Covariance evaluation of neutron cross sections in CENDL

Ruirui Xu[1*], *Zhigang* Ge[1], *Yuan* Tian[1], *Xi* Tao[1], *Yongli* Jin[1], *Yue* Zhang[1], *Duan* Wang[2], *Xiaodong* Sun[1], *Zhi* Zhang[1], *Jimin* Wang[1], *Dongdong* Wang[1] and *Zihao* Wei[3]

[1] China Nuclear Data Centre, China Institute of Atomic Energy, 102413 P.O.Box, Beijing, China
[2] China Institute of Atomic Energy, 102413 P.O.Box, Beijing, China
[3] Graduate School of China National Nuclear Corporation, China Industry College, 102413 P.O.Box, Beijing, China

Abstract: The covariance evaluation for neutron cross sections in CENDL is briefly introduced in this work. The methodology for evaluation contains the nuclear reaction theoretical model-dependent approach and the non-model dependent one according to the amount of experimental data. Both approaches are based on the Generalized Least-Squares (GLSQ) method. To obtain more reliable uncertainties from experimental measurement, the analysis of the sources of experimental uncertainties (ASEU) is used rigorously in the evaluation. Moreover, machine learning (ML) methods which can deal with the data mining with a more automatic way are employed to evaluate the cross sections in a large-scale nuclear mass region to compensate the uncertainties on some nuclides and reactions, lack of experimental data for, e.g., unstable nuclei and fission products. The covariance files for 70 fission product nuclei are obtained through the model-dependent method in CENDL-3.2, and the covariances for U and Pu isotopes have also been finished with high fidelity, which will be released as part of the next CENDL.

1 Introduction

Reasonable estimation for nuclear data covariance is very important in the study of sensitivity and uncertainty analysis, the nuclear data adjustment and so on for the advanced reactors [1]. Besides the early covariance databases such as COMMARA-2.0 [2], AFCI-1.2 [3] et al., the newly evaluated covariance files for MF=32, 33, 34, 35 are also released in the various latest evaluated nuclear data libraries, ENDF/B-VIII.0[4], JENDL-5[5], JEFF-3.3[6], CENDL-3.2[7] and TENDL-2021[8]. The total amount and quality of covariance data in these libraries have been greatly improved in the past decade. The nucleus and files involved in each library are show in Table 1. It is shown that covariances have been provided for average number of neutrons per fission (NU), resonance parameters (RES), cross sections (SIG), angular distributions (DA) and energy distributions of secondary particles (DE) in a large number. CENDL-3.2 also contains COV/SIG for 76 nuclei, which are mainly located in the fission product mass region and several light nuclei. Details will be introduced in Section 3.

Table 1. Status of covariance evaluations in international evaluated libraries.

ENDF MF	ENDF/B-VIII.0	JENDL-5	JEFF-3.3	CENDL-3.2	TENDL-2021
COV/NU	72	79	136	0	432
COV/RES	118	43	352	0	1
COV/SIG	221	102	442	76	2808
COV/DA	108	97	359	0	386
COV/DE	65	79	36	0	431

It is almost impossible to hand down the uncertainty information of experiments and theories among the nuclear data pipeline to covariance strictly. In order to achieve covariance data with better physics, great effort has been made in the past decades and the deterministic (Generalized Least-Squares, GLSQ) and stochastic (Monte Carlo, MC) approaches were developed, each with their advantages and disadvantages. They are both applied in the real covariance evaluation, LS approach is mainly adopted in ENDF/B, JENDL and CENDL, and MC is used in JEFF and TENDL. In addition to the traditional methods above, some innovative techniques, such as Machine Learning (ML) and Artificial Intelligence (AI), are also expected to join the nuclear data evaluation to automate evaluation work and uncover helpful information to improve data quality [6].

The total evaluation scheme and the derived covariance in CENDL will be briefly presented in this paper. The content following is laid out in three sections. Section 2 will provide the overview of methodology with LS. Section 3 will present some discussions on our derived cross sections covariance in CENDL-3.2 and the future CENDL. the summary of the conclusions and future work will be outlined in Section 4.

