

## Study of high-energy neutron-induced fission cross sections using Bayesian methods

**Authors:** Zhang, Dr. Peiyan Zhang Peiyan, Prof. Zhi-Qiang Chen, Han, Miss Rui, Roy, Prof. Wada, Tian, Dr. Guoyu, Dr. Bing-Yan Liu, Sun, Dr. Hui, Zhang, Dr. Xin, Guo, Mr. Rui, Zhang, Ze-Kun, Qiang, Dr. Li, Shi, Mr. Fudong, Zhi-Qiang Chen

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### Abstract

High-energy neutron-induced fission data for actinide nuclides form the foundation for the design of advanced nuclear energy systems such as accelerator-driven subcritical systems and fast neutron reactors, playing a vital role in their development. In this study, the INCL++ code is utilized to calculate neutron-induced fission cross sections in the energy range of 100 MeV to 1.2 GeV. Bayesian optimization is employed to refine parameters in the ABLA++ and GEMINI++ codes, ensuring closer alignment between computational results and experimental data. We train a Bayesian neural network using neutron-induced fission data, and its extrapolations are systematically compared with both theoretical calculations and experimental measurements. Results show that the Bayesian optimization method effectively reduces the chi-squared statistic between theoretical predictions and experimental data. Additionally, the Bayesian neural network demonstrates the ability to accurately reflect the trends of fission cross sections when provided with sufficient training data.

### Full Text

## Study of High-Energy Neutron-Induced Fission Cross Sections Using Bayesian Methods

Pei-Yan Zhang,<sup>1, 2</sup> Zhi-Qing Chen,<sup>1, 3, †</sup> Rui Han,<sup>1, 3</sup> Roy Wada,<sup>4</sup> Guo-Yu Tian,<sup>1</sup> Bing-Yan Liu,<sup>1, 3</sup> Hui Sun,<sup>1</sup> Xin Zhang,<sup>1</sup> Rui Guo,<sup>1</sup> Ze-Kun Zhang,<sup>1, 2</sup> Qin Li,<sup>1, 2</sup> and Fu-Dong Shi<sup>1</sup>

<sup>1</sup>Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou 730000, China

<sup>2</sup>School of Nuclear Science and Technology, University of Chinese Academy of

Sciences, Beijing 100049, China

<sup>3</sup>Gansu Isotope Laboratory, Lanzhou 730300, China

<sup>4</sup>Cyclotron Institute, Texas A&M University, College Station, Texas 77843

**Abstract.** High-energy neutron-induced fission data for actinide nuclides play a vital role in the design of advanced nuclear energy systems such as accelerator-driven subcritical systems and fast neutron reactors. In this study, the INCL++ code is utilized to calculate neutron-induced fission cross sections in the energy range of 100 MeV to 1.2 GeV. Bayesian optimization is employed to refine parameters in the ABLA++ and GEMINI++ codes, ensuring closer agreement between computational results and experimental data. We train a Bayesian neural network using neutron-induced fission data, and the extrapolations are systematically compared with both theoretical calculations and experimental measurements. The results show that the Bayesian optimization method effectively reduces the chi-squared statistic between theoretical predictions and experimental data. Additionally, the Bayesian neural network demonstrates the ability to accurately reflect the trends of fission cross sections when sufficient training data are provided.

**Keywords:** Bayesian neural network, Bayesian optimization, Fission, INCL, Spallation reaction

## INTRODUCTION

Since the discovery of uranium nuclear fission in 1938, this phenomenon has actively promoted the development of human society through applications such as nuclear energy utilization and medical technologies. Given the limited uranium resources on Earth, developing advanced nuclear energy devices such as fast neutron reactors and Accelerator-Driven Subcritical Systems (ADS) is of great significance. ADS utilizes a high-energy, intense proton beam generated by an accelerator to bombard a target nucleus, inducing spallation reactions that produce external neutrons [?]. These neutrons are then used to drive and sustain the operation of the subcritical reactor, offering inherent safety advantages compared to traditional reactors. Accurate and reliable nuclear data are essential for ADS design, particularly neutron-induced fission cross section data, which are crucial for investigating transmutation reactions in ADS.

Currently, the five major evaluated nuclear data libraries (ENDF, JENDL, JEFF, CENDL, BROND) provide neutron-induced fission data for actinides for ADS applications. However, they generally suffer from data shortages, with existing data predominantly concentrated below 20 MeV. Within most evaluated nuclear data repositories, a notable deficiency persists in neutron-induced fission cross section data sets for actinide nuclides at energies exceeding 20 MeV [?].

