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Title: How templates of expected measurement uncertainties and WPEC SG-50 might be helpful for EXFOR

Author(s): Neudecker, Denise

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How templates of expected measurement uncertainties and WPEC SG-50 might be helpful for EXFOR

Denise Neudecker

NRDC meeting 5/16/2022

LA-UR-24-

Templates of expected measurement uncertainties

How could templates help EXFOR compilers?

Templates document what experiment information and uncertainty sources are needed for evaluators to make most use of experimental data stored in EXFOR.

Templates could be used as a check-list by EXFOR compilers to see:

- What information is key to go into metadata of EXFOR,
- What corrections evaluators would look for,
- What uncertainties could be stored and could be asked for.

It would be very helpful if EXFOR compilers could record and ask for that unc. and experiment information. Having this information in EXFOR would positively impact the UQ of exp. data for evaluation and thus evaluated cov for users.

Where are templates documented?

General introduction	D. Neudecker et al., EPJ N 9, 35 (2023) , https://doi.org/10.1051/epjn/2023014
Fission cross section	D. Neudecker et al., NDS 163, 228 (2020), https://doi.org/10.1016/j.nds.2019.12.005
Total cross section	A. Lewis et al., EPJ N 9, 34 (2023) , **https://doi.org/10.1051/epjn/2023018**
Capture and charged particle cross section	A. Lewis et al., EPJ N 9, 33 (2023) , **https://doi.org/10.1051/epjn/2023015**
Scattering cross section	J. Vanhoy et al., EPJ N 9, 31 (2023) , **https://doi.org/10.1051/epjn/2023019**
Neutron multiplicity	D. Neudeckeret al., EPJ N 9, 30 (2023) , **https://doi.org/10.1051/epjn/2023016**
Prompt fission neutron spectrum	D. Neudecker et al., EPJ N 9, 32 (2023) , **https://doi.org/10.1051/epjn/2023013**
Fission yields	E. Matthews, *Advancements in the nuclear data of fission yields*, PhD thesis, Department of Nucl. Engineering, University of California, Berkeley, USA, 2021.

Templates document what information evaluators need for best inclusion of experimental data into evaluation.

What could EXFOR compilers use from templates:

- Lists of data,
- Metadata,

to be reported in EXFOR entry.

EPJ Nuclear Sci. Technol. **9**, 30 (2023)

https://doi.org/10.1051/epjn/2023016

EPJ Nuclear Sciences & Technologies

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Templates of Expected Measurement Uncertainties: a CSEWG Effort, Cyrille De Saint Jean and Denise Neudecker (Guest editors)

REGULAR ARTICLE — OPEN ACCESS

Templates of expected measurement uncertainties for average prompt and total fission neutron multiplicities

Denise Neudecker[1,*], Allan D. Carlson[2], Stephen Croft[3], Matthew Devlin[1], Keegan J. Kelly[1], Amy E. Lovell[1], Paola Marini[4,5], and Julien Taieb[4,6]

3 Information needed for evaluations

The incident-neutron energy, E_{inc}, and either $\overline{\nu}_p$ or $\overline{\nu}_t$ are used as a bare-minimum input for the evaluation. If $\overline{\nu}_p$ is evaluated and the measurement is of $\overline{\nu}_t$, the evaluator needs to correct for the delayed component. If the data were measured in ratio to a monitor, it would be desirable if the ratio data were reported. Otherwise, the nuclear data of the monitor observable, often ^{252}Cf(sf) or ^{235}U(n,f) $\overline{\nu}$, or a reference should be provided. It would be desirable to explicitly state what PFNS was used either by reference or model parameters. Given the convolution of the PFNS with many other observables in the analysis of $\overline{\nu}_p$ measurements in equations (4) and (6), it is difficult to correct with a new PFNS. However, if one knows how close the used PFNS was to current nuclear data, one can estimate potential missing uncertainties due to limited knowledge of the PFNS at the time of the experiment. Partial uncertainties for all uncertainty sources listed in the templates should be provided, if applicable to a particular measurement. The $\overline{\nu}_p$ and $\overline{\nu}_t$ can be measured to high precision. However, even small variations in $\overline{\nu}$ of major actinides can impact the simulated neutron-multiplication factor, k_{eff}, of critical assemblies by a substantial amount. For instance, a change of 0.1% in a relevant energy range of ^{239}Pu(n,f) $\overline{\nu}_t$ can lead to a 100-pcm (i.e., a 0.1%) change in k_{eff} of a Pu assembly, where approximately 210 pcm is the difference between a controlled critical assembly and an accident emitting lethal radiation doses [61]. Hence, reporting complete and realistic uncertainties for $\overline{\nu}_p$ and

