Letter

Deterministic sampling approach for the propagation of uncertainties in nuclear reaction models

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Uncertainty propagation of model parameters through nuclear reaction models is critical for nuclear data evaluation and other applications. Nuclear reaction models generally contain nonlinear functions of the model parameters, making the process of uncertainty propagation difficult. Usually stochastic approaches like the Monte Carlo method are employed to propagate the uncertainties through nuclear reaction models. The Monte Carlo method does provide proper results, but it takes a lot of computational power and time, which makes the process of uncertainty propagation difficult. Deterministic sampling approaches may provide results with accuracy using less computational time making the process of uncertainty propagation fast. In this study we have explored the use of a deterministic sampling approach called the unscented transform method for the uncertainty propagation in the nuclear reaction models. As a test case we have propagated the uncertainties of correlated optical model parameters through the optical model calculations for total and reaction cross sections of the $n + {}^{56}$Fe reaction. The results obtained using the unscented transform method are then compared with the results of the Monte Carlo method. It has been observed that the unscented transform method provides results practically similar to the Monte Carlo method in less computational time. It is concluded in this study that the unscented transform method can propagate uncertainties effectively through optical model calculations and there should be further investigation of the use of this method for other nuclear reaction models.

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Nuclear reaction data of good quality with a covariance matrix are crucial for safer and more advanced nuclear facilities, and this field has seen much progress in the past few decades [1–3]. Experimental measurement of nuclear reaction observables like cross sections, angular distributions, differential cross sections, etc., is a challenging and expensive task. Measuring all the physical quantities experimentally for a variety of nuclear reactions over a wide range of projectile energies is not feasible. Also some reactions of high importance may be impossible to measure directly due to the unavailability of targets or projectiles [4–6]. Therefore the use of the theoretical models is inevitable in this kind of situation, also such theoretical models are regularly used to interpolate and extrapolate the data in the absence of the experimental measurements, making them an integral part of the nuclear data evaluation [1,7]. Theoretical predictions are also associated with the uncertainties and may be correlated similarly to the experimentally measured data. These uncertainties can be attributed to different sources, e.g., uncertainties in the model parameters, uncertainties due to model deficiencies, algorithmic uncertainties, etc. [8,9]. Hence the quantitative knowledge of such sources of uncertainties and their effect on the final predictions of the model is very important.

In recent years there have been a renewed interest in the field of uncertainty quantification in low energy nuclear reactions [10–13]. Uncertainty quantification problems can be broadly classified into two categories, one is inverse problems; in which the model parameter uncertainties or model uncertainty itself are quantified using the well known final outcomes. The second is the forward problems, which are concerned with the determination of the uncertainties in the final outcomes of the models due to uncertainties in the input parameters [1]. In this study we will be focusing only on the forward uncertainty propagation of the model parameters. Input parameter uncertainties need to be propagated through nuclear reaction models, which generally contain nonlinear functions of the input parameters. When the statistical moments of the input parameters are known then there are two distinct approaches for calculating the statistical moment of the model outputs, these are the stochastic approach and deterministic approach [1,14]. In this study, we will be using a stochastic approach called the Monte Carlo method of uncertainty propagation, which provides accurate results even if the model functions are highly nonlinear [7,9]. In this method the input model parameters are sampled randomly from their joint probability distribution function and these random samples of the input parameters are then used to propagate the uncertainties through the theoretical model. But this method requires a very large number of random samples to be drawn so that it can give reliable results, which makes this method computationally expensive if the model calculations itself take large computational time. Deterministic sampling approaches may provide satisfactory results in less calculations as compared to the Monte Carlo method [15]. In this study we have also used a deterministic sampling approach called the unscented transform method [16–19]. This method was first proposed

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by Julier and Uhlmann for improving the performance of the Kalman filter in the presence of nonlinearities [16,18]. Since then this method has been used extensively in many fields of science and engineering successfully. There are different variants of the unscented transformation, and here we will be using the scaled unscented transform method [20,21]. In this method a few sample points (also called sigma points) are sampled using well defined deterministic equations and each sigma point is assigned with its corresponding weight. The weights and sigma points can be adjusted using an arbitrary scaling parameter to include information about the higher moments of the output probability distribution.