2 Methodology

* Corresponding author: xuruirui@ciae.ac.cn

2.1 Covariance evaluation based on the traditional GLSQ approach

The systematic technique to derive the covariance of cross sections for CENDL has been developed progressively in the past ten years [7]. The GLSQ approach is used in the whole process to perform the uncertainty propagation from the applied nuclear data experiment and theory. According to the abundance of experimental data for each physical quantity, we build the model dependent and non-model dependent approaches respectively, which have been described in [7, 8] and the details will not be talked too much in this paper.

It is worth mentioning that the central and most time-consuming process in GLSQ is to perform the reliable assessment of experimental data and their experimental covariance, particularly to deal with the multiple measurements to the same quantity from different laboratories. The analysis of the sources of experimental uncertainties (ASEU) is used rigorously in the evaluation. Noted that we try to follow the reported experimental errors in the references, but we also perform some variation to the experimental errors, such as when the data are measured for a long time, some important uncertainties are obviously missing in the report, and the pseudo-uncertainty will be supplemented. In other case, we rarely modify the experimental data error directly. In addition, some subjective effects are inevitable when determining the uncertainties from background subtraction, data normalization, detector counting statistics, detector efficiency as well as fundamental energy resolution of the machine in a cross-section measurement experiment, especially when analysing the measurements reported with scarce information in publications. In order to make compensation to the tractional GLSQ scheme, some innovative approaches such as machine learning are also involved in nuclear data study to reduce the subjectivity during covariance evaluation and make good predictions for the data without measurements.

2.2 Machine learning in the experimental cross sections analysis

Machine learning is a well-known promising data analysis technology that has been widely used in various scientific reach fields in recent years. It can convert the disordered data into useful information through some advanced computational algorithm, and is very effective to deal with complex nuclear data problems.

In the real nuclear cross section evaluation, one always meets with the cases the experimental information available is not enough to constrain all nuclear reaction theoretical parameters accurately to obtain the good description to nuclei cross sections without measurements. Therefore, we introduce the Artificial Neural Network (ANN) method to learning the experimental data available of a certain reaction (such as (n,2n), (n,3n)) systematically and to predict the nuclear cross sections (such as (n,2n)) without measurements; and then, we apply the predicted data in the theoretical calculation to further support the nuclear reaction model calculation to get better results.

In our scheme, a modified Bayesian Neural Network (BNN) with the Local Reparameterization Trick [9] is employed in the experimental data analysis and predictions. The designed BNN in our work is shown as Figure 1, which has the similar Topology structure with the so-called Variational Autoencoder (VAE) generator model [10]. Two intermediate variables ($\mu(X)$ and $\log(\sigma(X)^2)$) are first calculated and the output can be local reparametrized through the following relation,

$$output = \mu(X) + e^{\frac{1}{2}log(\sigma(X)^2)} \times \epsilon$$

where $\epsilon \sim N(0,1)$ is the normal distribution. In our scheme, the predicted cross sections of BNN are taken as an effective supplement measurement in the traditional GLSQ covariance evaluation scheme.

In the real calculations, eight physical parameters including proton number, mass number, single neutron separation energy, single proton separation energy, shell effect, level density parameter, pairing correlation, neutron incident energy are adopted in the input layer. Two hidden layers with each 128 nodes are contained in the network. The single task output means the obtained cross sections by BNN, and the uncertainties of output cross sections can be produced self-consistently.

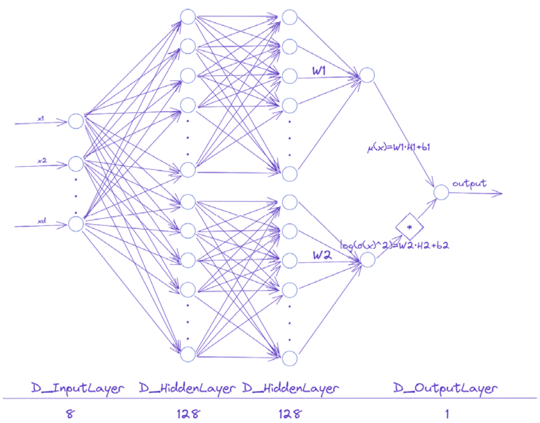

Fig. 1. Topology structure of BNN in this work.