$\overline{\nu}_t$ measurements is central for realistic application simulations and their bounds. Along the same lines, the experimental set-up (e.g., time the gate is open, size and isotopic composition of the neutron detector, through-tube size, neutron-producing reaction, impurity level), all pertinent corrections (e.g., background, foil thickness, angular distribution of fission fragments, dead-time, impurities, geometry, spurious structures in neutron flux, delayed γs, displacement of fission sample, false fissions, French effect) and analysis techniques should be documented in great detail, enabling the evaluator to judge the quality of the measurements and data reduction at a later time.

This is part of the section on "Information needed for evaluation." Similar sections should be in most template papers.

Templates help define what measurement type is given for a particular experiment. Knowing that is key for evaluators.

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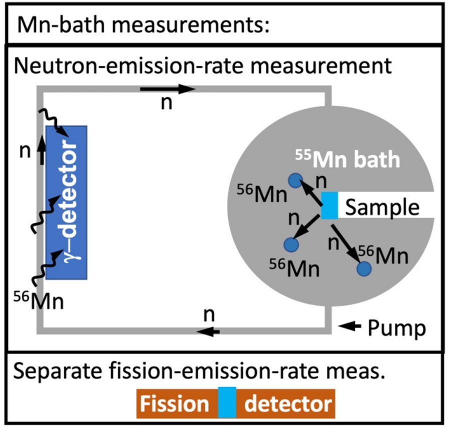
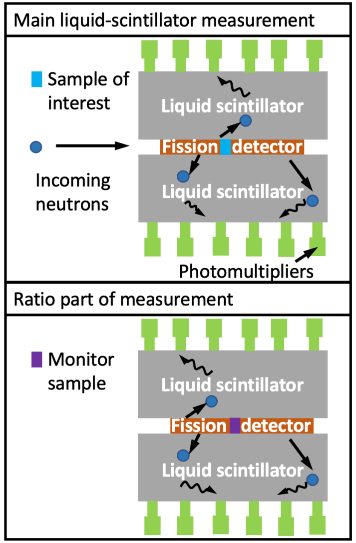
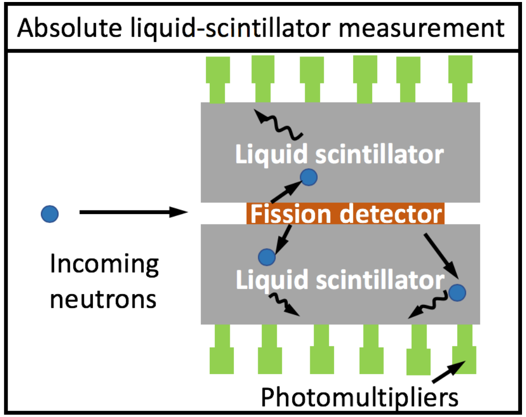
Knowing measurement type informs what:

- Uncertainties
- Metadata
- Corrections

Are needed to be reported in the EXFOR entry.







Templates document what uncertainties should be provided per measurement type.

What could EXFOR compilers use from templates. Lists of expected measurement uncertainties could be used to counter-check:

- If all pertinent partial uncertainties are provided that are expected.
- Ask the author for missing uncertainty sources (and the statement that they are negligible is important!)
- Could help pinpoint mistakes in uncertainties (unreasonably low).

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Table 1. Typical uncertainty sources encountered in absolute and ratio liquid-scintillator measurements of $\overline{\nu}_t$ are listed, along with realistic ranges of estimates that can be assumed if none are provided for a particular measurement. Also, off-diagonal correlation coefficients for each uncertainty source (for the same and different experiments) are roughly estimated. We implicitly assume that the typical tanks have high or similar detector efficiencies of ~80% which is indeed often the case. The correlation functions are defined in reference [62].