In this paper, we have propagated the optical model parameter uncertainties through the optical model calculations for the total and reaction cross sections of the $n + {}^{56}$Fe reaction for the neutron energies 1–20 MeV using the Monte Carlo and unscented transform methods. The final cross sections, their uncertainties, and correlation matrix obtained by using both methods are then compared to check the performance of the unscented transform (UT) method with respect to the Monte Carlo (MC) method.

Consider an n dimensional input vector $\mathbf{X}$ of correlated input parameters with $\mathbf{V}_x$ as their covariance matrix. Let $\mathbf{Y}$ be an m dimensional output vector derived from a collection of functions $y_k = f_k(\mathbf{X})$; $k = 1, 2, \ldots, m$; and $\mathbf{V}_y$ represents its covariance matrix. Generally such functions are nonlinear, and can be linearized by using the first two terms of the Taylor series expansion as

$$y_k \approx f_k(\mathbf{X}_0) + f_k'(\mathbf{X}_0)(\mathbf{X} - \mathbf{X}_0). \tag{1}$$

Here, $\mathbf{X}_0$ represents the vector of mean values of the input vectors, and the first term of the Taylor series expansion represents the mean of the output variables $\mathbf{Y}_0 = \mathbf{f}(\mathbf{X}_0)$. Then according to the general law of uncertainty propagation [14], we can write $\mathbf{V}_y \approx \mathbf{H}\mathbf{V}_x\mathbf{H}^T$, where $\mathbf{H}$ represents the Jacobian matrix of $\mathbf{Y}$ with respect to $\mathbf{X}$. This method does not provide satisfactory results if the functions are nonlinear, because then the higher order derivatives in the Taylor series will not be negligible [22]. Also calculating the Jacobian matrix and Hessian matrix is a cumbersome task if the functions are nonlinear. Hence, instead of using linearization, using the sampling methods reduces the need for the determination of derivatives.

In the MC method, a large collection of vectors $\mathbf{X}_l$ ($l = 1, 2, \ldots, L$) is sampled randomly from the joint probability distribution function of the input vector $\mathbf{X}$. Then an ensemble of the output vector $\mathcal{Y}_l^{\mathrm{MC}}$ is calculated [$\mathcal{Y}_l^{\mathrm{MC}} = \mathbf{f}(\mathbf{X}_l)$] corresponding to each randomly sampled input vector $\mathbf{X}_l$. From this ensemble, the mean ($\mathbf{Y}_0^{\mathrm{MC}}$) and covariance matrix of the output vector ($\mathbf{V}_{yij}^{\mathrm{MC}}$) can be calculated [14] as

$$\mathbf{Y}_0^{\mathrm{MC}} = \frac{1}{L}\sum_{l=1}^{L} \mathcal{Y}_l^{\mathrm{MC}}, \tag{2}$$

$$\mathbf{V}_{yij}^{\mathrm{MC}} = \frac{\sum_{l=1}^{L} (\mathcal{Y}_{li}^{\mathrm{MC}}\mathcal{Y}_{lj}^{\mathrm{MC}})}{L} - \mathbf{Y}_{0i}^{\mathrm{MC}}\mathbf{Y}_{0j}^{\mathrm{MC}}; i, j = 1, 2, \ldots, m. \tag{3}$$

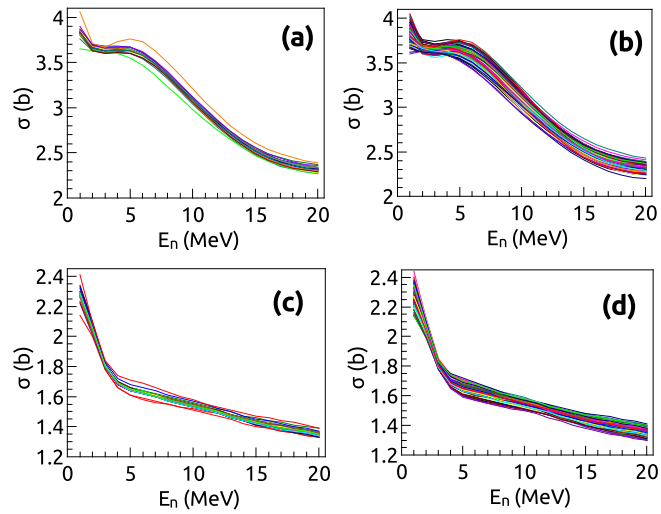

FIG. 1. Total and reaction cross sections calculated corresponding to the parameters sampled deterministically are presented in (a) and (c), respectively, calculated total and reaction cross sections corresponding to 100 out of 1000 random samples of parameters used in this study are presented in (b) and (d), respectively.