We take as example of ^{23}Na to ^{209}Bi (n,2n) cross sections, and predict them with a database of 5000 experimental data points. During BNN learning and validation processes, the learning set is built by randomly selecting 80% of the data, while the validation set is made up by the remaining 20%. Figures 2 and 3 are the derived (n,2n) cross sections of ^{89}Y and ^{209}Bi. It can be observed that after making full use of the existing experimental data, the BNN predictions are good enough to describe the physical curves and the relevant BNN uncertainty looks also reasonable regarding to the measurements. Both of the information will provide key input in GLSQ to improve the reliability of covariance, especially to the nuclear reactions without measurements.

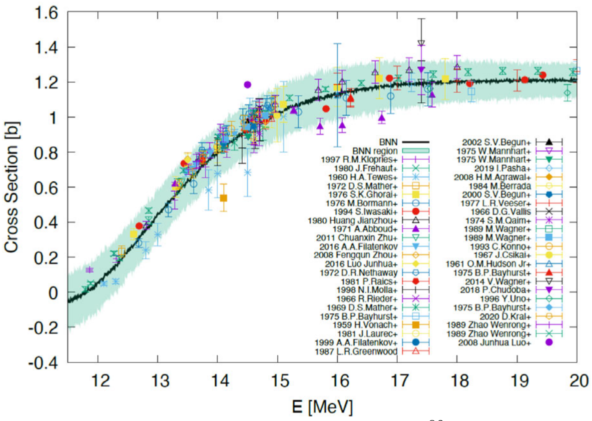

Fig. 2. The comparison of the obtained ^{89}Y(n,2n) cross sections and uncertainty and the relevant measurements.

3 Evaluated covariance in CENDL

Based on the methodology in Section 2, the covariance files of nuclear reaction cross sections are systematically generated for the light, medium heavy and fission nucleus, among which, 76 nuclei are released in CENDL-3.2 as listed in Table 2, and eight neutron reactions (n,total), (n,elastic), (n, γ), (n,inelastic), (n,p), (n,2n), (n,np) and (n,n α) are concerned for the medium heavy mass nucleus, two more reactions (n,fission) and (n,3n) are treated for the fission nucleus.

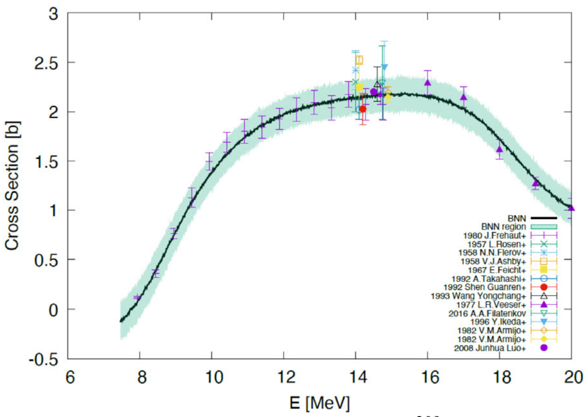

Fig. 3. The comparison of the obtained ^{209}Bi(n,2n) cross sections and uncertainty and the relevant measurements.

Table 2. The nucleus of covariance evaluation in CENDL-3.2.

Nucleus	Num.	Elements
Light	4	^{2,3}H, ^{3}He, ^{19}F
Structure	2	^{55}Mn, ^{56}Fe
Fission products	70	^{69,71}Ga, ^{71,73,74,75,76,77,78}Ge, ^{75,77,79}As, ^{89,91}Sr, ^{93,95}Zr, ^{95}Nb, ^{99}Tc, ^{99,100,101,103,104,105}Ru, ^{103,105}Rh, ^{105,108}Pd, ^{113}Cd, ^{121,125}Sb, ^{127,129,135}I, ^{124,132,134,135}Xe, ^{133,135,137}Cs, ^{130,134,135,136,137,138}Ba, ^{139}La, ^{141,144}Ce, ^{141}Pr, ^{143,145,146,148}Nd, ^{147,148,149}Pm, ^{150,151}Sm, ^{151,153,155}Eu, ^{154,155,156,157,158,160}Gd

The covariance of cross sections of 70 fission products are newly derived via the model-dependent methods in CENDL-3.2. The current model dependent covariance is mainly constructed from the uncertainty of theoretical model parameters, in the meantime, the outputs based on BNN are also partly referred in this work to compensate the scarcity of measurements in this mass region.