Unc.	Absolute (%)	Ratio (%)	Cor(Exp$_i$)	Cor(Exp$_i$,Exp$_j$)
δc	Must be provided	Must be provided (δc & δc^m)	Diagonal	None
δc_{DG}	0.1	0.12	Full	Full
δb	0.15	0.5	Gaussian	0.2 for same n source
				0 otherwise
δc_{ff}	–	0.22 (high α-activity sample)	Gaussian	0.2
	-	0.15 (low α-activity sample)		
δc_{FE}	0.1	–	Gaussian	0.2
$\delta\omega$	see Table 3	see Table 3	0.9	0.9 (same method & isot.)
				0.1 (different isotope)
$\delta\tau$	0.1	0.08	Full	Low (~0.2)
$\delta\varepsilon_\gamma + \delta\varepsilon_c$	0.2	N/A	Gaussian	Gaussian
$\delta\chi$	0.23	0.16	Gaussian	Full (same E_{inc})
		0.5 (2$^{\mathrm{nd}}$-chance fission)		Gaussian (different E_{inc})
δL_n	0.2	N/A	Full	0.5
δa	N/A (isotropic)	0.01–0.3	0.8–1.0	0.6
		0.5 at 2$^{\mathrm{nd}}$ c.f. and >10 MeV		
$\delta\overline{\nu}^m$	N/A	From libraries/reference	Full	Full
δd	N/A (point source)	0.1–0.3	Full	0.8–0.9 (not corrected)
$\delta d_{s/m}$	N/A	0.05	Full	None
ΔE_{inc}	–	Estimate from similar facilities at the same E_{inc}	Full in E_{inc} space	0

Templates describe in detail what corrections are expected to be undertaken for each measurement type.

It would be very helpful for evaluators if EXFOR compilers could list (and ask for) corrections that were undertaken by experimenter. It is also really important to know which corrections were NOT undertaken!

For this example, corrections would be:

- For the PFNS, angular distribution uncertainty, deadtime, backgrounds, random coincidences, etc.

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Corrections are described in the sections on the templates and measurement techniques and are often directly related to uncertainty sources that we need.

Summary: templates try to standardize information needed from experiments for best use in evaluations.

EXFOR is the starting point of many nuclear data evaluations. Descriptive metadata, information on corrections, and partial uncertainties in EXFOR enable evaluators to undertake a detailed uncertainty estimate for experiments entering nuclear data evaluations, and thus contribute to reliable evaluated covariances.

Would it be possible for EXFOR compilers to use templates as a checklist to:

- Put most relevant metadata into EXFOR for individual experiments?
- List what corrections were undertaken or not?
- Ask for partial uncertainties pertaining to the measurement?

We understand that EXFOR compilers rely on what is in the literature and the authors are willing to provide, i.e., there are limits to what you can put in.

WPEC SG-50 and how it might be helpful for EXFOR

WPEC SG50: Developing an Automatically Readable, Comprehensive, and Curated Experimental Reaction Database

- Goal: work towards a new database for experimental data that will build on EXFOR and will store “subjective” corrections to the data sets made by people other than the authors.
- Run-time: 2021-2024
- Coordinators: A. Lewis (Naval Nuclear Laboratory), D. Neudecker (LANL)
- Monitor: A. Koning (IAEA)
- Members: 57 members (and counting) from 11 countries and the NEA and IAEA, representing 5 libraries

This sub-group brought together several users of the EXFOR database.

How might the information from WPEC SG50 be helpful to EXFOR?

As part of WPEC SG-50, we:

- Collated typical EXFOR use cases,
- Summarized the requirements flowing from these use cases.
- We have built a requirement and specification document from that information.

EXFOR is an immeasurable asset to the nuclear data community that is the foundation of many nuclear data evaluations.

We hope that the information we provide here is helpful for future EXFOR developments.

Also, there is a difference between EXFOR and WPEC envisioned SG-50 databases.

<u>WPEC SG-50 database</u>

Layer 0	Layer 1	Layer 2	Layer 3
Same data as in EXFOR entry translated into WPEC SG-50 format	Added information that is in literature but not in EXFOR *-> needs user input*	• Objective corrections – new monitors • Highlighting missing uncertainties with template • Outlier identified	• Subjective corrections • Expert judgment from evaluators • Added unc. with template *-> needs user input*

Also, there is a difference between EXFOR and WPEC SG-50 databases.

Layer 0

Same data as in EXFOR entry translated into WPEC SG-50 format

Layer 1

Added information that is in literature but not in EXFOR

-> needs user input

Layer 2

- Objective corrections – new monitors
- Highlighting missing uncertainties with template
- Outlier identified

Layer 3

- Subjective ...s
- ...t judg...nt from ...ua...s
- ...ded u... ...ith ...ate

-> needs user input

Layers 0 and 1: This information could all be stored in EXFOR.

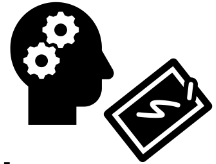
Layer 2: This information could be built into an API accessing the EXFOR database.