Nuclear fission data also play a crucial role in basic physics research, serving as indispensable inputs for understanding the evolutionary processes of elements in the universe and the fusion reactions of superheavy nuclides. They are particu-

larly important for simulation calculations of the rapid neutron capture process (R-process) in nuclear astrophysics. Precise calculations of the R-process can enhance the accuracy of elemental abundance calculations in the universe. Both advanced nuclear energy research and these basic physical studies rely on reliable nuclear fission data.

Since its inception in 2001, the neutron time-of-flight ( $n_{\text{TOF}}$ ) facility at CERN has undertaken a large-scale experimental program, resulting in a wealth of high-quality fission cross section data on actinide elements [?]. In recent years, the China Spallation Neutron Source (CSNS) has also made significant contributions to the measurement of fission reaction cross sections [?]. Thanks to these efforts and advancements in experimental techniques, the EXFOR database has collected numerous experimental data on neutron-induced fission cross sections of actinides above 100 MeV, including data for  $^{230,232}\text{Th}$  [?],  $^{233,234,235,236,238}\text{U}$  [?, ?, ?],  $^{237}\text{Np}$  [?, ?],  $^{239,240,241,242}\text{Pu}$  [?, ?, ?], and  $^{243}\text{Am}$  [?]. However, data for other actinide nuclides remain insufficient.

In 2014, S. Lo Meo et al. calculated the fission cross sections of actinides using the INCL++ Liège intranuclear cascade model combined with GEMINI++ and ABLA07 [?]. The (n,f) reaction cross sections of each nuclide were predicted based on (p,f) reaction cross sections, showing generally good agreement with experimental fission cross section data.

With the development of machine learning, these methods have been applied across various fields with promising results, and their introduction into nuclear data research has gained widespread acceptance. Machine learning can optimize parameters of physical models, particularly in nuclear reactions, fission processes, and data evaluation. By training on datasets, machine learning models can predict nuclear parameters and compare them with traditional models, thereby enhancing nuclear data assessment. Bayesian neural network (BNN) approaches have proven advantageous for evaluating nuclear data when experimental data are insufficient [?].

In this study, INCL++ version 6.33.1 [?] is used in conjunction with ABLA++ [?] and GEMINI++ [?] to calculate neutron-induced fission cross sections of actinides in the range of 100 MeV to 1.2 GeV. Additionally, Bayesian optimization is employed to refine critical physical parameters, improving theoretical calculations. We establish a BNN model and train it using available experimental data and theoretical calculation results. The trained BNN model output is then used to compare theoretical values with experimental data and perform analyses.

## II. METHODS

Bayesian optimization has long been used to address high-cost black-box optimization problems and is commonly employed to optimize hyperparameters of neural network models, effectively reducing computational costs while achieving optimal solutions. The Monte Carlo-based INCL++ method incurs high computational cost, making it suitable for parameter optimization of physical

models using Bayesian optimization. We use Bayesian optimization to optimize parameters in two de-excitation models: ABLA++ and GEMINI++.

The parameter to be optimized for the ABLA++ model is  $K_f \tilde{a}$ , where  $K_f$  is a tunable variable and  $\tilde{a}$  represents the asymptotic level density [?] (see formula (1)), and  $B_s$  is the same as in the liquid drop model. For the GEMINI++ model, the parameter to be optimized is  $a_f/a_n$ , where  $a_f$  is the level density parameter at the saddle point and  $a_n$  is the same quantity at ground-state deformation. The commonly optimized parameter is the fission barrier correction  $\Delta B_f$ .

$$\tilde{a} = 0.073A + 0.095B_{sA}^{2/3} \quad (1)$$

The quality of each parameter set is evaluated using  $\chi^2$ , defined as:

$$\chi^2 = \sum_{i=1}^N \left( \frac{\sigma_i^{\text{calc}} - \sigma_i^{\text{exp}}}{\Delta\sigma_i^{\text{exp}}} \right)^2 \quad (2)$$

In this work, the objective of Bayesian optimization is to minimize the chi-squared error between experimental points and theoretical calculations. Bayesian optimization is based on Bayes' formula:

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)} \quad (3)$$

where  $P(A|B)$  is the posterior probability,  $P(B|A)$  is the likelihood function,  $P(A)$  is the prior probability, and  $P(B)$  is the marginal likelihood.

[Figure 1: see original paper] Bayesian optimization flowchart.

