Verification of the databases EXFOR and ENDF

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Abstract. The objective of this work is for the verification of large experimental (EXFOR) and evaluated nuclear reaction databases (JEFF, ENDF, JENDL, TENDL...). The work is applied to neutron reactions in EXFOR data, including threshold reactions, isomeric transitions, angular distributions and data in the resonance region of both isotopes and natural elements. Finally, a comparison of the resonance integrals compiled in EXFOR database with those derived from the evaluated libraries is also performed.

1. Introduction

The Nuclear Energy Agency (NEA) Data Bank gathers and updates the data from different organisms for all nuclear reactions, and makes them available to scientists and engineers. The objective of this work is to improve the overall quality of these data.

In a previous work, the NEA Data Bank and the Société de Calcul Mathématique co-developed statistical methods to cross-check the consistency between experimental (EXFOR) and evaluated libraries (ENDF/B-VII.1 (USA), JEFF-3.2 (OECD/NEA), JENDL-4.0 (Japan), TENDL-2014 (Netherlands)).

In the present work we update this method to give a consistency ranking to each EXFOR entry that can be compared across all the reactions. The comparison is performed separately for each nuclear reaction between each experimental subentry and each evaluator.

The ranking allows directly seeing which EXFOR data and which reactions are the most suspicious, and which are reliable. This cross-checking allows not only reporting the suspicious EXFOR subentries, but it also helps identifying flaws in evaluated data files.

All the uncertainties available in both EXFOR and ENDF were taken into account, and most EXFOR data were used in this work.

2. Database description

The work is applied to induced neutron reactions in EXFOR data, including threshold reactions, isomeric transitions, angular distributions and data in the resonance regions. It is applied for isotopes and natural elements. In this work, a total number of 7,468 reactions were checked, corresponding to 26,634 EXFOR subentries and 3,955,254 points.

Each nuclear reaction is represented by two parameters: the abscissa corresponds to the incident energy

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(or the angle in angular distributions) and the Y axis corresponds to the cross-section (which may be considered as a probability of neutrons interaction).

Data contained in EXFOR are the result of the experimentations and considered as a set of points, whereas the data presented by the different evaluated libraries (e.g., JEFF) are the result of processing and considered as continuous functions.

The measurement points are attached with uncertainty in X and Y for EXFOR. For ENDF, only cross-section uncertainty is available.

The nuclear data may contain resonance zones: for certain energy intervals, the cross-section can vary widely. The comparison in such zones must be performed in a rougher way.

3. Principle of the method

The main idea of the consistency assessment is to calculate the distance between a curve and a set of points. For each single point, one computes the distance between the two vertical 95% confidence intervals of EXFOR and ENDF $[Q_{5\%}^{ENDF}, Q_{95\%}^{ENDF}]$ and $[Q_{5\%}^{EXFOR}, Q_{95\%}^{EXFOR}]$ as follows (see Fig. 1 at left):

$$\text{distance} = \left(\max Q_{5\%}^{\text{EXFOR or ENDF}} - \min Q_{95\%}^{\text{EXFOR or ENDF}}\right)^+ .$$

The confidence intervals are computed from the standard deviations, σ, of the cross-section denoted by:

$$\left[Y^{ENDF} - 1.96 \times \sigma^{ENDF}, Y^{ENDF} + 1.96 \times \sigma^{ENDF}\right] .$$

To take into account the horizontal uncertainty in EXFOR, one discretizes the 95% horizontal confidence interval and computes the minimal distance over the interval as shown at right in Fig. 1.

The higher the distance, the less consistency there is between the experimental data and the evaluated curve. A ratio is computed between this distance and the vertical
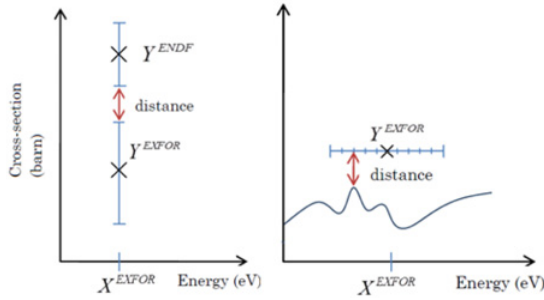
Figure 1. Uncertainties in Y (left) and in X (right).

uncertainty of EXFOR or ENDF (set to 10% when not specified):

$$\text{ratio} = \frac{\text{distance}}{\max(\sigma_{EXFOR}, \sigma_{ENDF})}.$$

For example, if the distance between the curve and the point is more than 5 times the vertical uncertainty, the ratio is equal to 5. Such a high ratio would mean that the point is quite suspicious. The smaller the uncertainties, the higher the ratio and the less consistency there is. This ratio can thus be compared across the reactions and the different subentries because it is not dependent upon the value of the cross-sections.