Layer 3: Outside of the scope of EXFOR.

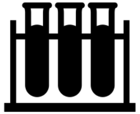
WPEC SG-50 use cases

Five different use cases were documented:

- Nuclear data evaluator

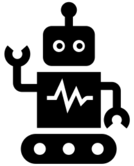


- Experimentalist

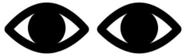


- Model development

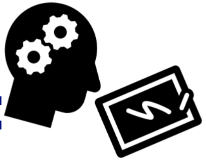
- Mining of data and metadata with Machine Learning and Artificial Intelligence



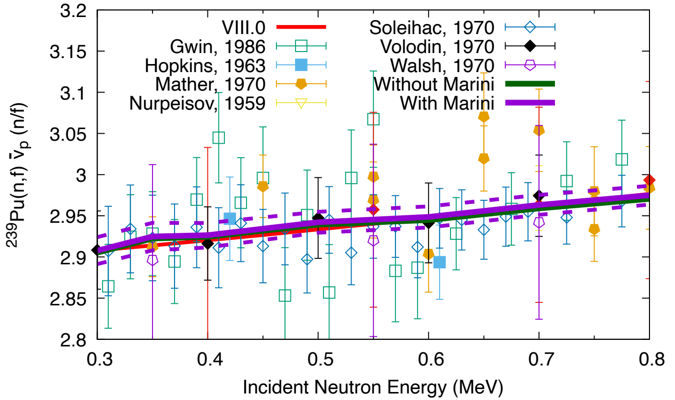
- Assessing quality of nuclear data libraries by comparing to experimental data.



Profile of use case “nuclear data evaluator”:



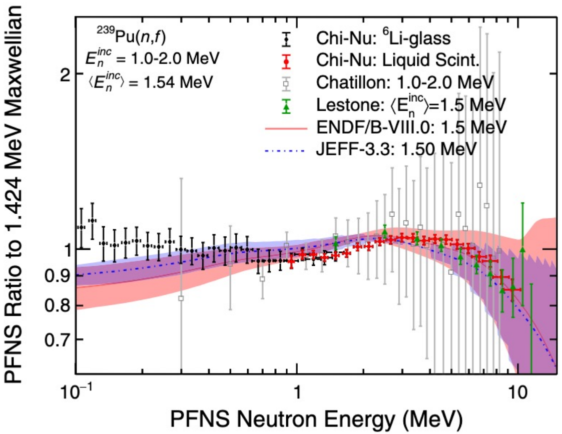
- Goal: evaluate one or more nuclear-data observable including the best understanding of experimental data and theory at the time.
- Use of retrieved data:
  - judges, corrects & re-normalizes data with new monitors,
  - estimates & adds missing unc., estimates cor, identifies outliers, builds a database for evaluation.
- Access:
  - downloads/ plots all data for observable(s) via API
  - needs metadata, data, unc., past judgments on the data.



Note: These are ***not*** the same exp. data as in EXFOR but ***augmented by evaluator knowledge.***

Profile of use case "experimentalist":

- Goal: to provide the best possible measurement of an observable at a time.
- Use of retrieved data:
  - justifies the need for new experiment;
  - finds out how experiments were previously undertaken (analysis techniques, hardware & total unc.);
  - compare to historic data to understands possible biases past data.
- Accesses:
  - downloads/ plots all data for observable(s) using an API
  - needs metadata, data, unc., past judgments on the data
  - searches with API by clearly defined observable or by metadata.



These are data as in EXFOR.

From K. Kelly et al., Phys. Rev. C 102, 034615 (2020).

Profile of use case “model development”:

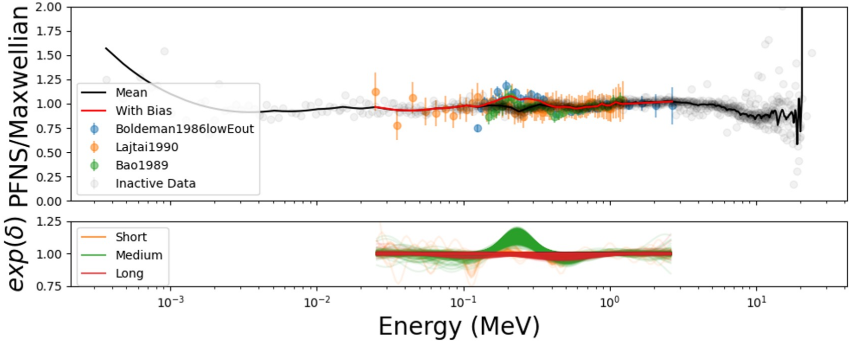
- Goal: model developer develops model to predict available exp. data accurately; model user fits parameters such that model values predict exp. data to its best ability.
- Use of retrieved data:
  - uses large amounts of EXFOR across many nuclides and observables;
  - compares model-predicted quantities to reliable/ curated exp. data including curated unc.
- Accesses :
  - downloads large parts of EXFOR at once;
  - needs curated exp. data (i.e., outliers removed, re-normalized to newest monitor, complete total unc.).

