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The need for new EXFOR formats to apply machine learning techniques to its data

Denise Neudecker

Nov. 11-15, 2022
Nuclear Data Retrieval, Dissemination, and Data Portals

IAEA Nuclear Data Section database online tools are immeasurable assets to the community!

I use EXFOR from https://www-nds.iaea.org/exfor/exfor.htm, and

ENDF tools from https://www-nds.iaea.org/exfor/endf.htm

Finding most of the data online is the basis for streamlined evaluation!

- It makes progress faster as it saves us time to find pertinent data.
- It stores information that might otherwise be lost to some or all of us as some journals are out of print or in languages that some cannot read.
- It helps us to intuitively understand the quality of nuclear data.

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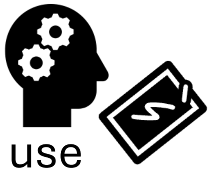
- It helps us to intuitively understand the quality of nuclear data.

Even great things can become better. ☺

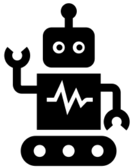
What kind of a user am I? Evaluator, validating nuclear data versus EXFOR data, and AI/ ML user.



- Weekly, I use EXFOR APIs to find data for evaluation. I read the whole entry, use metadata and data for detailed experimental uncertainty quantification. The more information is in EXFOR, the easier my job (and the happier I am).

- Weekly, I plot various libraries versus EXFOR data to understand how close our evaluated data are, where the problems are, etc.

- I apply ML techniques to EXFOR data and metadata to understand what part of measurements drive bias in data. Understanding the physics root cause of bias is crucial to design future experiments that resolve biases in data.



Where do I hit limits of EXFOR or loose time?

- Evaluation:
  - Uncertainty heading cannot be automated for exp. UQ. Very much **“by-hand process”.**
  - Concerns on data from other evaluators not stored. I **re-invent the wheel constantly!!!**

- Validation:
  - I need curated experimental data to **correctly judge evaluated data**: outliers removed, complete experimental uncertainties, all data re-normalized to newest standard.
  - I need evaluated uncertainty bands around the mean to **judge if unc. cover experiments**.

- ML:
  - Retrieving key-words for ML analysis is painful and prohibitive for far-reaching applicability. **Not having features in that way impedes scientific progress**.
  - I need metadata cast in uniquely identifiable language.

Where do I hit limits of EXFOR or loose time?

- Evaluation: 
  - Uncertainty heading cannot be automated for exp. UQ. Very much **“by-hand process”.**
  - Concerns on data from other evaluators not stored. I **re-invent the wheel constantly!!!**

ERR-4	ERR-5	ERR-6	ERR-7	ERR-8	ERR-9	MONIT	
PER-CENT	PER-CENT	PER-CENT	PER-CENT	PER-CENT	PER-CENT	PER-CENT	PRT/FIS
0.05	0.05	0.2	0.1	0.05	0.1	3.732	

ENDCOMMON

These descriptors are NOT helpful!

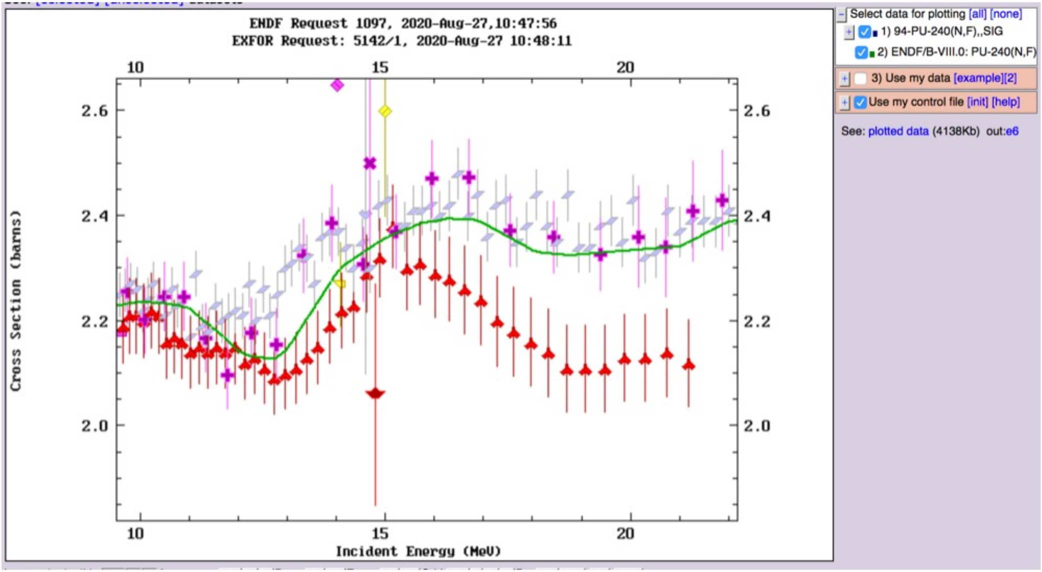
within the limits of the statistical error.
ERR-ANALYS By compiler (2020-09-24):
The compiler assumed all uncertainties in Table 1 of CEA-R-4626 except for neutron scattering by Pt are relevant to the nu-bar determination.
(ERR-S) purely statistical
(ERR-1,0.1,0.3) Background (0.1-0.3%)
(ERR-2,0.1,0.2) Dead time (0.1-0.2%)
(ERR-3,0.05,0.42)Spectrum difference (0.05-0.42%)
(ERR-4) Relative sample position (0.05%)
(ERR-5) Impurities (0.05%)
(ERR-6) Anisotropy in fragment emission (0.2%)
(ERR-7) Fission event loss (0.1%)
(ERR-8) French effect (0.05%)
(ERR-9) Delyaed gamma-rays (0.1%)