Using Gaussian process estimation, the approximate process of Bayesian optimization proceeds as follows: First, several parameter groups are selected within the defined parameter space and the objective function values are calculated. The prior distribution of a surrogate function is initialized based on these calculated values. Based on the prior distribution of the surrogate function and the sampling function, several data points are sampled to find the point with the highest probability of being the minimum. New objective function values are obtained according to the sampling results, and the prior distribution of the surrogate function is updated simultaneously. This iteration is repeated to find the global optimal solution. The optimization flowchart is shown in Fig. 1.

There are many third-party Python libraries for implementing Bayesian optimization, such as Bayesian Optimization, Scikit-Optimize, GPyOpt, and others. This work is based on Scikit-Optimize.

The training data for the Bayesian neural network consist of experimental data with incident neutron energy above 20 MeV, and theoretical calculation data corresponding to each experimental point with incident neutron energy above

100 MeV. The input parameters are: incident neutron energy  $E$ , mass number  $A$ , proton number  $Z$ , and the optimized parameters. The parameters in the initial Bayesian neural network follow a normal distribution with an expected value of 0 and a variance of 1. A single hidden layer with ReLU activation function is used and the number of neurons is 130. The BNN model was trained using Variational Inference with the Adam (Adaptive Moment Estimation) optimizer. The Bayesian neural network is implemented based on Pyro. The structure of the Bayesian neural network is shown in Fig. 2.

[Figure 2: see original paper] Bayesian neural network structure.

### III. BAYESIAN OPTIMIZATION RESULTS

We input the parameters obtained from Bayesian optimization and the default parameters into GEMINI++ and ABLA++ for calculations. Additionally, we randomly extract 10 reference experimental points from the Bayesian optimization to compute and compare their  $\chi^2$  values. Table 1 presents the parameter results from the Bayesian optimization. The direct output of the optimized parameters is given in 16 decimal numbers, but only the first 6 decimal numbers are effective for the  $\chi^2$  value. Comparative calculations indicate that retaining the directly output parameters to six decimal places has a negligible effect on the  $\chi^2$  value. Therefore, we retain the optimized parameters to six decimal places and the  $\chi^2$  value to two decimal places. The default values for parameters in GEMINI++ and ABLA++ are:  $a_f/a_n = 1.036$ ,  $K_f = 1$ ,  $\Delta B_f = 0$ . Comparing the  $\chi^2$  values shows that using the parameters from Bayesian optimization significantly reduces  $\chi^2$ . The calculation results are shown in Figs. 3 and 4.

For  $^{239}\text{Pu}$  in Fig. 4(c) and  $^{235}\text{U}$  in Fig. 3(e), the experimental data for neutron-induced fission cross sections are limited. If only the available neutron-induced fission cross sections are considered, the  $\chi^2$  values for  $^{239}\text{Pu}$  and  $^{235}\text{U}$  could be further reduced. Since the  $\chi^2$  values include the proton-induced fission cross sections, the following treatment is conducted. Due to the scarcity of neutron-induced experimental data and the concentration of data below 300 MeV, which cannot fully reflect the overall trend of data in the 100 MeV–1.2 GeV energy range, a common issue arises for these nuclei. A similar issue also arises for  $^{240,241,242}\text{Pu}$  in Figs. 4(d)–(f), respectively: theoretical calculations agree well with experiments in energy regions with available data but may appear unreasonable in regions without experimental data. Therefore, we added proton-induced fission cross section data for  $^{239}\text{Pu}$  and  $^{235}\text{U}$ . For  $^{240,241,242}\text{Pu}$ , proton-induced fission cross section data are unavailable, precluding their inclusion in Bayesian optimization. Future experimental measurements are anticipated to address this limitation.

With the default parameters, the calculated fission cross sections show poor agreement with experiments in the energy range of 100 MeV–300 MeV, which is most obvious for  $^{230,232}\text{Th}$  in Figs. 3(a), (b) and  $^{243}\text{Am}$  in Fig. 4(g). For  $^{234}\text{U}$  in Fig. 3(d) and  $^{237}\text{Np}$  in Fig. 4(b), the calculation results with default parameters

significantly overestimate the fission cross sections in the energy range of 500 MeV–1000 MeV. The use of optimized parameters can fix this problem and achieve better agreement with experimental data.