In total, the assessed uncertainties for the nuclear reactions for 70 fission produce nuclei are about less than 10% for (n,total); 20% for (n,inelastic); 20% for (n,2n); 30% for (n, γ); 80% for (n,n α); 50% for (n,np), which can be evidenced by Figure 4-6. In these figures, the isotopes of Ge are sampled and the uncertainties of neutron cross sections look all reliable in magnitude.

To further compare the current results with other libraries, ^{95}Zr(n,inl) and (n,2n) reactions are plotted with the evaluated uncertainties available in ENDF/B-VIII.0, JEFF-3.3 and CENDL-3.2. The uncertainties in ENDF/B-VIII.0 are the largest one comparing to the others, because data are directly adopted from COMMARA-2.0, which contains evaluated low-fidelity covariances [11]. The data in JEFF-3.3 are generated by the Monte Carlo TASMAN code in TALYS, the uncertainties mainly rely on the MC samples and build the margin of the theoretical parameter, and the absolute values look identical to CENDL-3.2. The deviation illuminates the obtained covariance through different approaches, and the covariance passed from the real nuclear data evaluation process is always more reliable to show the confidence interval of evaluated nuclear cross sections.

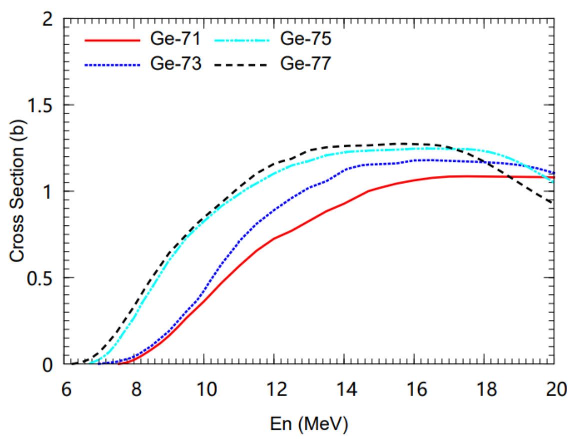

Fig. 4. The evaluated cross sections of ^{71,73,75,77}Ge(n,2n) in CENDL-3.2.

Besides the new evaluations for fission produce nuclei, the covariance for actinide nuclei is also built together with the evaluation for cross sections. Figure 7 shows the data for ^{235}U(n,2n) and (n3n), and the results are achieved through the combination of model dependent and non-model dependent methods. It can be seen that the experimental data are almost in the uncertainty bands. In addition, the correlated coefficient between the different reactions are also shown in Figure 8, which provide more complete information to the nuclear application.

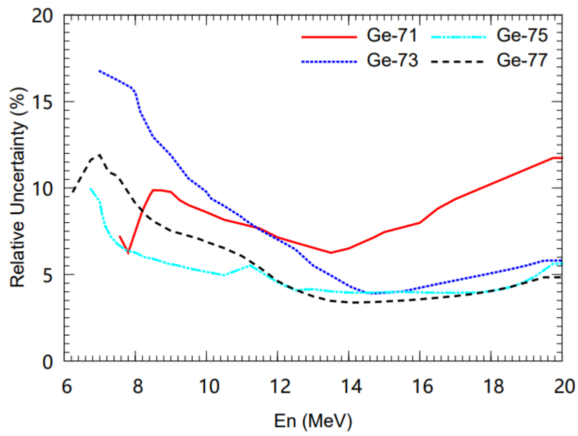

Fig. 5. The evaluated uncertainties relevant to the cross sections in Fig. 4.

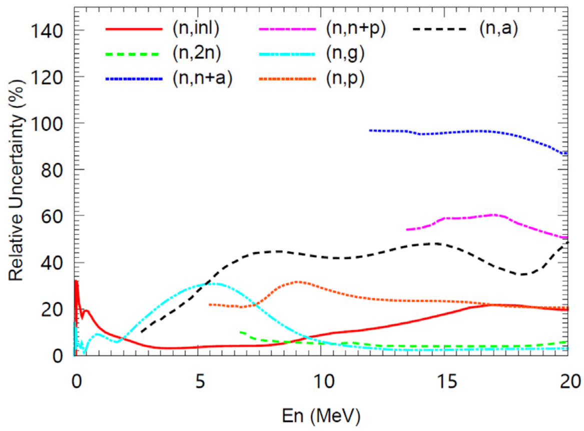

Fig. 6. The uncertainties of seven neutron cross sections of ^{75}Ge CENDL-3.2.