This method is robust against the nonlinearities and also provides complete information about the probability distribution function of the output vector. The results of this method are not unique as the mean and covariance are functions of the number of samples, hence in order to achieve the better convergence a large number of samples should be used.

In the UT method instead of using random samples, $(2n + 1)$ sigma points ($\boldsymbol{\chi}_i$; $i = 0, 1, \ldots, 2n$) are sampled from the input vector $\mathbf{X}$ using deterministic equations. The transformation equations [20,21] are as given below:

$$\begin{aligned}
&\boldsymbol{\chi}_0 = \mathbf{X}_0,\\
&\boldsymbol{\chi}_i = \mathbf{X}_0 + (\sqrt{(n+\lambda)\mathbf{V}_x})_i \quad (i = 1, \ldots, n),\\
&\boldsymbol{\chi}_i = \mathbf{X}_0 - (\sqrt{(n+\lambda)\mathbf{V}_x})_{i-n} \quad (i = n+1, \ldots, 2n).
\end{aligned} \tag{4}$$

Here, $\lambda = \alpha^2(n + \kappa) - n$. The matrix square root in above equations can be calculated using algorithms like Cholesky decomposition, which is numerically stable. Every sigma point $\boldsymbol{\chi}_i$ is assigned with its corresponding weight [21] using the following equations:

$$W_0^{(m)} = \lambda/(n + \lambda), \tag{5}$$

$$W_0^{(c)} = \lambda/(n + \lambda) + (1 - \alpha^2 + \beta), \tag{6}$$

$$W_i^{(m)} = W_i^{(c)} = 1/\{2(n + \lambda)\} \quad (i = 1, \ldots, 2n). \tag{7}$$

The parameters α, β, and κ are called the scaling parameters. The value of α controls the spread of the sigma points around the mean value of the parameter, the secondary scaling parameter κ also determines the spread of the sigma points. If the number of parameters involved in the calculations is large ($n > 3$) then κ is generally set to be zero and the value of α varies between $1 \geqslant \alpha \geqslant 10^{-4}$. The value of β does not effect the sigma points but rather it incorporates information about the probability distribution function of the input parameters

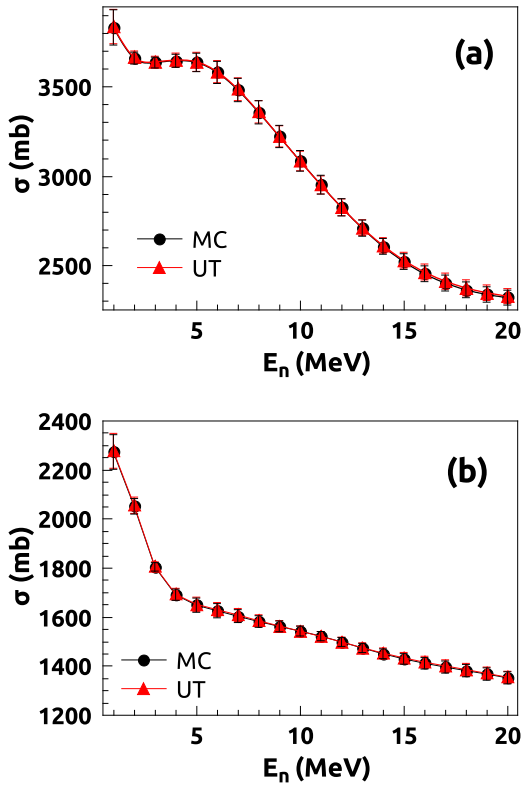

FIG. 2. (a) Mean and standard deviation of total cross sections calculated using the MC and UT method. (b) Mean and standard deviation of reaction cross sections calculated using the MC and UT method.

