



## Cross-checking of Large Evaluated and Experimental Nuclear Reaction Databases

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Automated methods are presented for the verification of large experimental and evaluated nuclear reaction databases (e.g. EXFOR, JEFF, TENDL). These methods allow an assessment of the overall consistency of the data and detect aberrant values in both evaluated and experimental databases.

## I. INTRODUCTION

The Nuclear Energy Agency (NEA) Data Bank is a member of the network of Nuclear Reaction Data Centres that maintains large nuclear databases and makes them available to scientists and engineers worldwide [1]. Within the context of WPEC Subgroup 30 activities [2], the NEA Data Bank, the Société de Calcul Mathématique (SCM) and the Nuclear Research and Consultancy Group (NRG) have developed statistical methods to help improve the quality of the nuclear reaction databases.

An outline of the NEA-SCM procedure to check the mutual consistency of experimental data is described in Ref. [3]. The focus of the present contribution is to describe methods developed by NEA-SCM and NRG to check the consistency of data from different evaluated libraries (e.g. JEFF, TENDL) and to cross-check these evaluated data with experimental data (EXFOR).

This approach aims to use the valuable information stored in both experimental and evaluated database, and help assess the quality of evaluated data by comparison with experimental data (and vice-versa) to identify flaws in the evaluated and experimental databases.

## II. DATABASE DESCRIPTION

We only consider the case of cross section  $y = f(x)$ , where  $x$  is the energy of the incident particle. However, there are some features that must be taken into account: (i) an experimental point may be associated with an uncertainty and/or a resolution; (ii) both experimental and evaluated data may contain resonance regions characterized by large fluctuations in cross section values; (iii) low cross sections may lead to large relative discrepancies.

## III. METHOD DEVELOPED BY NEA-SCM

The main idea of the consistency assessment is to calculate the mean distance between (i) two curves in the case of evaluated data; (ii) a curve and a set of points when comparing evaluated and experimental data.

The comparison is performed separately for each nuclear reaction by means of relative and absolute “distances” between experimental points and each of the evaluated curves. Subsequently, the available nuclear reactions are rated by combining the two types of distances. The same procedure is applied when checking the mutual consistency of evaluated data: each library is compared with all available evaluations of the same reaction and then rated according to its similarity with the others.

The absolute distance between two libraries describing the same reaction is calculated as the integral of the difference between two continuous functions

$$d = \int_a^b |f(x) - g(x)| dx. \quad (1)$$

The absolute distance between a curve and a set of points is the average of the differences observed at the same abscissa (energy)

$$d = \frac{\sum_{i=1}^N |y_i - y'_i|}{N}, \quad (2)$$

where  $y_i$  is the experimental value,  $y'_i$  is the evaluated (interpolated) value, and  $N$  is the number of experimental data points. The relative distance is deduced by dividing the absolute distance by the average of compared values. This method is implemented in six steps.

(1) *Representation of the data:* An essential point is to define the optimal scales that allow the data to be represented as evenly spaced as possible [3].

(2) *Discretization:* The energy range common to all data sets is discretized in 50 subintervals of the same size.

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(3) *Construction of the resonance indicator:* Before making a comparison, resonance regions must be distinguished. We calculate a “relative variance” for each discretization interval,  $i$ , using the formula

$$\text{var}_i^{\text{rel}} = \frac{\sum_{n=1}^{N_i} \frac{|Y_n - \bar{Y}|}{(Y_n + \bar{Y})/2}}{N_i}, \quad i = 1, \dots, 50 \quad (3)$$

where  $N_i$  is the number of measurements, and  $Y_n$  and  $\bar{Y}$  are the cross section and its average value, respectively. A resonance region is empirically defined by a “relative variance” larger than 0.18. Fig. 1 shows an example of computing of such relative variance for a given nuclear reaction so that the resonance region is clearly defined.