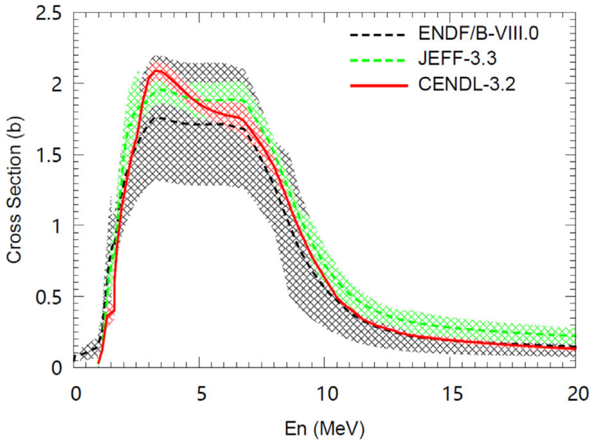

Fig.7. The comparison of evaluated ^{95}Zr(n,inl) cross sections and uncertainties in ENDF/B-VIII.0, JEFF-3.3 and CENDL-3.2.

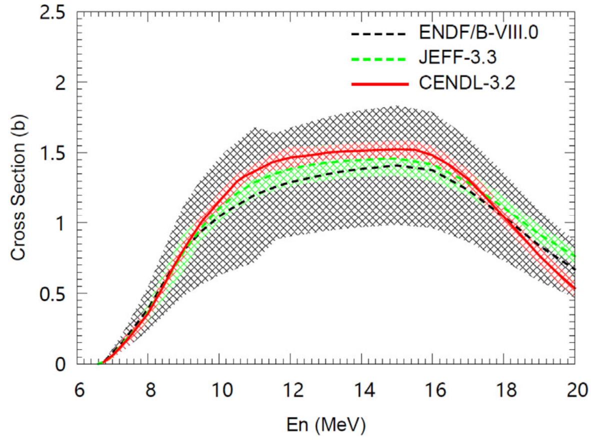

Fig.8. The comparison of evaluated ^{95}Zr(n,2n) cross sections and uncertainties in ENDF/B-VIII.0, JEFF-3.3 and CENDL-3.2.

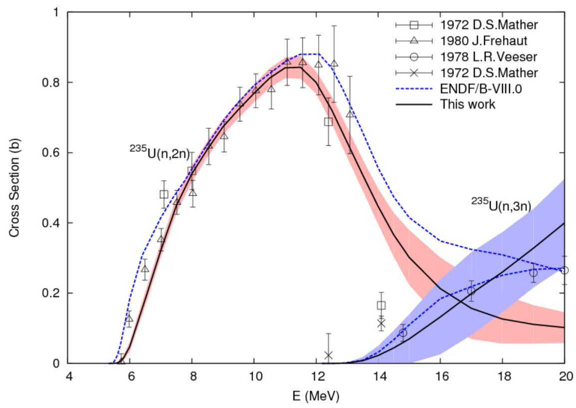

Fig.9. The comparison between the evaluated ^{235}U(n,2n) and (n,3n) cross sections and uncertainties and the measurements [8].

4 Conclusion and perspective

The methodology of nuclear cross section covariance evaluation in CENDL is introduced, meanwhile the new evaluated results for fission products and actinides are also discussed. As a result, the current covariance in CENDL seems confident to describe the uncertainties of most important neutron data, which could supply nuclear application with a good database. In addition, the new covariance for actinides will be released in the next CENDL.

To involve more information from experimental data, the machine learning approach BNN is employed in an exploratory study. Joining the BNN outputs of cross sections and uncertainties in GLSQ are promising to increase the reliability of the traditional covariance results in future.

