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Definitions for Testing Whether Evaluated Nuclear Data Relative Uncertainties are Realistic in Size

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Contents

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Abstract

Keywords: Nuclear Data, Relative Uncertainties, Expert Judgment Limits, Physics Uncertainty Boundaries, Templates of Expected Measurement Uncertainties.

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This document describes various tests that can be used to check whether evaluated relative uncertainties stored in nuclear-data covariances are realistic. To be more specific, these tests check whether nuclear-data uncertainties could be either over- or under-estimated given the input that usually enters the evaluation of nuclear-data mean values and covariances. Warning and error messages on the reliability of nuclear-data uncertainties will result from these tests. If uncertainties of one specific nuclear-data observable trigger warning messages from multiple tests, an evaluator should counter-check the reliability of the relative uncertainties of this particular nuclear-data covariance matrix.

1 Why Should We Test Whether Evaluated Nuclear Data Relative Uncertainties Are Realistic in Size?

Nuclear-data covariances quantify the limited knowledge we have on the associated nuclear-data mean values. The covariance matrix provides in the diagonal a measure of the precision of an individual nuclear-data value, while the off-diagonal entries measure the linear dependence of a set of nuclear-data values. Nuclear-data covariances often contain information from nuclear theory and several differential experimental data sets.

Nuclear data are used as input for neutron-transport simulations of various applications. Nuclear-data covariances can be forward-propagated to assess the bounds on an application calculation due to imprecise nuclear data. If the nuclear-data uncertainties are either over- or under-estimated, the bounds on applications due to these nuclear data become unrealistic. Unrealistic bounds on application simulations can raise concerns on adequate safety and operational margins but can also have an economic impact if larger than necessary safety margins need to be applied to a nuclear technology due to unreasonably large evaluated uncertainties.

To give an example, ENDF/B-VIII.0 [1] uncertainties for the ^{239}Pu(n,f) fission cross section increased significantly [2] compared to its previous version [3] (see Fig. 1). This led to a three time larger uncertainty contribution to the simulated criticality of the Jezebel critical assembly [4], namely from 331 pcm to 903 pcm [5], far beyond the difference between prompt and delayed critical ($\sim$ 220 pcm) for this assembly. It was shown in Ref. [6] that this increase for ENDF/B-VIII.0 was justified and that uncertainties reported in the previous nuclear-data library, ENDF/B-VII.1 [7], were underestimated. It is important for the nuclear-data community as well as for nuclear-data users to develop a suite of tests that can automatically detect over- or under-estimated nuclear-data uncertainties early on. It would be best practice to apply these tests before the release of a new nuclear-data library.

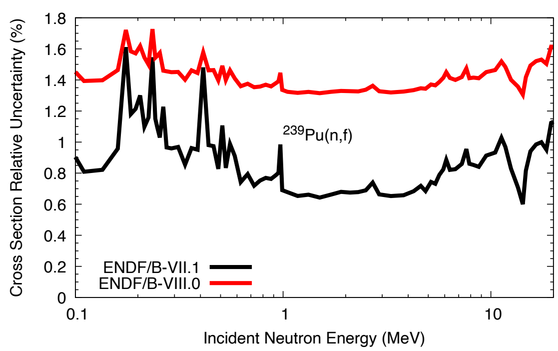

Figure 1: Relative uncertainties of the neutron-induced ^{239}Pu fission cross section are compared for ENDF/B-VII.1 and ENDF/B-VIII.0.

Here, various tests are described that check whether relative uncertainties of nuclear data are over- or under-estimated. These tests are summarized in Section 2 such that they can be easily implemented in various nuclear-data covariance processing and testing codes. An example of applying these tests is discussed in Section 3. For each test, some background explaining the reasoning behind the test is given along with the upper/ lower limits used for testing, and limitations of the test. It should be mentioned that most of these tests can only yield warning messages that the relative uncertainties could be possibly over- or under-estimated as they all rely on approximations of various granularity on the information that enters the evaluation of the studied observables. These warning messages are meant as an indication to evaluators to take a second look at the covariances and let then these expert judge if the uncertainties are realistic. If one applies such tests consistently on large parts of nuclear-data libraries, unrealistic covariances can be more easily spotted.

2 Tests

2.1 Expert Judgment Test

Background D.L. Smith, the previous chair of the CSEWG [1] covariance session, established in Ref. [8] lower limits for the relative uncertainties of various nuclear-data observables. Nuclear-data observables are, for instance, the total or fission cross section (CS), the average prompt-fission neutron multiplicity ($\overline{\nu}_p$) or the prompt-fission neutron spectrum (PFNS). The lower limits in Ref. [8] were defined by expert judgment taking into account how well each of these observables can be measured in a single measurement.

The reasoning behind using experimental uncertainties as the limiting factor on nuclear-data uncertainties is the fact that experimental data are often the constraining factor on nuclear-data evaluations. While nuclear theory provides important information on the shape of nuclear data and allows for extrapolation to energy ranges and observables with little or no experimental information, uncertainties in model parameters often allow for a wide variation of nuclear data that can be determined distinctly more precise with experimental data. To give a specific example, neutron-induced fission cross sections can be reliably measured for many cases with a precision of 1% [9], while small and defensible variations in fission model parameters can easily change predicted fission cross sections by 20% or more [10].

Description and Limits The 1-σ lower limits defined by D.L. Smith in Ref. [8] are summarized in Table I for all available observables. No lower limit was given for the PFNS. However, the PFNS is an important observable for any application simulation relying on fission. Hence, I provided rough 1-σ lower expert-judgment limits for the PFNS in Table II based on my own experience evaluating PFNS.