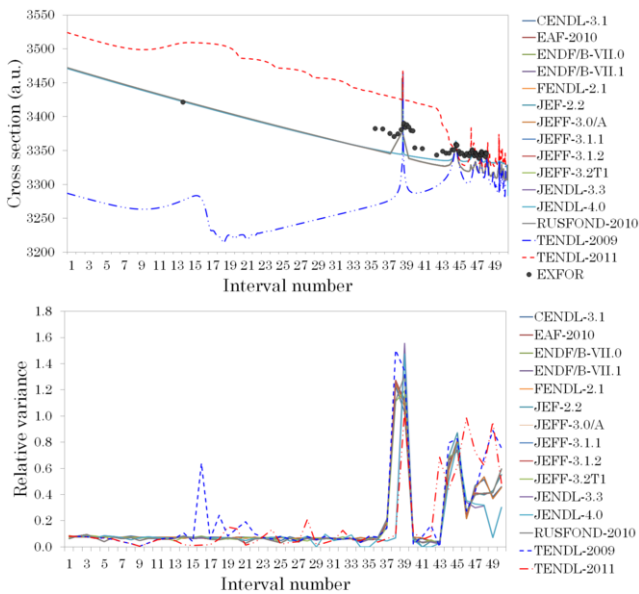


FIG. 1. Data from the EXFOR database (points) and evaluated libraries (lines) for the  $^{11}\text{B}(n, \gamma)$  cross section (top) and values of relative variance for each interval (bottom).

(4) *Consistency of evaluated and experimental data:* The comparison is performed subject to the value of the resonance indicator: (i) in a resonance region, the distance is computed as the difference of integrals

$$d = \left| \int_a^b f(x) dx - \int_a^b g(x) dx \right|, \quad (4)$$

where the integral for the EXFOR data is made using interpolation between points from the same data set; (ii) otherwise Eq. (2) is applied.

(5) *Mutual consistency of evaluated data:* (i) in a resonance region, the distance is computed using Eq. (4); (ii) otherwise Eq. (1) is used. As an example, Figs. 2 and 3 present the distances calculated for the reaction given in Fig. 1. The greater the distance, the worse the library. Thus, in this case, the calculated distances confirm that the TENDL libraries are suspicious compared to other libraries and experimental data.

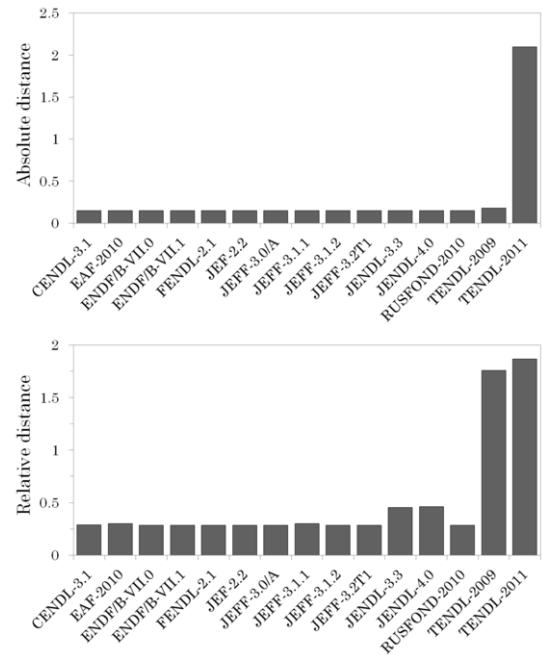


FIG. 2. Assessment of the self-consistency of evaluated data: absolute (top) and relative distances (bottom).