This free-text description is very helpful but cannot be automated and causes repetitive work.

Where do I hit limits of EXFOR or loose time?

Validation:

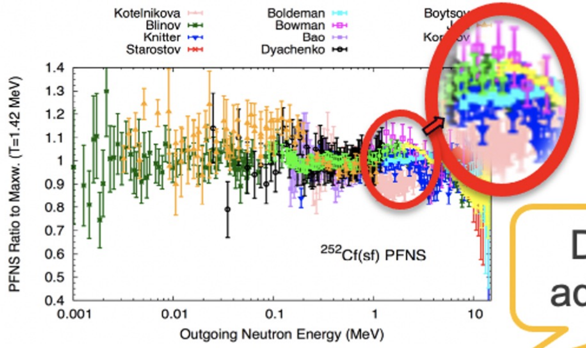
- I need curated experimental data to **correctly judge evaluated data**: outliers removed, complete experimental uncertainties, all data re-normalized to newest standard.
- I need evaluated uncertainty bands around the mean to **judge if unc. cover experiments**.



Three examples

- Applying AI/ ML to metadata in EXFOR.
- WPEC SG-50 requirement and specification documents.
- Templates.

AIACHNE applied ML techniques (sparse Bayesian methods) to identify drivers of systematic bias between ^{252}Cf PFNS exp.



Developing advanced ML

Using state-of-the-art LANSCE equipment

Correcting past data and assessing impact

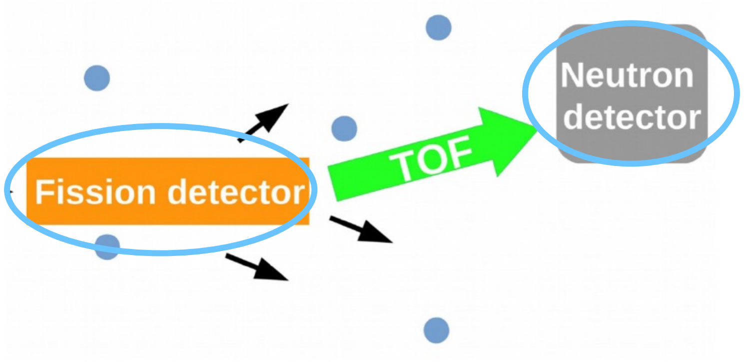
Discrepant experiments (exp.) → **ML indicates features of exp. related to bias** → **Simulations explore features and bias** → **Low-bias exp** / **Low-bias exp. + feature related to bias** → **Correction factor** → **Improve ND**

Simulated correction factors

Knowing what hardware or analysis techniques drive bias between different experiments helps us design experiments to resolve that and drive scientific progress. **It hinges on knowing metadata describing the experiment!**

We collected features by hand for categories describing the experiment from the literature & EXFOR entries.

Here, we analyze features related to neutron and fission detectors.