Table I: 1-σ lower limits for uncertainties of various neutron-induced nuclear-data observables are provided based on Ref. [8].

Observable	Lower Uncertainty Limit (%)
Total Cross Section	1.0
Elastic Cross Section	2.0
(n,γ) Cross Section	2.0
Inelastic Cross Section	3.0
Fission Cross Section	1.0
(n,p) Cross Section	3.0
(n,α) Cross Section	3.0
Other Cross Section	3.0
Average Prompt/ Delayed Neutron Multiplicity	1.0

Table II: 1-σ lower limits for evaluated PFNS uncertainties are provided based on expert judgment.

Outgoing-neutron Energy (MeV)	Lower Uncertainty Limit (%)
0.01	10
1.0	1
5.0	3
10.0	20

If nuclear-data uncertainties are below the limits put forth in Tables I and II, these uncertainties should be flagged via a warning message as potentially too low.

[1] CSEWG assembles, validates and disseminates US nuclear-data libraries. Several national laboratories, industry and universities are contributing to CSEWG and its nuclear-data libraries.

Limitations of the Test It should be mentioned that the lower limits put forth in Tables I and II constitute the first attempt in the field of nuclear data to formalize common-sense lower limits for evaluated nuclear-data uncertainties. They are very roughly estimated and were meant to be broadly applicable for nuclear data across the chart of nuclides.

As such, they capture the typical uncertainty level of many observables and isotopes but are not sufficiently fine-grained enough, both for specific isotopes and in energy. One limitation, for instance, is that these limits are rather high when applied to isotopes with abundant differential data available in the EXFOR database [11] [2]. For instance, the fission cross sections and $\overline{\nu}$ of major actinides have been measured multiple times with a combined precision that can reach credibly lower uncertainties than put forth in Table I. Also, the expert-judgment limits described here do not vary with incident-neutron energy. For instance, data above 14 MeV can become scarce for many isotopes and the lower limit should then be higher.

Hence, I would recommend to only give a warning message if relative uncertainties are below the limits defined in Tables I and II. An evaluator should certainly take a look if a warning message with this test occurs for all isotopes ***excluding*** the following isotopes: major actinides (^{235,238}U, ^{239}Pu), isotopes often used in applications (any component that appears to more than 10% in steel, water, air, *etc.*) nor a standard reaction as defined in Ref. [2]. For those isotopes called out as excluded, an evaluator should take a look if warning messages from several tests described in this manuscript occur for one and the same observable.

[2] The EXFOR database contains more than 20,000 data sets that serve as input for evaluations of nuclear data.

2.2 Neutron Data Standards Test

Background Many nuclear-data observables are measured relative to a standard observable. These standards are defined and evaluated by the IAEA-co-ordinated Neutron Data Standards committee. The current standards observables and the energy range where they are applicable are defined in Table 1 of Ref. [2].

The advantage of measuring an observable as a ratio to a standard one is that many systematic correction factors drop out of the measurement. For instance, one might not need to determine the detector efficiency or the neutron fluence for a particular measurement. The determination of these two analysis components is a challenge and often leads to associated uncertainties being the major contributions to total measurement uncertainties. On the other hand, one obtains ratio data as a final results, i.e., x/s where x is the desired observable and s the standard one. The evaluator has to then multiply the ratio, x/s, with evaluated nuclear data for s to obtain x that is actually used for the evaluation. Hence, uncertainties on the standard nuclear data reported in Ref. [2] need to be forward-propagated to give total uncertainties on experimental data x.

If many measurements for one and the same observables were measured as ratios to a specific standard s, the standard nuclear-data uncertainty becomes a common uncertainty source across all these measurements. Hence, the final evaluated uncertainty should be limited by the uncertainty on s. Many nuclear-data observables are measured relative to one of the standards defined in Table 1 of Ref. [2]. Consequently, the applicable standard uncertainty constitutes a firm lower limit for many nuclear-data observables.

Description and Limits Table III shows which specific standard uncertainties can be used as a firm lower limit for particular nuclear-data observables. If evaluated nuclear-data uncertainties are below this firm lower limit, an error message should be given. While it is possible to have reliable evaluated uncertainties below a standard uncertainty, it is the exception rather than the rule. In any case where the evaluated uncertainties are below its associated standard, an evaluator should take a closer look on whether the flagged evaluated nuclear-data uncertainties could possibly be underestimated.

Table III: This table shows which standard observables are frequently used as monitors for measurements of various neutron-induced nuclear-data observables. "CS" is short for cross section, while the variable $\overline{\nu}_t$ and $\overline{\nu}_p$ denote the average total- or prompt-fission neutron multiplicity. PFNS stands for prompt-fission neutron spectrum.