The ratio is averaged for all EXFOR points to obtain a final ranking of the subentry. This rank is computed as follows:

- rank = A if $0 < \text{ratio} \leq 1$
- rank = B if $1 < \text{ratio} \leq 2$
- rank = C if $2 < \text{ratio} \leq 3$
- rank = D if $3 < \text{ratio} \leq 8$
- rank = E if $\text{ratio} > 8$.

A subentry with a rank of D or E is considered as a potential outlier.

4. Implementation steps

The implementation of the method is carried out following different steps:

1) Finding the right scale for the abscissa: the data must be plotted as evenly as possible, see details in [1];
2) Defining the common borders of the subentry and the available ENDF;
3) Discretizing the abscissa in 50 interval
4) Distinguishing between resonance and no-resonance interval before marking a comparison. The comparison must be rougher in the resonance area because of large fluctuation of data. For each interval, a resonance indicator is calculated as the "relative variance":

$$\text{relative\_variance} = \frac{1}{N} \sum_{n=1}^{N} \frac{|Y_n - \overline{Y}|}{(Y_n + \overline{Y})/2}, i = 1, 2, \ldots$$

Where N is the total number of measurements in the interval, Y_n is the cross-section of the n-th point and $\overline{Y}$ is the average. When the variance is higher than 0.18 (defined empirically) the interval is considered in a resonance area. Sometimes, when the resonance spikes are far from one another, the discretization with 50 intervals
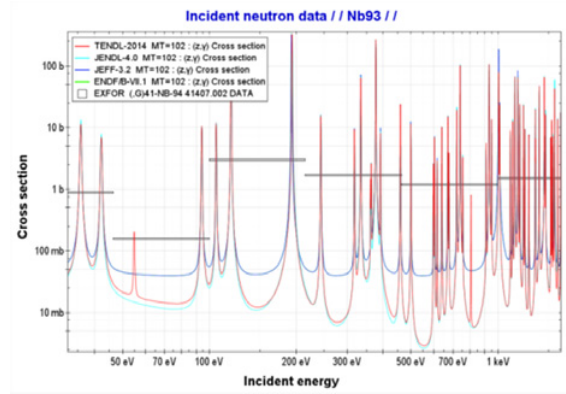

Figure 2. Suspicious subentry in resonance zone for ^{93}Nb(n,γ).

is too precise, resulting in low relative variance for all intervals. Resonance intervals may thus be considered as no-resonance intervals by the algorithm.

5) Computing the distance and the ratios for each interval:

In a **no-resonance interval**, the mean ratio of all the EXFOR points-i is computed as follows:

$$\text{ratio\_interval} = \frac{1}{N} \sum_{i=1}^{N} \frac{\text{distance}_i}{\max(\sigma_i^{EXFOR}, \sigma_i^{ENDF})}.$$

Where "distance$_i$" is computed as shown in Fig. 1. The cross-sections and standard deviations of ENDF corresponding to each EXFOR point's abscissa are obtained by linear interpolation. In practice ENDF is not really a curve but a very dense set of points, so there is not necessarily an ENDF point at the exact same abscissa as EXFOR.

In a **resonance interval**, the distance is the difference between the integral of ENDF and EXFOR. The interval is discretized in 10 subintervals. The integrals of EXFOR or ENDF are computed as below:

$$\overline{Y}^{\text{EXFOR or ENDF}} = \frac{1}{10} \sum_{j=1}^{10} \frac{1}{N_j} \sum_{i=1}^{N_j} Y_i^{\text{EXFOR or ENDF}}.$$

Where N_j is the number of points in the subinterval-j. The ratio is computed as follows:

$$\text{ratio\_interval} = \frac{\overline{Y}^{EXFOR} - \overline{Y}^{ENDF}}{\max(\overline{\sigma}^{EXFOR}, \overline{\sigma}^{ENDF})}.$$

Where $\overline{\sigma}$ is the mean vertical standard deviation. The horizontal uncertainties are not taken into account in a resonance interval.

This method has several limitations for resonance intervals. In the example Fig. 2, the mean values of EXFOR and ENDF do not match, but if one considers the large horizontal uncertainty, the subentry appears less suspicious. In addition, comparing the mean value is not suitable when the EXFOR point is located on a spike.

6) Averaging the ratios of the 50 intervals;
7) Computing the rank for the complete entry based on the average ratio, and computing the rank of the worst single EXFOR point (only in no-resonance interval). This allows to detect a single aberrant point in a subentry that is globally correct.

Table 1. Subentries checked, cases with a rank D or E (in %).