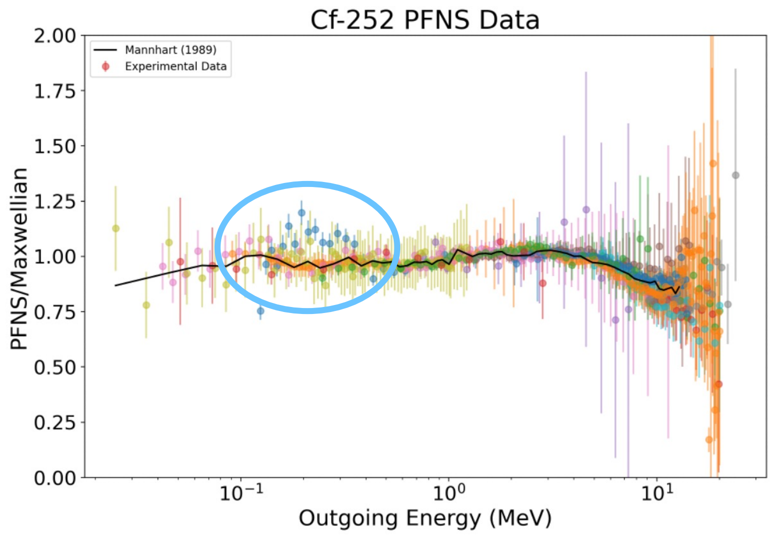


	Correction Features	Hardware Features	Method Features
0	ShadowBarBackground	FissionDetector1_raw	RandomCoincidence
1	BackgroundCorrected	FissionDetector1_caseA	BackgroundGeneral
2	RandomCoincidenceBackground	FissionDetector1_caseB	BackgroundAlpha
3	GammaBackground	FissionDetector1_caseC	GammaBackground
4	AlphaBackground	FissionParticleDetected	MSinSample
5	WrapAroundBackground	FissionFragmentDetectorEfficiency	MSinSurrounding
6	MultipleScatteringSampleBackingCorrected	FissionDetectorGas_raw	FissionDetectorEfficiencyMethod
7	MultipleScatteringSurroundingCorrected	FissionDetectorGas_caseA	FFAbsorptionAngularDistributionMethod
8	AttenuationSampleBackingCorrected	AngularAcceptanceofFFDetector	NeturonDetectorResponseMethod
9	AttenuationSurroundingCorrected	NeutronDetector_raw	NeturonDetectorEfficiencyMethod
10	FissionDetectionEfficiencyCorrected	NeutronDetector_caseA	DeadtimeDeterminationMethod
11	NeutronDetectionEfficiencyCorrected	AngularCoverageofNeutronDetector	
12	NeutronDetectionResponseCorrected	NeutronDetectorSizeCM	
13	SampleDecayCorrected	NeutronDetectorStructuralMaterialAu	
14	FissionFragmentAbsorptioninSampleCorrected	NeutronDetectorStructuralMaterialAl	
15	SignalPulsePileupCorrected		
16	DeadtimeCorrected		
17	AngularDistributionFissionFragmentsCorrected		
18	ImpuritiesCorrected		

This is a *filtered* list of feature categories!!!

It took months to collect features & put them in an ML interpretable format!!!

In order to test algorithm, we look for known issue in data, namely, bias due to Li-6 peak from 100-300 keV.