Observable	Standards used for Limit
Total Cross Section	None
Elastic Cross Section	^{1}H(n,n) CS (left-hand side of Fig. 2), C(n,n) CS ($\sim$ 0.7%)
(n,γ) Cross Section	None
Inelastic Cross Section	^{1}H(n,n) CS (left-hand side of Fig. 2), C(n,n) CS ($\sim$ 0.7%)
Fission Cross Section	^{235}U(n,f) CS (left-hand side of Fig. 2)
(n,p) Cross Section	None
(n,α) Cross Section	None
Other Cross Section	None
$\overline{\nu}_t$ and $\overline{\nu}_p$	^{252}Cf(0,f) $\overline{\nu}_t$ (0.43%)
PFNS	^{252}Cf(0,f) PFNS (right-hand side of Fig. 2)

Limitations of the Test As mentioned above, there are cases where evaluated nuclear-data uncertainties can be lower than the standard uncertainties associated with this observable in Table III. If, for example, multiple measurements exist for a specific observable and many of those were measured

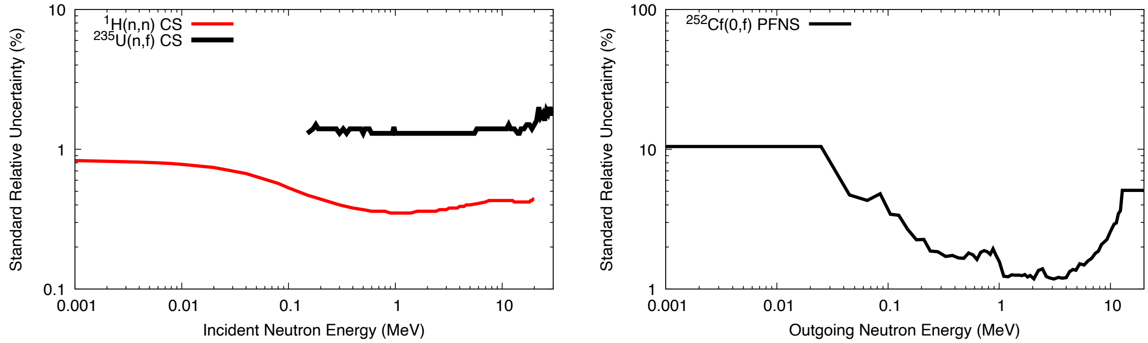

Figure 2: The uncertainties associated with the ^{1}H(n,n) and ^{235}U(n,f) cross-section standards are displayed on the left-hand side. On the right-hand side, the uncertainties associated with the standard ^{252}Cf(sf) PFNS are given. Both plots show data of the 2018 standards reported in Ref. [2]

absolutely rather than as a ratio to a standard, then the final evaluated uncertainty can be lower than the standard. For instance, several ^{235}U(n,f) $\overline{\nu}_p$ measurements were absolute ones and did not rely on a standard.

However, determining the detector efficiency and the neutron fluence can be extremely challenging. Both have to be determined if one does not rely on a ratio measurement to a standard. So, it is indeed difficult to get lower uncertainties than the standard one. One should also consider that many standards observables were measured partially absolutely and also as a ratio to other standards, with extreme care taken to reduce any pertinent biases and uncertainties. So, standards observables usually already come along with the lowest-achievable evaluated uncertainties in the field. Hence, I would treat any evaluated uncertainty for non-standard observables reported to be significantly below the associated standard uncertainties, with caution and study in detail if such low uncertainties are indeed justified.

One word of warning: The IAEA-co-ordinated Neutron Data Standards committees does regularly revise their uncertainties. For instance, the ^{239}Pu(n,f) cross-section uncertainties shown in Fig. 1 were both released by that committee. It is obvious that they are very different, and constitute always only the best knowledge at the time of the release of the data. Hence, it is important to always use the newest standards values and uncertainties for these tests.

2.3 Templates Test

Background Templates of expected measurement uncertainties are defined for various nuclear-data observables in Refs. [9, 12]. They summarize what uncertainty sources apply to typical nuclear-data measurements of an observable. These uncertainty sources correspond, in a sense, to all independent physics processes occurring in a nuclear-data measurement that in their combined entirety yield the reported experimental value for the observable of interest. Uncertainty values were provided for all uncertainty sources listed based on a broad literature review across many measurements, an in-depth review of information in the EXFOR database, and by consulting experimentalists executing such experiments. These uncertainties can be used as a stand-in value by nuclear-data evaluators, if no uncertainty values were provided for a particular uncertainty source in a past measurement.

These template uncertainties can also be applied to counter-check the evaluated nuclear-data uncertainties. As mentioned before, experimental uncertainties are often the limiting factor of evaluated nuclear-data uncertainties as nuclear theory is usually less constraining. The template uncertainties can yield total uncertainties of a typical measurement for a nuclear-data observable. Given that nuclear-data uncertainties are often bounded by uncertainties on experimental data, these template uncertainties can provide a limit for how low or high nuclear-data uncertainties can be.

Description and Limits The uncertainty sources encountered in typical measurements of nuclear-data observables are listed in Table IV. For each of these uncertainty sources, a typical value is provided in Refs. [9, 12]. These uncertainty values were added up in quadrature to yield total uncertainties of a typical measurement for a particular nuclear-data observable. Adding the individual uncertainties up in quadrature is appropriate as the uncertainty sources were established to be independent.

Table IV: The template uncertainty sources considered for estimating the limits in Table V are listed for specific nuclear-data observables. The relevant uncertainty sources per observable were defined in Refs. [9, 12].