MF	MT	Number of subentries	Rank of D or E	D or E in (%)
3	(n,tot)	3742	142	3.8
3	(n,el)	1195	61	5.1
3	(n,nonelastic)	279	87	31.2
3	(n,n)	258	63	24.4
3	(n,2n)	1593	46	2.9
3	(n,3n)	66	0	0.0
3	(n,fission)	1440	45	3.1
3	(n,nalpha)	56	11	19.6
3	(n,2nalpha)	5	0	0.0
3	(n,np)	75	9	12.0
3	(n,nX)	3400	229	6.7
3	(n,n4)	28	2	7.1
3	(n,gamma)	3697	566	15.3
3	(n,p)	1913	29	1.5
3	(n,d)	43	2	4.7
3	(n,t)	157	16	10.2
3	(n,He)	38	15	39.5
3	(n,alpha)	1123	39	3.5
3	(n,2alpha)	4	0	0.0
3	(n,2p)	14	9	64.3
10	(n,n)	262	8	3.1
10	(n,2n)	1148	60	5.2
10	(n,3n)	20	4	20.0
10	(n,nalpha)	20	2	10.0
10	(n,np)	21	0	0.0
10	(n,n4)	3	0	0.0
10	(n,gamma)	496	113	22.8
10	(n,p)	690	29	4.2
10	(n,t)	45	5	11.1
10	(n,He)	6	1	16.7
10	(n,alpha)	310	25	8.1
10	(n,2p)	1	1	100.0
4	(n,el)	4549	1099	24.2

5. Results

Only 2% of the subentries have been classified in the lowest rank "E". The numbers of subentries that have obtained a ratio superior to several thresholds are presented below:

– Ratio > 2: 3665 subentries;
– Ratio > 3: 2937 subentries;
– Ratio > 5: 1932 subentries;
– Ratio > 10: 284 subentries;
– Ratio > 20: 45 subentries.

For natural elements, 3118 subentries were checked: 173 obtained a ratio > 8, and 20 have ratio > 20. All the subentries that have obtained a rank of D or E (ratio > 3) with all evaluators are reported for each type of reaction in the Table 1.

Based on this checking, the most suspicious data are (n,n α), (n,He), (n,2p), (n,nonelastic), (n,nX) and (n, γ). The proportion of potential outliers might seem high, but the method is based on uncertainties, so a point can receive a bad ranking when the uncertainties of both ENDF and EXFOR are very small with respect to the distance, and this situation is very frequent.
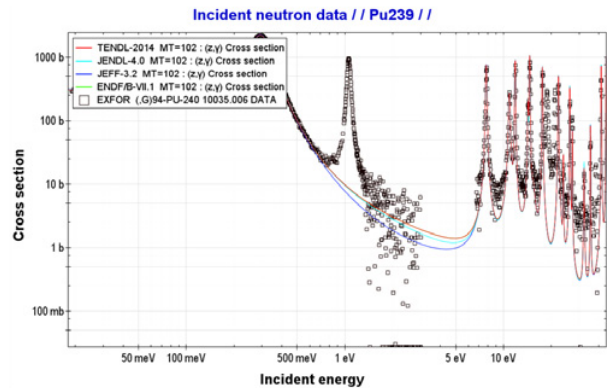

Figure 3. EXFOR entry 10035.005 for ^{239}Pu (n, γ). The resonance at 1eV is due to the contribution of ^{240}Pu in the experiment.
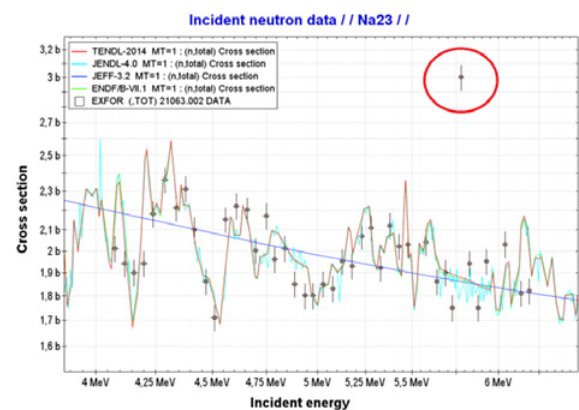

Figure 4. Suspicious single point for ^{23}Na (n,total).
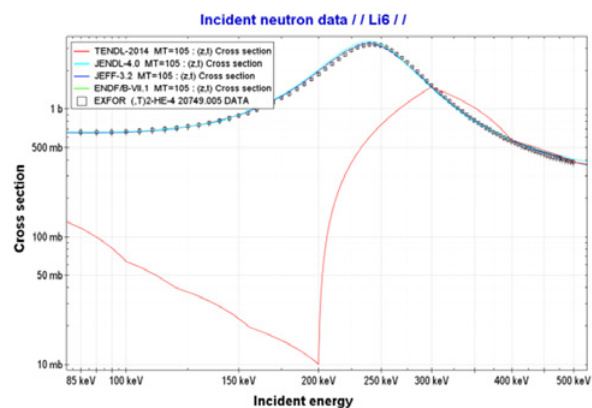

Figure 5. ^{6}Li(n,t) reaction showing large difference in TENDL.