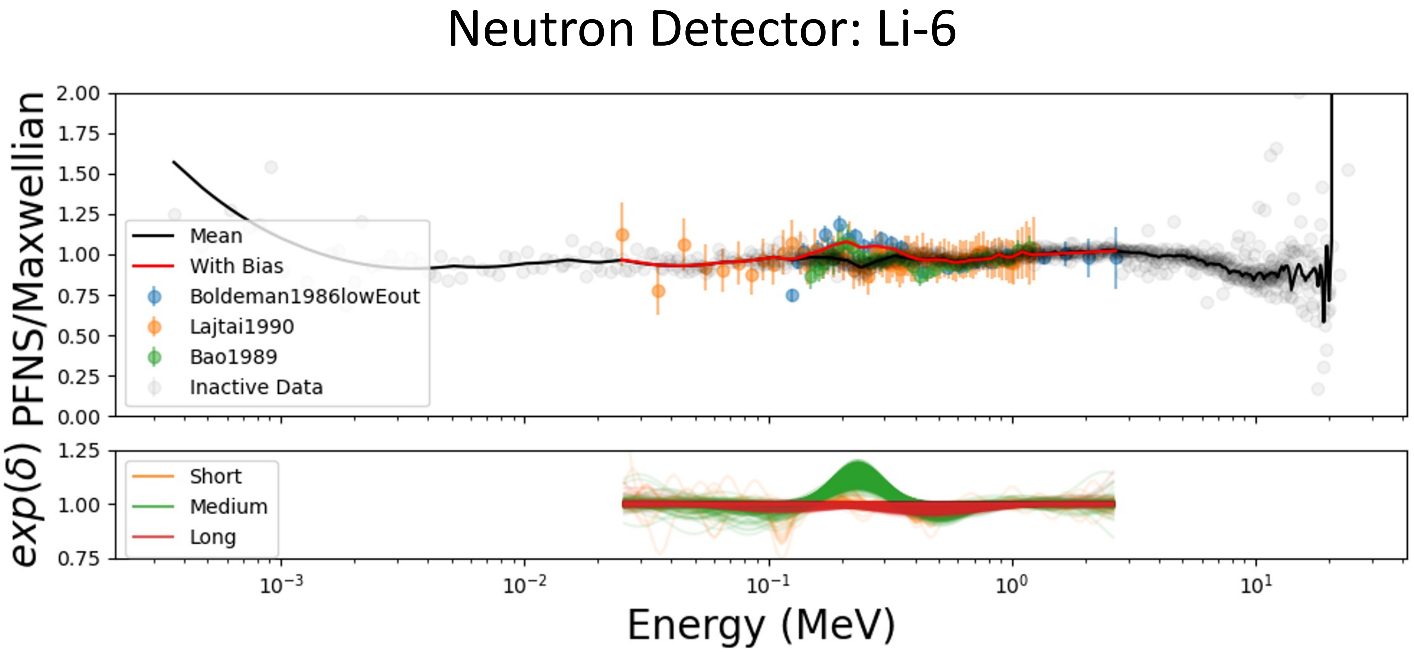


Dataset	NeutronDetector_raw	NeutronDetector_caseA
Boldeman1986lowEout	Scin (6li)	(6li)
Lajtai1990	Glasd (6li)	(6li)
Blinov1973	Ioch (235u(n,f) chamber)	Ioch (235u(n,f) chamber)
Poenitz1982	Scin	Scin
Boytsov1983ant	Scin (anthracene)	Scin (anthracene)
Maerten1990_0deg	Scin (liquid)	Scin (liquid)
Maerten1984	Scin (liquid)	Scin (liquid)
Blain2017highEout	Scin (liquid)	Scin (liquid)
Chalupka1990	Scin (liquid)	Scin (liquid)
Maerten1990_60deg	Scin (liquid)	Scin (liquid)
Boettger1990	Scin (liquid)	Scin (liquid)
Kornilov2015	Scin (liquid)	Scin (liquid)
Boldeman1986highEout	Scin (plastic)	Scin (plastic)
Blain2017lowEout	Scin (plastic)	Scin (plastic)

Experimental features are expected to guide if datasets are grouped as biased.

This example shows that standardized EXFOR identifiers were not unique enough.

Results for Neutron Detector Case A: algorithm correctly identified expected bias due to Li-6 peak – algorithm works!



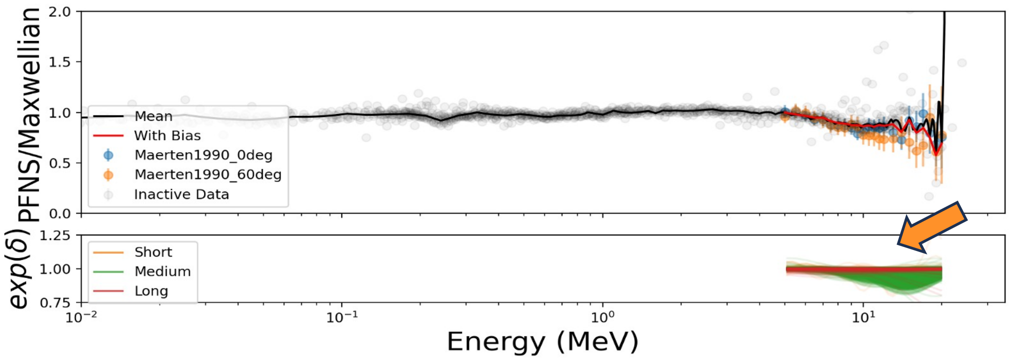
Advantage of algorithm: Enables to more quantitatively identify bias in exp. data as a function of energy and study experiments based on that.

High-E bias identified across several feature groups, less obvious but experimentally explainable.

Effect at high energies was attributed to many features. Detailed expert discussion and analysis of data pointed to fission detection (angular dependence of fission fragments).