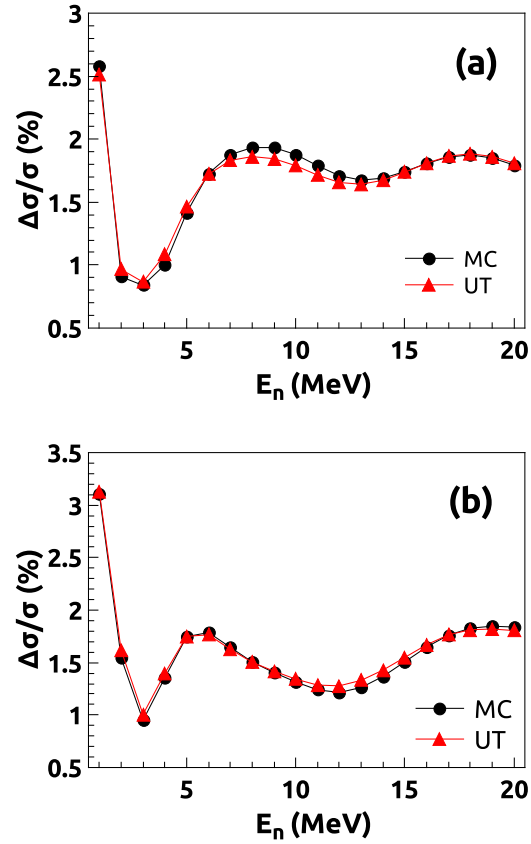

FIG. 3. Fractional uncertainties in the total and reaction cross sections calculated using the UT and MC methods are presented in (a) and (b), respectively.

by including the contributions from higher order moments of the parameters in the covariance of the output vector. Weights represented by the superscripts 'm' and 'c' are used for calculating the mean and covariance matrix, respectively. Then an ensemble of $(2n+1)$ output vectors is calculated corresponding to each sigma point; $\mathcal{Y}_i^{UT} = \mathbf{f}(\boldsymbol{\chi}_i)$, $i = 0, \ldots, 2n$. The mean and the covariance matrix of the output vector can be calculated using the following equations:

$$\mathbf{Y}_0^{UT} = \sum_{i=0}^{2n} W_i^{(m)} \mathcal{Y}_i^{UT}, \tag{8}$$

$$\mathbf{V}_y^{UT} = \sum_{i=0}^{2n} W_i^{(c)} \left(\mathcal{Y}_i^{UT} - \mathbf{Y}_0^{UT}\right)\left(\mathcal{Y}_i^{UT} - \mathbf{Y}_0^{UT}\right)^T. \tag{9}$$

An optical model potential contains real and imaginary parts, which further contains volume central, surface central, and spin orbit parts

$$\mathcal{U}(r, E) = \mathcal{V}(r, E) - i\mathcal{W}(r, E). \tag{10}$$

There are different parametrizations available to represent the strength and shape of these parts [23–26]. We have used a common Woods-Saxon phenomenological optical model potential parametrization that has been used extensively in recent years [23].

In this study we have compared two approaches of uncertainty propagation as described above by propagating the optical model parameter uncertainties for the reaction and total cross section for the $n + {}^{56}$Fe reaction. Total and reaction cross sections are the basic observables in optical model calculations [27] and may be expressed as

$$\sigma_{\text{reaction}} = \frac{\pi\lambda\!\!\!^{-2}}{2} \sum_{lj} (2j+1)\left(1 - \left|S_l^j\right|^2\right), \tag{11}$$

$$\sigma_{\text{total}} = \pi\lambda\!\!\!^{-2} \sum_{lj} (2j+1)\left(1 - ReS_l^j\right). \tag{12}$$

Here, S_l^j represents S-matrix element, l and j represents the orbital and total angular momentum; for neutrons $j = l \pm 1/2$, and $\lambda\!\!\!^{-}$ is the reduced wavelength of the neutrons.

In our previous study [12], we have optimized the optical model parameters and their correlation matrix for $n + {}^{56}$Fe and some other reactions. It was concluded in Ref. [12] that the optical model parameters are correlated to each other, therefore in this study, we will be using the correlated optical model parameters and their covariance matrix calculated in Ref. [12] as our inputs for the optical model calculations. We have used TALYS-1.95 nuclear reaction code [28] for the optical model calculations.