<u>Data automatically retrieved</u> from EXFOR and some post-processing.

Profile of use case “mining of data and metadata with Machine Learning and Artificial Intelligence”:

- Goal: Find trends in data and metadata to better understand the physics represented by experiments; informs models with data; finds issues in nuclear-data libraries.
- Use of retrieved data:
  - identifies outliers in exp. data;
  - correlates outlying data with metadata.
- Accesses:
  - large parts of EXFOR are downloaded at once
  - Needs curated data, total unc., partial unc., flags identifying possible outliers/ biases, metadata, and comments from previous users.

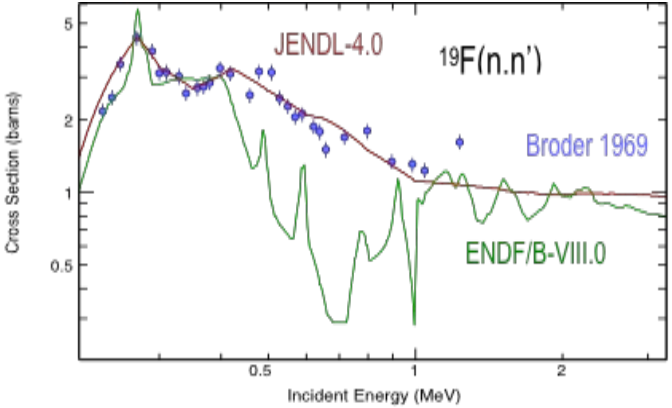
Neutron Detector: ^{6}Li*



These are ***not*** the same exp. ***data and metadata*** as in EXFOR but augmented by evaluator knowledge.

Profile of use case “assessing Quality of nuclear data libraries by comparing to experimental data”: 👁👁

- Goal: understands if data from a nuclear data library are realistic given differential experimental data.
- Use of retrieved data: curated data and unc. are compared to nuclear data.
- Accesses:
    - plots curated data and total unc. via API for one reaction at a time and compares to nuclear data;
    - wants to retrieve data used for a specific evaluation.



These are data as in EXFOR and in nuclear data libraries. ***<u>Curated data would help!</u>***

High-level requirements of interest to EXFOR format and its API based on needs from the different users.

High-level requirements from different use cases:

Access of data (of interest for EXFOR API):

- Download of a large amount of data at once,
- API to access and plot the data of all different layers,
- Uploading user-defined data for plotting to compare to data in EXFOR.

Format:

- Create a format that is easy to read automatically for a large amount of data,
- Clear identification of what observable was measured and how it relates to ENDF-6 formatted nuclear-data observables,
- Using common units for all data in the database to make them easily comparable,
- Using unique identifiers for meta-data to easily find common features among experiments.

High-level requirements from different use cases: cntd.

Data treatment (part of an EXFOR API):

- Converting ratio data to absolute data,
- Re-normalizing to newest standard and reference reactions,
- Automatically flagging and identifying outliers with various algorithms,
- Automatically flagging missing or suspiciously low uncertainties via templates,
- Automatically adding missing uncertainties via templates,
- Estimating total covariances using existing uncertainties and templates,

Storing past judgements (outside of EXFOR scope):

- Storing past judgments on the data,
- Identifying if a data set was used for an evaluation.

Each requirement is documented in the requirement document. The specification document is also being worked on based on these requirements.

WPEC SG-50 use cases, requirements and specification documents might be helpful for EXFOR developments.

- WPEC SG-50 brought many EXFOR users together.
- We documented use cases.
- The requirement document collects needs flowing from these use cases.
- A specification document was made based on the requirements. It is just a start of the discussion.
- Boris Pritychenko proposed a new sub-group continuing the SG-50 work. He will connect more tightly to NRDC.

- We hope some of the information is helpful for the NRDC/ EXFOR!

Thank you for your attention!