Observable	Uncertainty Sources Included
Total Cross Section	Statistical, target density, flux
Elastic Cross Section	Statistical, neutron-production target, neutron-flux monitor, sample, geometry, multiple scattering, nuclear data, detector efficiency, peak identification
(n,γ) Cross Section	Statistical, flux normalization, target density, sample composition
Inelastic Cross Section	Statistical, neutron-production target, neutron-flux monitor, sample, geometry, multiple scattering, nuclear data, detector efficiency, peak identification
Fission Cross Section	Statistical, normalization, detector efficiency, background, deadtime, impurity, nuclear data, attenuation, multiple scattering, angular distribution of fission fragments
(n,p) Cross Section	Statistical, normalization, flux normalization, angle, multiple scattering, deadtime, detector efficiency

(n,α) Cross Section	Statistical, normalization, flux normalization, angle, multiple scattering, deadtime, detector efficiency
$\overline{\nu}_p$ and $\overline{\nu}_t$	Statistical, delayed gammas, background, false fissions, deadtime, PFNS, angular distribution of fission fragments, sample thickness, sample displacement, impurity
PFNS	Statistical, nuclear data, background, multiple scattering, impurity, deadtime, angular distribution of fission fragments

Lower and upper limits, put forth in Table V, were established based on the following considerations:

- The lower limits were derived by multiplying the total uncertainties obtained in quadrature from the individual template uncertainties by a multiplicative factor between 0.5–0.8. The total template uncertainties were reduced for the lower bound, because in many cases multiple experimental data sets are available for the evaluation of one nuclear-data observable. The uncertainty sources in Table IV come along with estimates of their correlation coefficients across energies and experiments. As many uncertainty sources are not fully correlated between two different measurements, the evaluated uncertainties from these two measurements should be reduced. Reducing total template uncertainties accounts for this reduction of evaluated uncertainties if several measurements are considered.

- The upper limits in Table V were obtained by multiplying the total template uncertainties by a factor of 3. This increase accounts for the fact that it can be extremely challenging to measure observables of specific isotopes, due to, e.g., short half-lives, low sample mass or very small values (e.g., at the threshold) for the particular observable.

Table V: Upper and lower limits (1-σ) for uncertainties of various neutron-induced nuclear-data observables are listed. These limits were estimated based on templates of expected measurement uncertainties [9, 12].

Observable	Lower Uncertainty Limit (%)	Upper Uncertainty Limit (%)
Total Cross Section	0.9	3.4
Elastic Cross Section	3.0	18.2
(n,γ) Cross Section	1.7	6.4
Inelastic Cross Section	3.9 (discrete), 8.1 (continuum)	23.2 (discrete), 48.3 (continuum)
Fission Cross Section	Fig. 3	Fig. 3
(n,p) Cross Section	3.0	11.2
(n,α) Cross Section	3.0	11.2
Other Cross Section	None	None
$\overline{\nu}_p$ and $\overline{\nu}_t$	Fig. 4	Fig. 4
PFNS	Fig. 5	Fig. 5

If evaluated nuclear-data uncertainties are below the lower limits defined in Table V, they should be flagged by a warning message as possibly too low. In turn, if evaluated nuclear-data uncertainties are above the higher limits defined in the same Table, a warning message should be triggered that the evaluated uncertainties are possibly too high.

Limitations of the Test Contrary to the Neutron Data Standards tests, these template limits do not constitute firm upper or lower bounds. It is indeed possible to reach credible evaluated nuclear-data uncertainties below the lower limits put forth in Table V. One should remember that the template

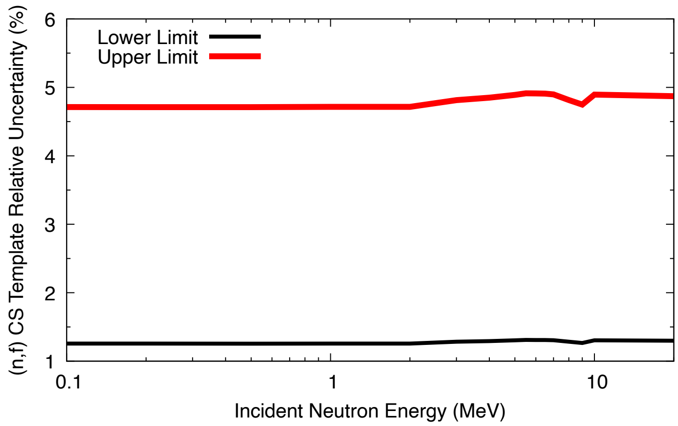

Figure 3: Upper and lower limits for (n,f) cross-section uncertainties are shown. These limits were estimated based on templates of expected measurement uncertainties [9].

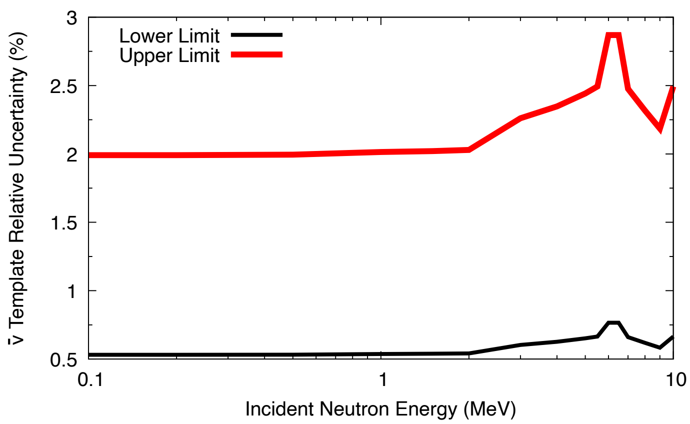

Figure 4: Upper and lower limits for $\overline{\nu}_p$ and $\overline{\nu}_t$ uncertainties are shown. These limits were estimated based on templates of expected measurement uncertainties [12].