We have used 18 energy independent optical model parameters. For propagating their uncertainties through optical model calculations using MC method, 1000 samples of 18 optical model parameters were randomly sampled from the

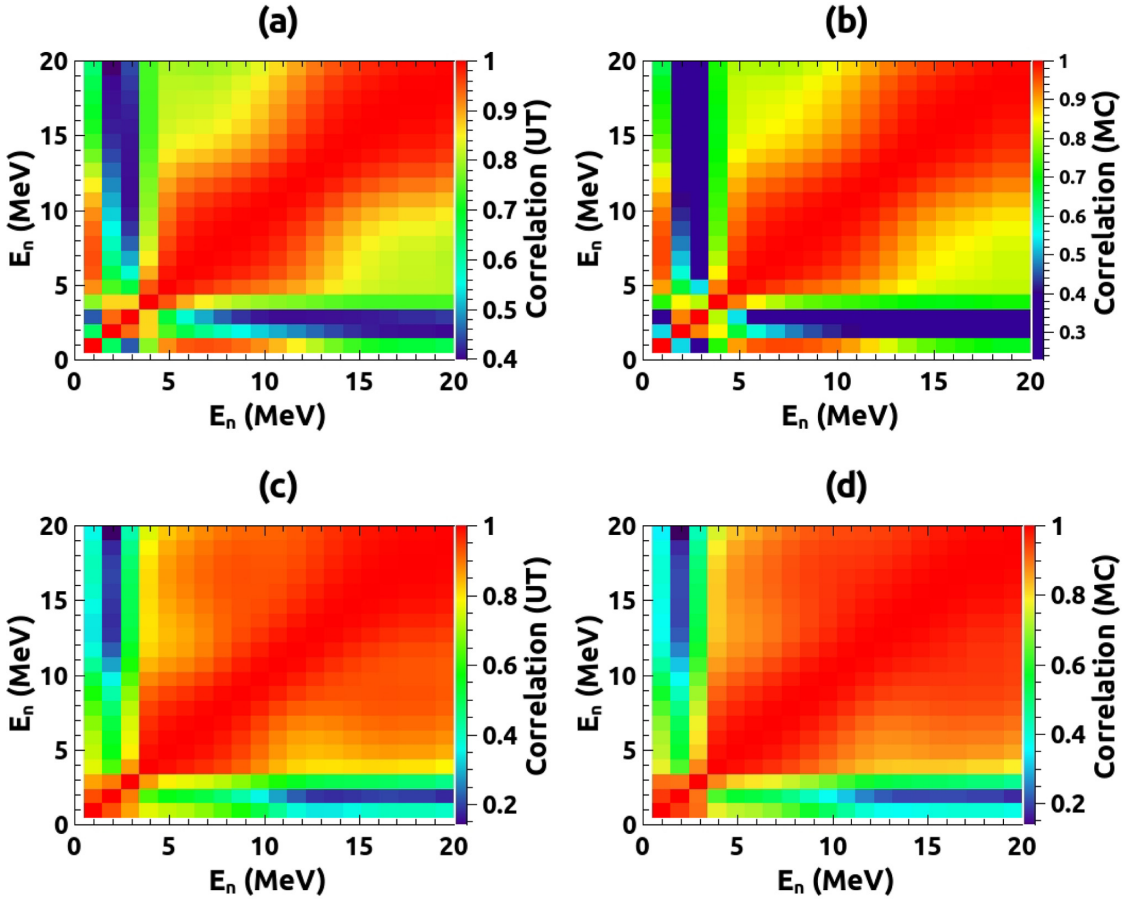

FIG. 4. Correlation matrix for total cross sections calculated using the UT and MC methods are presented in (a) and (b), respectively, and in (c),(d) the correlation matrix for reaction cross sections calculated using the UT and MC methods, respectively, is presented.

multivariate normal distribution functions. Then optical model calculations were performed for each random vector of optical model parameters and 1000 corresponding vectors of total and reaction cross sections for the neuron energy range 1 to 20 MeV were calculated. From this ensemble of total and reaction cross sections their mean and covariance matrix were calculated using Eqs. (2) and (3). Similarly for propagating these uncertainties using the UT method, 37 deterministic sigma points of 18 optical model parameters were generated using Eq. (4). We have used scaling parameters with values $\alpha = 0.55, \kappa = 0$, and $\beta = 0.177$ in this study. Then 37 vectors of total and reaction cross sections corresponding to each sigma point were calculated using optical model calculations. From the ensemble of cross sections the mean and covariance matrix of the cross sections were calculated using Eqs. (8) and (9).