Using the optimized parameters to calculate the proton-induced fission cross section (see Fig. 5), it is found that, compared with default parameters, the optimized parameters increase the fission cross sections at 100 MeV for  $^{232}\text{Th}$  as shown in Fig. 5(a),  $^{233,235,238}\text{U}$  in Figs. 5(b)-(d), and  $^{237}\text{Np}$  in Fig. 5(e). This may be attributed to the reduction in the fission barrier. For  $^{237}\text{Np}$ , the calculation results above 400 MeV with optimized parameters are lower and exhibit a rapid downward trend because Bayesian optimization also incorporates the experimental data of neutron-induced fission. In neutron-induced fission,  $^{237}\text{Np}$  shows a steep decline above 400 MeV, which affects the calculation results of the proton-induced fission cross section.

It may be insufficient to consider only two parameters for the optimization of  $^{237}\text{Np}$ , and other corrections may need to be taken into account, but this is beyond the scope of this work.

Calculation of (n,f) Reaction Cross Sections Using GEMINI++ and ABLA++ and Evaluation of Bayesian Optimization Results

#### IV. BAYESIAN NEURAL NETWORK RESULTS

The dataset was divided into 90% training data and 10% testing data. For the trained BNN model, the mean absolute error (MAE) on the training data is 42.43 mb, and that on the testing data is 40.54 mb. The slight difference between the two MAE values indicates a low risk of overfitting in the BNN model. The formula for MAE is:

$$\text{MAE} = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i| \quad (4)$$

where  $y_i$  is the true value of the  $i$ -th sample,  $\hat{y}_i$  is the predicted value of the  $i$ -th sample, and  $n$  is the number of samples.

[Figure 6: see original paper] Predictions by Bayesian neural network for  $^{230,232}\text{Th}$  and  $^{233,234,235,236}\text{U}$  are compared with theoretically computed and experimental data.

As shown in Figs. 6 and 7, the neutron-induced fission cross sections are predicted using the BNN model and are denoted by light blue bands around black solid lines. The blue region represents the 95% confidence interval, and the black solid line denotes the mean value of the probability distribution. The BNN model is extrapolated to incident neutron energies up to 1.2 GeV and compared with theoretical calculations. For  $^{230,232}\text{Th}$  in Figs. 6(a), (b), the predictions of the BNN model generally agree well with both experimental data and theoretical calculations. However, for  $^{232}\text{Th}$  in the higher energy region,

there are significant discrepancies between the predictions of the BNN model and the calculation results of ABLA++. For  $^{233,234,235,236,238}\text{U}$  in Figs. 6(c)-(f) and 7(a),  $^{237}\text{Np}$  in Fig. 7(b), and  $^{243}\text{Am}$  in Fig. 7(g), the predictions of the BNN model show excellent agreement with both theoretical calculations and experimental data in the low-energy region where abundant experimental data exist. On the other hand, in the higher incident energy region, due to the scarcity of experimental data, there are noticeable differences between the predictions of the BNN model and the calculation results of ABLA++ and GEMINI++.

For  $^{239,240,241,242}\text{Pu}$  in Figs. 7(c)-(f), the BNN model shows notably wide confidence intervals because the experimental data are concentrated below 200 MeV, and no data are available above 200 MeV, which causes significant discrepancies and makes extrapolation unreliable. Combined with the issues mentioned in the previous chapter, the lack of experimental data prevents the BNN model from making accurate predictions of the fission cross section trend. However, for nuclides such as  $^{230,232}\text{Th}$  and  $^{233,234}\text{U}$  in Figs. 6(a)-(d), the comparisons between BNN model extrapolation and theoretical calculations indicate that the extrapolated trends agree well with theoretical predictions. We conclude that the BNN model can capture the trends of fission cross sections when sufficient training data are available.

[Figure 7: see original paper] Predictions by Bayesian neural network for  $^{238}\text{U}$ ,  $^{237}\text{Np}$ ,  $^{239,240,241,242}\text{Pu}$  and  $^{243}\text{Am}$  are compared with theoretically computed and experimental data.

## V. SUMMARY AND CONCLUSIONS

In this study, the INCL++ code version 6.33.1 coupled with the ABLA++ and GEMINI++ models is used within a BNN framework to calculate total neutron-induced fission cross sections, and the BNN model is established. The Bayesian optimization algorithm is implemented using the Python library Scikit-Optimize to optimize the parameters of the ABLA++ and GEMINI++ models. This optimization significantly improves theoretical predictions for experimental neutron-induced fission cross sections and demonstrates the potential capability of Bayesian optimization. By avoiding the high computational cost and unclear specific form of the objective functions, Bayesian optimization provides an excellent solution. By comparing the extrapolations of the BNN model with theoretical calculations, it is concluded that the BNN model extrapolations can predict the trends of fission cross sections when sufficient training data are available. It is hoped that the Bayesian optimization method can be widely applied in more research studies.

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