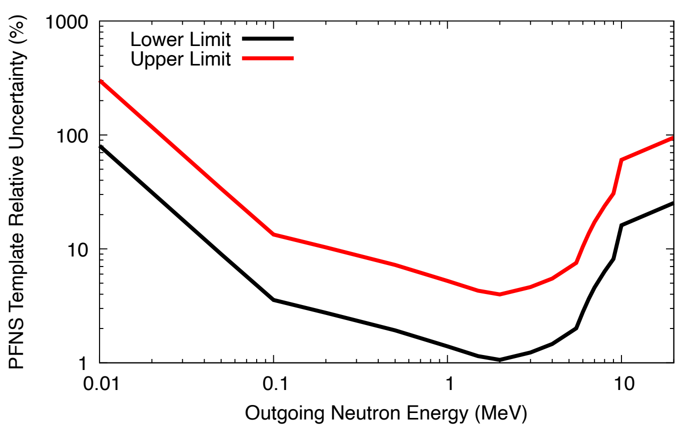

Figure 5: Upper and lower limits for PFNS uncertainties are shown. These limits were estimated based on templates of expected measurement uncertainties [12].

uncertainties were established with ***typical*** measurements in mind and often conservative estimates are provided for template uncertainties. However, for highly important nuclear-data observables (e.g., standard observables) measurement campaigns were and are undertaken with the explicit aim to reduce uncertainties to the best of the ability of the experimental team. Hence, measurements entering these evaluations frequently have lower uncertainties than estimated for the templates. In turn, the resulting evaluated uncertainties are below the template uncertainty bounds in Table V and with a good reason.

On the other hand, it is also possible that evaluated nuclear-data uncertainties larger than the upper limits defined in Table V can be encountered and are justified. The reason for that could be, for instance, that no experimental data were available for that particular observable and energy range. Hence, the template limits do not apply for this particular case.

Due to these limitation, the choice was taken to only generate warning messages if evaluated nuclear-data uncertainties fail the template test. However, evaluators should take a look at the evaluated uncertainties if nuclear-data uncertainties of one particular observable fail this and other tests.

2.4 Test versus Spread in Experimental Differential Data

Background In a recent publication of an IAEA working group [13], clues were identified that point towards the possibility that "unrecognized sources of uncertainties" (USU) could potentially be present in a body of experimental input data. These USU could potentially lead to under- or over-estimated nuclear-data uncertainties. Some of these clues can only be studied by evaluators at the time of their evaluation or require too much in-depth information on the experimental data entering the evaluation to enable automatic testing whether evaluated uncertainties are over- or under-estimated. However, Clues 1, 3, 4 in Ref. [13] can be easily used to craft a test to identify potentially over- or under-estimated nuclear-data uncertainties.

All three Clues rely on comparing evaluated nuclear-data uncertainties to the spread in differential experimental data, that often bound evaluated uncertainties. Clue 3 in Ref. [13] states that one would expect under the assumption of a normal distribution that roughly one third of existing data points would fall within the evaluated nuclear-data uncertainties. Excessive number of data points lying outside the 1-σ evaluated nuclear-data uncertainties could point towards underestimated nuclear-data uncertainties, while too many data points within the 1-σ bound raise the question whether the nuclear-data uncertainties could be over-estimated. It should be mentioned that this clue implicitly assumes that the experimental data are curated, i.e., all data known to be outlying or biased were removed by the evaluator.

Description and Limits Here, Clue 3 of Ref. [13] is used to quantify whether evaluated nuclear-data uncertainties are over- or underestimated. To that end, the 1-σ lower bounds on a nuclear-data observables are defined as 1.41 times the nuclear-data uncertainties added to the nuclear-data mean values. An example of the 1-σ bounds relative to the spread in differential data is shown in Fig. 6. While the uncertainties are not multiplied with a factor of 1.41, it is clear that the evaluated uncertainties around 100 keV to 2 MeV contain much less than one thirds of the experimental data.

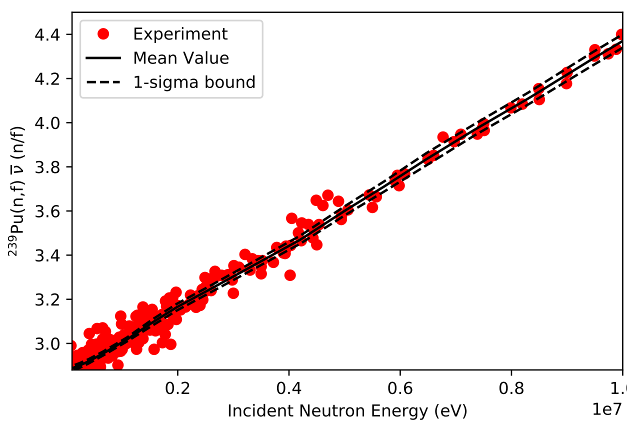

Figure 6: The spread in ^{239}Pu(n,f) $\overline{\nu}_p$ differential data is compared to ENDF/B-VIII.0 mean values and uncertainties to illustrate that less than one third of data points from 0.1–2 MeV are within the evaluated uncertainties.

The multiplicative factor of 1.41 in this test accounts for the fact that in many evaluations two sources of information enter: (1) differential experimental data, and (2) theory. Usually, these two contributions to the evaluation should be independent, and, hence, uncertainties could reduce by up to a factor of 1.41, if one assumes the model uncertainties to be at the level of those of experimental data. This assumption is likely not satisfied in many cases—usually theory is less precise than experimental data—but it makes this test less restrictive. If less than 50% of the differential experimental data points lie within the range spanned between the above-defined nuclear-data uncertainties, one might question whether the evaluated uncertainties could possibly be under-estimated.

Alternatively, one can test whether the evaluated nuclear-data uncertainties are over-estimated by assigning upper and lower bounds around the nuclear data by adding the 1-σ bounds to the mean values. If more than 90% of the differential experimental data lie within these bounds, one should check whether evaluated nuclear-data uncertainties could potentially be over-estimated.

