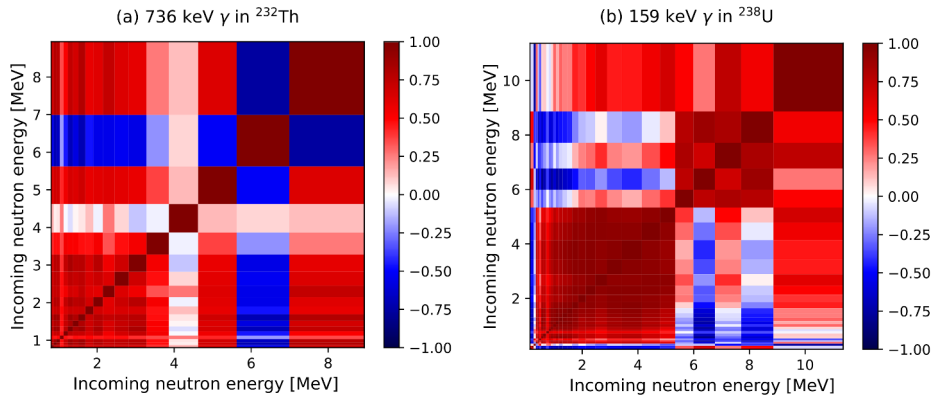


Figure 3. Correlation matrices of the $(n, n'\gamma)$ cross section, computed with the Monte Carlo method, for (a) the 736 keV γ -ray in ^{232}Th (preliminary results) and (b) the 159 keV γ -ray in ^{238}U .

The ability to simply turn *off* or *on* uncertainties in the Monte Carlo code makes it easy to study the impact of one particular source of uncertainty on the final values. This is something that has not been fully studied yet, but will help us understand our result better in the future, as well as target the relevant source of uncertainty to increase the precision of our work.

In conclusion, this partial Monte-Carlo analysis, using intermediate results to produce the final values, total combined uncertainties, and covariance matrix, produces comparable results as the analytical one, with the addition of correlation information and can even take into account some less evident sources of uncertainty out of the box. It is a good compromise between full analytical or full Monte-Carlo methods.

The use of intermediate results from previously finalized analysis highlights the importance of keep this kind of data file available even after the results has been published and reinforce the importance of data archiving and open data strategy.

As the code is application specific, there is no plan, as of today, to publish it as an Open Source project. It might be part of future release of experimental results obtained using this method in an Open Science approach. However, the key code elements are either part of publicly available library (numpy [18], matplotlib [19], Monte-Carlo Variable [20], data file reader [21]).

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