Uncertainty quantification in optical model calculations using deterministic sampling method

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Introduction

Nuclear reaction data of good quality with complete uncertainty information is important for the future nuclear technologies [1, 2]. There have been efforts for improving the theoretical models in order to produce more reliable data to meet this high demand. Just like the experimental data [2, 3], theoretical predictions are also associated with the uncertainties. These uncertainties are due to different sources, e.g. uncertainties in the model parameters, model itself may be not accurate etc. The uncertainty quantification can be classified in two parts, forward problems and inverse problems. Forward problems are well posed while the inverse problems are ill posed, therefore they are more difficult to deal with. In this study, we have tried to answer both of these problems using a deterministic sampling method called Unscented Transform (UT) [4]. We have used Unscented Transform Kalman filter for the inverse problem, i.e. determining the model parameters and their associated uncertainties from the available experimental data. We have also propagated the parameter uncertainties through the reaction model using UT method for determining the uncertainties in the final result. Results of the UT method are also compared to the the Monte Carlo (MC) method.The main advantage of using deterministic sampling approach is that it uses far less calculations as compared to the Monte Carlo approaches of uncertainly quantification. In this study we have used optical model calculations for elastic differential cross section of p+^{48}Ca at energies 12 and 9 MeV as the test case.

Methodology

Experimental data for p+^{48}Ca elastic scattering at energies 12 and 9 MeV was retrieved from the EXFOR data library. For the DWBA calculations, we have used TALYS nuclear reaction code. We have used the global optical model parameters of Koning and Delaroche as our initial estimates of the parameters. We then employed Unscented Transform Kalman filter technique for the optical model parameters optimisation. Complete procedure of the optimisation can be found in our recent study Ref. [5]. This method provides the new better estimates of the optical model parameters and their covariance matrix. We then propagated this covariance matrix through the DWBA calculations using UT and MC method. For UT method, we sampled 39 sigma points corresponding to the 19 input parameters deterministically and then calculated the elastic differential cross sections corresponding to each sigma point. From the output ensemble the mean and covariance matrix of the differential cross sections were calculated. For propagating the uncertainties using MC method we used 100 correlated random samples of each optical model parameter and computed the mean and covariance in the elastic differential cross sections.

Results

The elastic differential cross sections for p+^{48}Ca using initial parameters and the new parameters from this study are presented in Fig. 1 (a) and (b) for energies 12 and 9 MeV respectively. The correlation matrix of the optical model parameters is presented in Fig. 2. It is clear from Fig. 1 that the new parameters reproduces the experimental data well, while the initial parameters does not reproduce the experimental data properly. From Fig. 2 it

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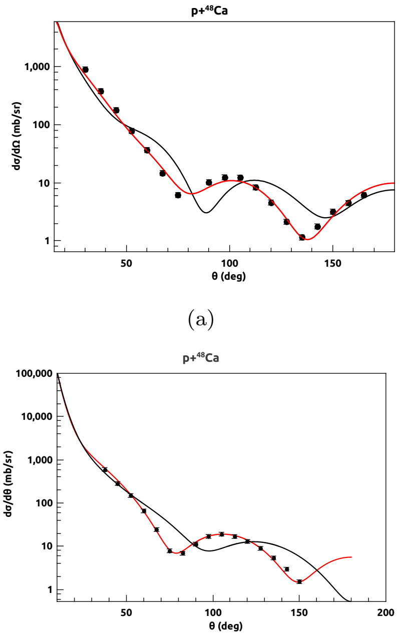

(a)

(b)

FIG. 1: Predictions for elastic scattering differential cross sections for $p+^{48}$Ca, using new parameters (in red) and initial parameters (in black) (a) for $E_p = 12$ MeV (b) for $E_p = 9$ MeV

can be observed that some of the parameters are highly correlated, hence these correlations should not be ignored while predicting using the optical model. Therefore in this study we have also used new parameters with their covariance matrix to determine the uncertainties in the final predictions of elastic differential cross sections at energy 12 MeV using UT method. We have also propagated these uncertainties using the MC method for comparing the two methods. The results obtained using UT and MC method are presented in Fig. 3. It is clear from this figure that although UT method take very less computational time as compared to MC method, yet the UT method has given the uncertainty estimates in the final outcomes similar to the MC method. In this study we have successfully demonstrated the forward and inverse uncertainty quantification using a deterministic sampling approach for the optical model calculations.

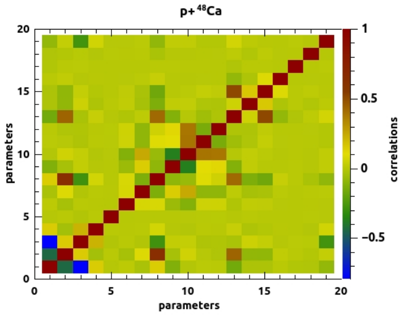

FIG. 2: Correlation matrix of the optical model parameters (the parameters are identified as the serial numbers 1 to 19 for r_v, a_v, v_1, v_2, v_3, w_1, w_2, r_d, a_d, d_1, d_2, d_3, r_{so}, a_{so}, v_{so1}, v_{so2}, w_{so1}, w_{so2} and r_c respectively).

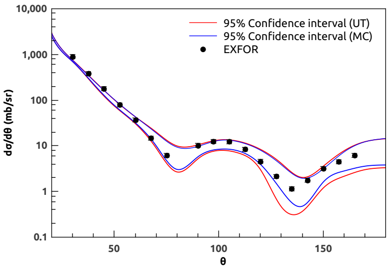

FIG. 3: Elastic differential cross sections for p+ ^{48}Ca at energies 12 MeV from EXFOR with the 95% confidence interval calculated through Unscented Transform method and Monte Carlo method.

References

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