Limitations of the Test One critical barrier to this test is that it requires curated experimental data as its basis. In the best-case scenario, one should use the exact database as used as input for the nuclear-data evaluation producing the uncertainties. However, differential data as used for an evaluation are rarely stored and only in exceptional cases openly available.

Hence, one has to take recourse to extracting data from the EXFOR database [11]. However, these data are not curated. For instance, outliers are not removed, known biases in data are not reported, and ratio data are not re-normalized to the newest standard. These issues lead to a larger spread in differential data than is justified. In addition to that, it is difficult to extract data from the EXFOR database [11] automatically; the format is cumbersome and increasingly more difficult for observables beyond cross sections. Hence, the test designed above can only be done for in-house calculations at the moment. However, this might be a test that can be easily implemented in nuclear-data evaluation codes to counter-check whether resulting evaluated uncertainties are realistic.

Also, right now, an international working group, WPEC SG-50 [14], aims at increasing the readability of EXFOR data and implementing outlier identification codes automatically to EXFOR data to flag questionable data. In the future, the resulting WPEC SG-50 database, might also store differential experimental data as used for a particular evaluation.

2.5 Physical Uncertainty Bounds Test

Background The Physical Uncertainty Bounds (PUBs) method developed by Vaughan and Preston [15] aims to bound a composite quantity of interest. In general, his method estimates bounds on a quantity of interest by first parting it into all its independent constituting physics sub-processes and assessing then bounds on those sub-processes that non-negligibly impact the make-up of the quantity of interest. For instance, the quantity of interest, $q = f(a, b, c)$, is obtained by independent sub-processes, a, b, and c. If one can vary the sub-process a widely without impacting q, then one has to just bound b and c. The individual physics sub-processes are bound by considering (a) realistic experimental data and associated uncertainties, and (b) governing physics laws directly related to them.

The PUBs method was applied in Ref. [6] to establish minimal realistic and conservative bounds on the ^{239}Pu(n,f) cross section. The evaluated nuclear data of this observable was exclusively obtained by experimental data as part of the Neutron Data Standards project (version 2018 [2]). However, the experimental data themselves are composite measurements with many separate physics sub-processes (e.g., detector efficiency, and sample mass determination). Hence, bounds had to be established on the separate sub-processes. From bounds on the individual sub-processes, total conservative and minimal realistic PUBs bounds were estimated. These bounds were then used to counter-check whether evaluated uncertainties in ENDF/B-VIII.0 were realistic. If the evaluated uncertainties were below the minimal realistic bounds estimated by PUBs, the evaluated uncertainties were deemed to be under-estimated. If the evaluated uncertainties were above the conservative bounds estimated by PUBs, the evaluated uncertainties were likely over-estimated.

Minimal realistic and conservative PUBs bounds were also estimated for ^{239}Pu(n,f) $\overline{\nu}_p$ and PFNS. The bounds for the former are documented in Ref. [16]. All these bounds were estimated considering constraints on physics processes governing the experimental data rather than based on physics laws. The reason for this is that physics laws would result in much larger bounds. This emphasizes again the fact that differential experimental data are in many cases more constraining for nuclear data than physics laws and theory considerations. However, physics laws come into play in two instances: In cases with sufficient differential experimental data, they often provide constraints on the expected shape of evaluated data. For instance, in some energy ranges, we expect no sharp peaks in specific observables due to the underlying physics (e.g., no resonance behavior is expected in the ^{239}Pu(n,f) fission cross section from 0.5–20 MeV as resonances are so close together that the cross section is smooth). Nuclear theory encoding physics laws can also help provide bounds on observables or energy ranges without differential data. However, as mentioned above, the bounds will be very large.

Description and Limits Lower (minimal realistic) and upper (conservative) PUBs limits were only estimated for three observables so far as shown in Table VI. They were obtained for only ^{239}Pu based exclusively on experimental information. One should keep in mind that the measurement methods applied to determine ^{239}Pu experimental data are usually employed for many other isotopes. Hence, bounds relevant for ^{239}Pu can also be applied to isotopes with comparable amount of differential experimental data. Hence, these bounds can also be used for the same observables of ^{235,238}U. Factors to multiply the PUBs bounds of other isotopes are given in Table VII. These should be used to multiply upper bounds shown in Figs. 7 and 8 before utilizing them to test evaluated relative uncertainties of isotopes beyond ^{235,238}U and ^{239}Pu.

The PUBs bounds can be used in the following manner: If the evaluated relative uncertainties are below the lower PUBs bounds (both 1 σ), the evaluated uncertainties should be flagged as under-estimated. If the evaluated relative uncertainties are above the upper PUBs bounds (both 1 σ), the evaluated uncertainties should be flagged as over-estimated. Given that these bounds were estimated for ^{239}Pu and not for all isotopes specifically, warning rather than error messages should be given.

Table VI: It is shown in this table for which observables PUBs bounds are currently available.

Observable	Lower Uncertainty Limit (%)	Upper Uncertainty Limit (%)
Total Cross Section	None	None
Elastic Cross Section	None	None
(n,γ) Cross Section	None	None
Inelastic Cross Section	None	None
Fission Cross Section	Fig. 7	Fig. 7
(n,p) Cross Section	None	None
(n,α) Cross Section	None	None
Other Cross Section	None	None
$\overline{\nu}_p$ and $\overline{\nu}_t$	Fig. 7	Fig. 7
PFNS	Fig. 8	Fig. 8

Table VII: Multiplicative factors for various PUBs bounds dependent on isotope are shown.