Table 1 includes only the subentries that might have a global problem (see Fig. 3), but it does not include the subentries that contain a single aberrant point (Fig. 4).

There are multiple types of problems in resonance zones: i) EXFOR data shows spikes but ENDF is flat (Fig. 3); ii) EXFOR data vertically shifted from ENDF, or vertically/horizontally compressed; iii) data are erratic and do not match ENDF at all (middle of Fig. 3).

In no-resonance zones, the aberrant subentries are often constituted of only one single point that is much lower or higher than ENDF (see Fig. 4).

The proportion of subentries that disagrees with at least one evaluator is obviously much greater. An example of disagreement is shown in Fig. 5.

Table 2. Comparison of calculated (C) and EXFOR (E) values. Number of cases given in log(|C/E|) units.

# Cases in log (|C/E|) units	ENDF/ B-VII.1	JEFF- 3.2	JENDL- 4.0	TENDL- 2014
≤ 1	780	768	782	760
2	7	16	5	22
3	2	5	2	6
4	1	1	1	2

6. Resonance integral

To complete the checking in the resonance energy range, a comparison of the resonance integrals has been performed. In the Atlas of Neutron Resonances [2], the epi-cadmium dilute resonance integral for a particular reaction in a 1/E spectrum, is givens as:

$$RI = \int\limits_{E_{min}}^{E_{max}} \frac{\sigma(E)}{E} dE,$$

The term 1/E represents the neutron spectrum for fission reactors between the Maxwellian and the fission spectrum. The upper energy bound is assumed $E_{max} = 100$ keV and the lower energy bound E_{min} corresponds to the cadmium cutoff energy, equals 0.50 eV. E_{max} and E_{min} are mostly taken from the Atlas, which provides values calculated using all of the resonance within that energy range, as well as a contribution from the 1/v cross section background. Some of these values are a compilation of experimental values while others are derived from the resonance parameters included in the Atlas [3]. In this work, a comparison of 790 EXFOR recommended (RECOM) and calculated (CALC) entry values to some major nuclear data libraries is carried out. Few deficiencies in EXFOR entries (wrong compilation of energy limits...) were found and reported to NRDC. Table 2 summarizes this comparison.

Then, large differences between evaluations have been found. As an example, Table 3 shows the large overestimation given by JEFF-3.2 for the calculated integral resonance of ^{50}Ti(n,γ). In Fig. 6, the cross-section of ^{50}Ti(n,γ) is illustrated showing large difference between JEFF-3.2 and other evaluations.

Table 3. EXFOR values for the integral resonance of capture in ^{50}Ti. Relative error ((C-E)/ΔE).

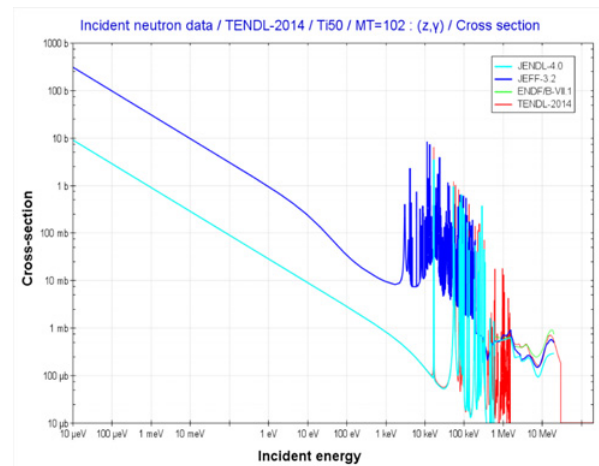| Reference	RI (b)	DRI(b)	(Calc.-EXFOR)/ΔEXFOR	
			ENDF/B-VII.1 TENDL2014 JENDL-4.0	JEFF-3.2
V1001.169	8.3E-02	6.0E-03	1	392

Figure 6. Comparison of ^{50}Ti (n,γ) cross section.

7. Conclusion

The algorithm allowed to focus on the most suspicious data among the whole set of data of 26,636 EXFOR subentries. More than 459 subentries have been classified in the lowest rank. This analysis might be useful for NRDC to find potential outliers, and for evaluators to improve current evaluations.

Future activities will be focused on the development of a new methodology to tackle the difficulties to assess the resonance energy range. Finally, this study has been applied to induced neutron reaction, but can be extended to other induced reactions (e.g. charged particles, ...).

References

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