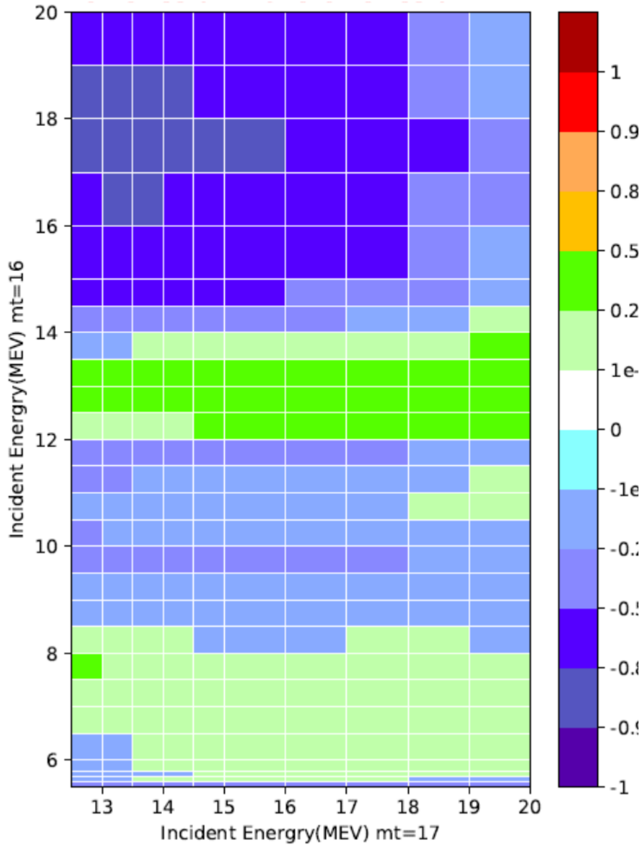

Fig. 10. The correlated coefficient of cross sections between ^{235}U(n,2n) and (n,3n) reactions [8].

The authors thanks Prof. *Yingxun* Zhang from China Institute of Atomic Energy for his kind discussion about application of machine learning in nuclear physics. This work has been supported by the National Natural Science Foundation of China (Grants No. 11875321, No. 11790320, No. 12005303).

References

1. V. Sobes, W. J. Marshall, D. Wiarda, F. Bostelmann, A. Holcomb, B. T. Rearden, ORNL/TM-2018/1037 (2019)
2. M. Herman, P. Oblozinsky, C.M. Mattoon, M. Pigni, S. Hoblit, S.F. Mughabghab, A. Sonzogni, BNL- 94830-2011 (2011)
3. P. Oblozinsky, Report BNL-90897 (2009)
4. D. A. Brown, et al., Nuclear Data Sheets 148, 1–142 (2018)
5. O. Iwamoto, N. Iwamoto, K. Shibata, A. Ichihara, S. Kunieda, F. Minato, and S. Nakayama, EPJ Web of Conferences, 239, 09002_1-6 (2020)
6. Plompen, A.J.M., Cabellos, O., De Saint Jean, C. et al., JEFF-3.3. Eur. Phys. J. A 56, 181 (2020).
7. Zhigang Ge, Ruirui Xu, Haicheng Wu et al., EPJ Web of Conferences 239, 09001 (2020).
8. A.J. Koning, D. Rochman, J.-Ch. Sublet, N. Dzysiuk, M. Fleming, and S. van der Marck, Nuclear Data Sheets 155, 1–55 (2019).
9. https://www-nds.iaea.org/exfor/endf.htm
10. R. Capote, D.L. Smith, A. Trkov, EPJ Web of Conferences 8, 04001 (2010)
11. P. Vicente-Valdez, L. Bernstein, M. Fratoni, Annals of Nuclear Energy 163, 108596 (2021)
12. R. Xu, Q. Zhang, Y. Zhang, T. Liu, Z. Ge, H. Lu, Z. Sun, B. Yu, and G. Tang, Nuclear Data Sheets 123, 16–20 (2015)
13. Z. Zhi, Y. Zhang, Y. Tian, R. Xu, J.M. Wang, X. Tao, Y.L. Jin, X.D. Sun, Z.G.Ge, Atomic Energy Science and technology, 056, 1599(2022)
14. D. P. Kingma, T. Salimans, arXiv:1506.02557v2 (2015)
15. D. P. Kingma, M. Welling, arXiv:1312.6114 (2013)
16. M.T. Pigni, M. Herman, P. Oblozinsky, BNL-79985-2008-IR (2008)