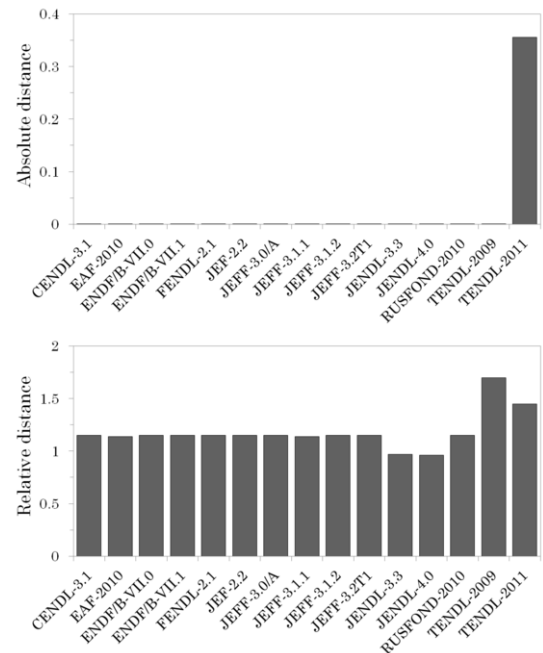


FIG. 3. Assessment of the consistency between measured and evaluated data: absolute (top) and relative distances (bottom).

(6) *Classification:* A single indicator combining the absolute and relative distances is implemented as follows: (i) compute the absolute (*abs*) and relative (*rel*) distances for each single library; (ii) calculate  $\log_{10} \text{abs}$ ; (iii) us-

ing all examined reactions, normalize these values between  $[0.005-1.005]$ ; (iv) the final indicator is given by  $rel \times (log_{10} abs)^{norm}$ . Note that this indicator is still relative, and only helps identify on a consistency scale the best and worst cases among all cases studied.

#### IV. METHOD DEVELOPED BY NRG

A quality score should be given to each EXFOR sub-entry to verify and improve the database efficiently. This is no small task given the total size of EXFOR, as summarized in Table I. Out of a total of 134,941 data sets, 83,084 have been translated by the IAEA into the extended computational format (XC4), which makes EXFOR more easily readable for further processing, and 97% of these have been identified as usable data and categorized in a directory-structured database developed at NRG with the preliminary name “Newbase”. Finally, 52% of these sub-entries (at the moment cross sections only) have been compared with the latest version of the major evaluated libraries (CENDL-3.1, EAF-2010, ENDF/B-VII.1, IRDFF-1.0, JEFF-3.1.1, JENDL-4.0 and TENDL-2012). The main goodness-of-fit estimator we are using is the F-factor

$$F = 10 \sqrt{\frac{1}{N} \sum_i^N \left( \log \frac{\sigma_T^i}{\sigma_E^i} \right)^2}, \quad (5)$$

although we also monitor the  $\chi^2$  estimator

$$\chi^2 = \frac{1}{N} \sum_i^N \left( \frac{\sigma_T^i - \sigma_E^i}{\Delta \sigma_E^i} \right)^2, \quad (6)$$

and the absolute deviation

$$\Delta = \frac{1}{N} \sum_i^N |\sigma_T^i - \sigma_E^i|, \quad (7)$$

in which the subscript T stands for TENDL or another evaluated library, E for experiment, and N is the number of data points. Thus, the F-factor can be given per data point, in which case this factor is a distorted C/E ratio, per data set summed over all points, per reaction summed over all data sets and/or nuclides, per projectile summed over all reactions, and finally for the whole EXFOR database and each of the evaluated libraries.

If we want a *quality score* for each data set in such a large database, initially these scores will be assigned automatically. Then, paper reviews and possible corrections

TABLE I. Total contents of EXFOR and derived databases.

Database	# entries	# sub-entries	# data points
EXFOR	19,764	134,941	11,882,567
XC4	13,621 (69%)	83,084 (62%)	7,572,483 (64%)
Newbase	13,342 (98%)	80,660 (97%)	7,471,028 (99%)
Evaluations	7,829 (59%)	41,958 (52%)	4,062,317 (54%)

may be performed, and sub-entries placed in a different class. A preliminary classification is proposed as follows:

- Class 1:  $1 \leq F \leq 1.2$
- Class 2:  $1.2 < F \leq 2$
- Class 3:  $F > 2$

At the moment, the class “3” is always reviewed by checking the publication for possible compilation mistakes, while class “2” is reviewed if in addition  $\Delta$  is more than 10% of the total nonelastic cross section and if  $\chi^2$  is larger than 20. After such an exercise, the data set is assigned a “R” (reviewed) flag or an “E” (error) flag. Note that “reviewing” here has nothing to do with the intrinsic quality of the measurement, but rather a check that the correct quality was compiled into EXFOR.