We have performed an uncertainty propagation of the optical model parameters as described above. The total cross sections and reaction cross sections for the $n + {}^{56}$Fe reaction corresponding to 37 sigma points of optical model parameters obtained using UT are presented in Fig. 1(a) and 1(c), respectively. Also the optical model results for the total and reaction cross sections corresponding to 100 out of 1000 random vectors of optical model parameters have been shown in Fig. 1(b) and 1(d), respectively, for more clarity. These figures represent the ensemble of the model outputs which are highly correlated and information about the statistical moments of the cross sections can be extracted from them. From the ensembles of reaction and total cross sections obtained using the MC and UT methods, the mean and covariance matrix of the cross sections were calculated. Total and reaction cross sections along with their standard deviations have been presented in Fig. 2(a) and 2(b), respectively. The results obtained using the MC method have been presented by black dots, while results of the UT method are presented using red triangles. These results show that the UT method provides results similar to that of the MC method. Calculation time for a single run for the present problem in TALYS-1.95 take ≈25 s, in MC method time required for 1000 runs is ≈25000 s or ≈416 min, while the calculation time using UT method is ≈925 s or ≈15 min only. This difference in the computational time of two approaches will be more drastic if the model calculations themselves take computational time of minutes or hours. The difference between the MC and UT results for total cross sections are between 0.1 mb to 11 mb (the results of the UT method differ from the MC method between 0.02% to 0.46% for total cross sections). Also the deviations of the uncertainties for total cross sections from these methods differ to each other in the range of 0.007 to 3 mb. Similarly for reaction cross sections the results from the two methods differ

in the range of 0.001 mb to 5 mb (results of the UT method differ from that of the MC method by 0.006 to 0.34 %) also the uncertainties deviate from each other by 0.01 mb to 1.5 mb.

We have also calculated the fractional uncertainties $[\Delta\sigma/\sigma(\%)]$ in the total and reaction cross sections for both MC and UT methods and are presented in Fig. 3. From Fig. 3 it is clear that the fractional uncertainties calculated using the UT method are very close to those calculated using the MC method. The difference between fractional uncertainties calculated from two methods for total cross sections is between 0.001 to 0.09 and for reaction cross sections it differs between 0.003 to 0.07. From the ensemble of outputs the covariance matrix for total and reaction cross sections were also calculated. From these covariance matrices, we calculated the correlation matrix of the cross sections. The correlation matrix calculated using the MC and UT methods for total and reaction cross sections have been presented in Fig. 4(a), 4(b), 4(c), and 4(d). These figures clearly show that the cross sections are correlated to each other and also the correlation matrices calculated by using both the methods show the same structures. The correlation coefficients calculated using both methods for total cross sections [Fig. 4(a) and 4(b)] are comparable and the maximum difference between them is 0.19. Also the correlation matrix from both methods for reaction cross sections [Fig. 4(c) and 4(d)] is comparable and the maximum difference between the correlation coefficients is 0.04. The rapid change in the correlations for neutron energies below ≈4 MeV can be attributed to the sensitivity of the total and reaction cross sections to the perturbations in the optical model parameters [29].

In the present study the uncertainties of the optical model parameters have been successfully propagated through optical model calculations using the UT method and MC method for the $n + {}^{56}$Fe reaction. The cross sections, their uncertainties, and correlation matrix calculated using both methods have been compared. It is found that the total and reaction cross sections show positive correlations among themselves. It is also established in this study that, although the UT method takes less calculation time in comparison to the MC method, yet the mean, uncertainties, and the correlation matrix of the cross sections are comparable to the MC method. This study successfully demonstrated that the UT method can be used for calculating the estimated cross sections and their covariance matrix with good accuracy in few calculations. This study also advocates for the further investigation of the UT method for propagating the uncertainties in other nuclear reaction models of interest.

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