Observable	^{235,238}U, ^{239}Pu	Other Actinides
Fission Cross Section - Lower Bounds	1.0	2.0
Fission Cross Section - Upper Bounds	1.0	4.0
$\overline{\nu}_p$ and $\overline{\nu}_t$ - Lower Bounds	1.0	2.0
$\overline{\nu}_p$ and $\overline{\nu}_t$ - Upper Bounds	1.0	4.0
PFNS - Lower Bounds	1.0	2.0
PFNS - Upper Bounds	1.0	4.0

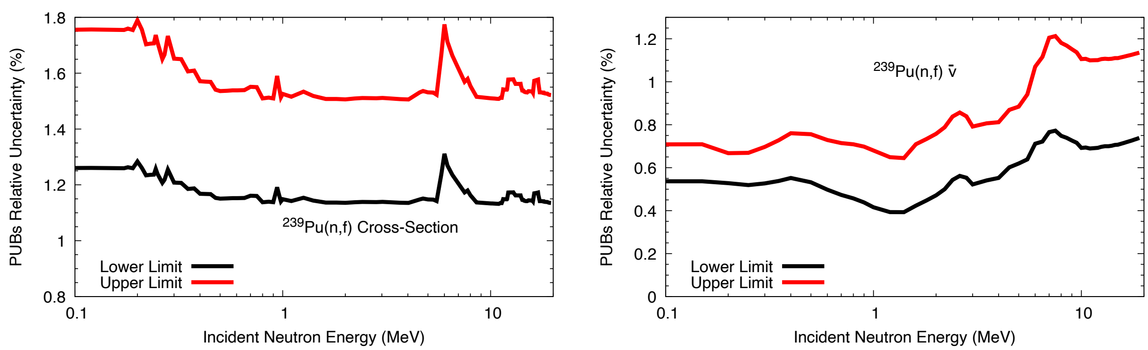

Figure 7: PUBs bounds (1 σ) for the neutron-induced fission cross section (left-hand side), the $\overline{\nu}_p$ and $\overline{\nu}_t$ (right-hand side) are shown as estimated in Refs. [6, 16]. Lower (minimal realistic) and upper (conservative) limits are shown in black and red, respectively. The multiplication factors of Table VII apply dependent on isotope.

Limitations of the Test One obvious limitation of the PUBs test is that limits for only three observables are given. Bounds for more observables should be estimated. In addition to that, PUBs bounds were only estimated for ^{239}Pu and are applied to other isotopes. While they likely provide a good bound for other isotopes, given that the same measurement methods are usually used for several isotopes, the PUBs bounds shown are not as exact for other isotopes. Hence, the decision was taken to give warning rather than error messages, if evaluated relative uncertainties of another isotope than ^{239}Pu fail the PUBs test.

PUBs bounds were also given so far only for those observables with reasonable amount of differential experimental data. Bounds would need to be estimated based on physics laws (nuclear-theory

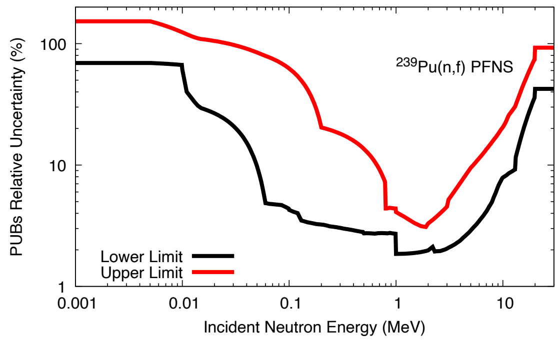

Figure 8: PUBs bounds (1 σ) for the neutron-induced PFNS are shown. Lower (minimal realistic) and upper (conservative) limits are shown in black and red, respectively. The multiplication factors of Table VII apply dependent on isotope.

considerations) for cases with scarce or no experimental information; they will be significantly larger than for cases where experimental information is available. One major stumbling block to applying these exclusively theory-based bounds is that automatic codes would need to know whether reliable experimental data are available or not for an observable. One would need to automatically load in data from the EXFOR database and know whether the available data are realistic. As mentioned in Section 2.4, automatically accessing large parts of EXFOR is a challenge and only small parts of the data are curated. Hence, these two limitations of the database form a critical barrier to applying such tests easily.

Another limitation applies only to the PFNS: Only one set of PUBs bounds is provided for all incident-neutron energies. These bounds would be expected to change dependent on the physics happening at each incident-neutron energy. For instance, experimental PFNS uncertainties are usually largest at second-chance fission. This could not be accounted for given the lack of differential experimental data.

Last but not least, PUBs bound need to be applied to light elements. So far, only bounds for actinides are estimated. Light elements have more stringent bounds coming in from physics laws (unitarity constraints through R-matrix theory) that need to be taken into account when estimating PUBs bounds.

3 Example of Applying These Tests

In Fig. 9, the tests described above were used to test whether the evaluated ^{239}Pu(n,f) $\overline{\nu}_p$ relative uncertainties in ENDF/B-VIII.0 are realistic. The figures are shown as they are coming out of the current python prototype code for testing whether evaluated relative uncertainties are realistic. All five tests indicate that the evaluated uncertainties are likely underestimated which was the expected result in agreement with Ref. [16].