As an example, Fig. 4 and Table II show a comparison between experimental data and evaluated libraries for the  $^{72}\text{Ge}(n,p)$  cross section. On the basis of this study, the data set #11274047 was reviewed, and it was concluded that the compiled value was as reported. This exercise could be performed for the entire EXFOR database.

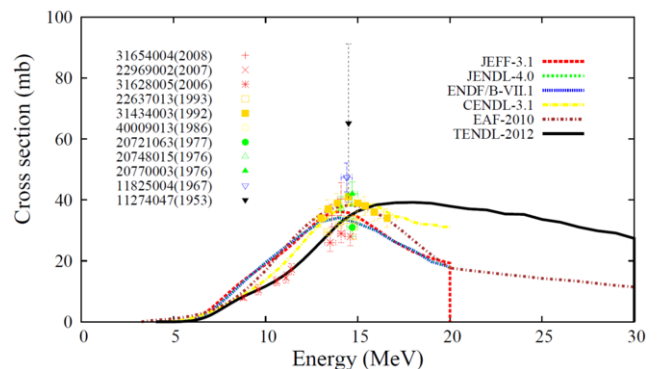


FIG. 4. Comparison of experimental data and evaluated libraries for the  $^{72}\text{Ge}(n,p)$  cross section.

#### V. CONCLUSIONS

This work is a follow-up of activities initiated within WPEC Subgroup 30 [2]. The NEA-SCM method was successfully validated on a selection of two hundred cross sections. Further testing is under way involving the full database of the JANIS application [4] and including future JEFF test libraries. The method developed at NRG is being used to assign quality scores to the EXFOR data set with the ultimate objective to improve the accuracy of TENDL libraries. These initiatives will help improve the quality of the EXFOR database, JEFF and TENDL libraries for the benefit of all nuclear data users.

TABLE II. F-values for all  $^{72}\text{Ge}(\text{n,p})$  cross section data sets available in EXFOR [1].

Sub-entries	<F>	CENDL-3.1	EAF-2010	ENDF/B-VII.1	JEFF-3.1	JENDL-4.0	TENDL-2012
31654004	1.13	1.05	1.06	1.13	1.08	1.13	1.20
22969002	1.44	1.25	1.51	1.64	1.62	1.64	1.04
31628005	1.26	1.34	1.36	1.22	1.30	1.22	1.17
22637013	1.11	1.16	1.18	1.08	1.12	1.08	1.04
31434003	1.15	1.05	1.03	1.18	1.13	1.18	1.18
40009013	1.16	1.24	1.23	1.05	1.13	1.05	1.15
20721063	1.16	1.24	1.23	1.06	1.14	1.06	1.14
20748015	1.08	1.01	1.02	1.09	1.02	1.09	1.13
20770003	1.20	1.09	1.10	1.28	1.19	1.28	1.19
11825004	1.35	1.24	1.24	1.42	1.32	1.42	1.39
11274047	1.85	1.69	1.71	1.96	1.82	1.96	1.89
Average	1.29	1.21	1.30	1.33	1.31	1.33	1.21

[1] N. Otuka *et al.*, NUCL. DATA SHEETS **120**, 272 (2014).[2] A.J. Koning *et al.*, Quality Improvement of the EXFOR Database, WPEC, Vol. 30, OECD NEA, Paris (2011).[3] E. Dupont *et al.*, NEA NEWS MAGAZINE **29.1**, 30 (2011).[4] N. Soppera *et al.*, NUCL. DATA SHEETS **120**, 294 (2014).