Prior estimation of covariance matrix of reaction cross sections using Unscented Transform Method

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Introduction

Nuclear data with complete uncertainty information is of great importance for designing and running of nuclear facilities. Uncertainty information in the form of error bars is not sufficient for application part, therefor for more accurate calculations we also need covariance information of nuclear data. To evaluate nuclear data we need a prior estimate and then new experimental measurements can be combined with the prior estimate to give new evaluated data. In evaluation process prior estimate can be given using theoretical models or a prior evaluation of experimental data. These days different nuclear reaction codes are commonly used to give a prior estimate, and uncertainty in theoretical model parameters are propagated by using Monte Carlo (MC) method through the codes [1]. But such methods involve a very large number of calculations before it can produce satisfactory results. In present study, we have used Unscented Transform (UT) method [2] instead of Monte Carlo method to propagate uncertainty of nuclear model parameters through nuclear reaction code TALYS 1.9 [3]. UT is a deterministic method and uses very less calculations as compared to Monte Carlo method. We have presented some of our preliminary results for $^{60}Ni(n,p)^{60}Co$ reaction, we have propagated uncertainties of optical model parameters through TALYS 1.9.

General Unscented Transform Method

In this method, instead of using random numbers, we use well calculated deterministic sigma points. Consider a primary variable vector x with mean vector $\bar{x}$ and covariance matrix P. If we find a set of deterministic vectors called sigma points whose ensemble mean and covariance are same as that of x . Then we can use these sigma points on the known nonlinear functional relationship $(y = f(x))$ to obtain m dimensional transformed vectors y, and then we can calculate mean and covariance of transformed vectors. Consider x is an $n \times 1$ vector. We choose $2n + 1$ sigma points $(x^{(i)})$ as: $x^{(0)} = \bar{x}$; $x^{(i)} = \bar{x} + \widetilde{x}^{(i)}$ for $i = 1, 2, 3...2n$

where

$$\widetilde{x}^{(i)} = \sqrt{(n + k)P}$$

for $i = 1, 2, 3...n$
and

$$\widetilde{x}^{(i+n)} = -\sqrt{(n + k)P}$$

for $i = 1, 2, 3...n$

$2n + 1$ transformed vectors $(y^{(i)})$ are then calculated using these sigma points by applying them to the functional relationship. The vector of means and covariance matrix are given as

$$\bar{y} = \sum_{i=0}^{2n} W^{(i)} y^{(i)}$$

$$Cov = \sum_{i=0}^{2n} W^{(i)}(y^{(i)} - \bar{y})(y^{(i)} - \bar{y})^T$$

where $W^{(0)} = \frac{k}{n+k}$ and $W^{(0)} = \frac{1}{2(n+k)}$ are weighting coefficients. Here k is parameter and for Gaussian distribution n+k=3.

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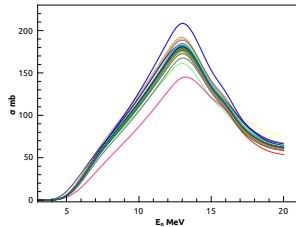
FIG. 1: Different outputs of TALYS 1.9 for $^{60}Ni(n,p)$ corresponding to different sets of input parameters produced by using unscented transform.
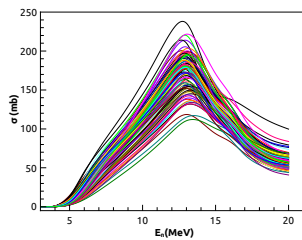

FIG. 2: 100 outputs of TALYS1.9 for $^{60}Ni(n,p)$ corresponding to 100 sets of random input parameters.

Calculation of covariance using TALYS

We selected $^{60}Ni(n,p)$ reaction as our test case, first of all we adjusted optical model and level density parameters to fit the available experimental data of this reaction. We made a list of optical potential parameters of ^{60}Ni with neutrons and ^{60}Co with protons. Un-
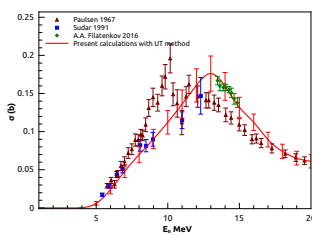

FIG. 3: Present calculations in comparison with some experimental data from EXFOR.
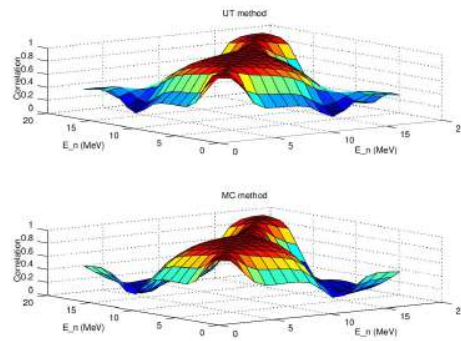

FIG. 4: Correlation matrices for $^{60}Ni(n,p)$ reaction calculated using UT and MC method.

certainty of these parameters were taken from ref. [1]. Then we have transformed these parameters using UT and calculated $^{60}Ni(n,p)$ cross sections using TALYS 1.9 for each set of parameters, results are presented in Fig. 1. From ensemble of outputs we calculated mean and covariance matrix using equations given above, calculated mean in comparision with experimental data from EXFOR is presented in Fig. 3. For comparison with Monte Carlo method we also did the same calculations using MC method for 100 trials, results are presented in Fig. 2. Random input parameters were generated in MATLAB according to their mean and uncertainty values considering normal distribution. Methodology for Monte Carlo calculations can be found in ref.[1]. In Fig. 4, we have compared the correlation matrices calculated by UT and MC method. This study is just a proof of concept that UT can also be used instead of MC to give prior estimations of covariance matrices. Further in this study uncertainties for a number of input parameters will be considered to give more accurate estimates.

References

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