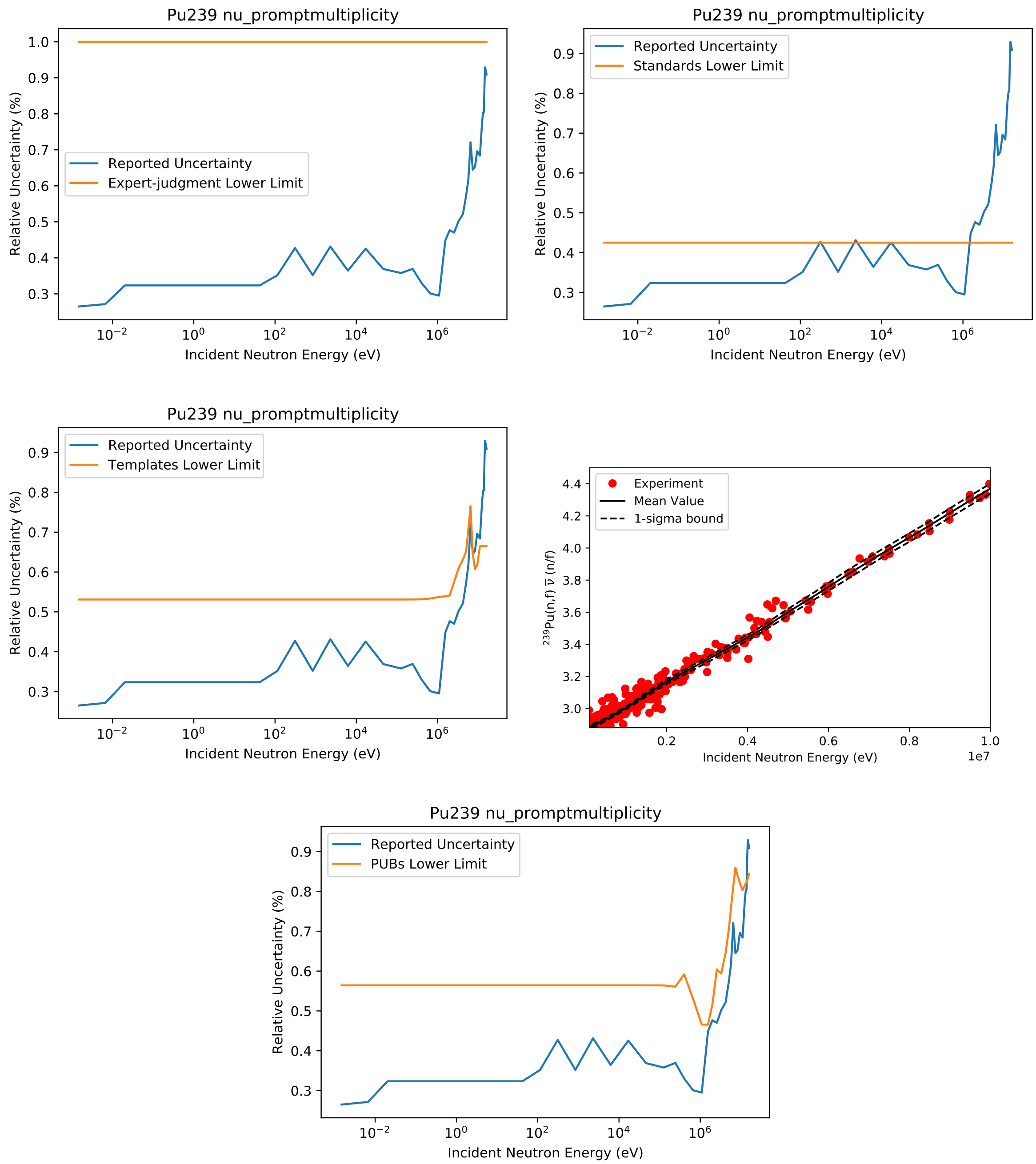

Figure 9: Different tests were applied to counter-check whether the evaluated ^{239}Pu(n,f) $\overline{\nu}_p$ relative uncertainties in ENDF/B-VIII.0 are realistic.

One might question whether some of the tests are redundant. For instance, if the standards test (which provides a hard limit) already triggers an error message that the uncertainties are likely under-estimated, one might not need to counter-check the same uncertainties with other tests anymore (e.g., expert-judgment, templates, and PUBs test). However, the standard test does not apply (i.e., provide bounds) for all observables we have relative uncertainties in nuclear-data libraries for. Hence, for these cases other tests need to be applied.

At the moment, I am working on summarizing the results of the various tests. The current plan is to write out error and warning messages if relative uncertainties of one particular observable fail multiple of these tests as then there is more likely an issue. The ^{239}Pu(n,f) $\overline{\nu}_p$ uncertainties in ENDF/B-VIII.0 are a good example for such a case.

4 Summary and Future Work

In this report, various tests are summarized that counter-check whether evaluated relative uncertainties are realistic. These tests can be applied across whole nuclear-data libraries to pin-point over- or under-estimated uncertainties in our nuclear-data covariances given the input that usually enters their evaluation. Many of these tests trigger warning or error messages that then can be passed on to evaluators that they then take a second look at the covariances and see if they are realistic.

Currently, these tests have been implemented in a python prototype code and applied to counter-check evaluated relative uncertainties of ^{239}Pu ENDF/B-VIII.0 uncertainties. This code, or the tests in them, will be implemented in a processing and V&V covariance toolset by Nathan Gibson to counter-check future nuclear-data covariance libraries for unrealistic uncertainties.

In the near future, a testing hierarchy will be developed that summarizes the output of many of these tests for one nuclear-data observable at a time on a high level. This step should help avoid too many error/ warning messages that make it hard to digest the V&V results. If time permits, PUBs test might be extended to cover more observables and those cases without differential experimental information.

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