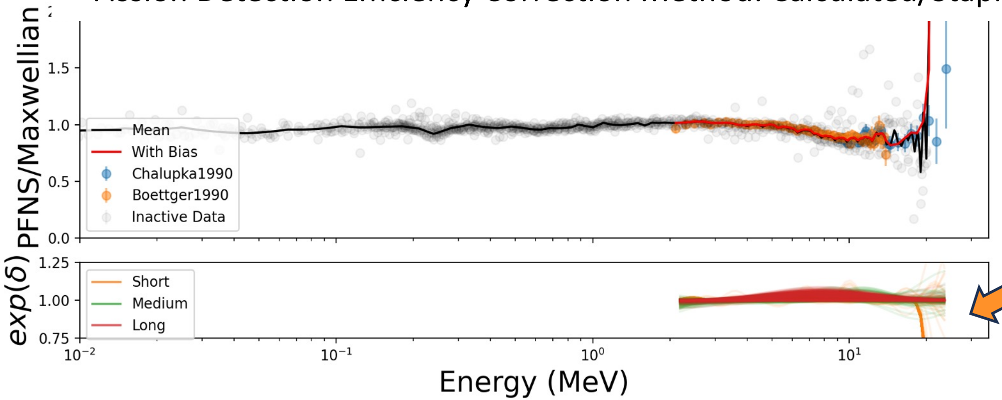
Effects suspected leading to bias can be now studied by experts! AI/ ML is key to point expert into the right direction. BUT WE NEED METADATA IN UNIQUE FORMAT FOR ML!!!

Fission Detection Efficiency Correction Method: Calculated/Measured



~30% of samples

Fission Detection Efficiency Correction Method: Calculated/Stapre



~10% of samples

SG-50 gave requirements & specifications for an automatically readable, comprehensive & curated experimental database.

- WPEC SG-50:
  - Run-time: 2021-2024
  - Team: coordinators A. Lewis and D. Neudecker; monitor A. Koning; 57 members from 11 countries, NEA & IAEA, representing 5 libraries
- Requirement document:
- 5 use cases: evaluator, validation, AI/ML users, large-scale modeling & experimenter; for each their use of data, goals, needs and access of databases were described.
- Requirements flowing from these use-cases on access of data, format, data treatment, and storing of past data (see back-up for details).
- Summarized the broad need of SG-50 members.
- Specification document:
- Gave new format recommendations made based on the requirements.
- It is just a start of the discussion. Will be continued in WPEC SG-54.

Templates of expected measurement unc. can complete unc. for curated data and can aid in EXFOR compilation.

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.

Having this information in EXFOR would positively impact the UQ of exp. data for evaluation and thus evaluated cov for users.

Templates **can be used in an API connected to EXFOR to complete unc.** to save UQ time & better comparison to eval. Requires clear identification of unc. sources.

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.

Final recommendations:

- Please, consider standardizing metadata compilation for EXFOR to render entries more comparable, get better input for ML, and enable estimating cross-experiment correlation. WPEC SG-50 could be a starting point for this standardization.
- Please, ask compilers if they would be willing to use templates of expected measurement uncertainties to ask experimenters for more uncertainty information.
- Please, consider curating the experimental data you plot from EXFOR to compare to evaluated data and adding evaluated uncertainty bands.
- **Please, continue to maintain these excellent databases!!!**

Thank you for listening!

Research reported in this publication was supported by the U.S. Department of Energy LDRD program at Los Alamos National Laboratory, the DOE Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the Department of Energy and the ASC program.

LDRD

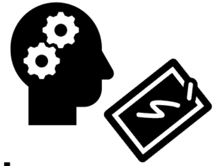
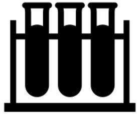
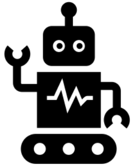
NCSP
NUCLEAR CRITICALITY SAFETY PROGRAM

Research reported in this publication was supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics, under the Nuclear Data InterAgency Working Group Research Program.

Back-up

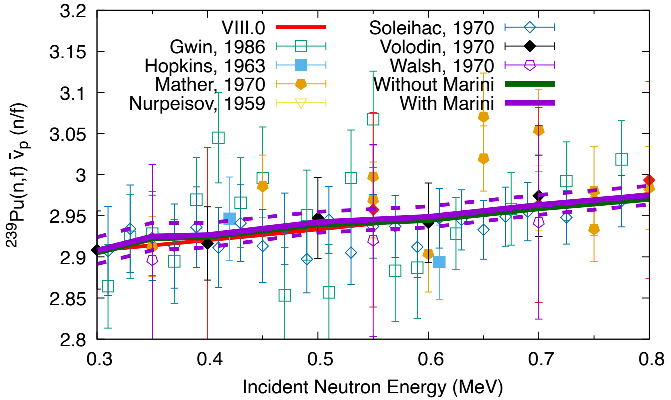
WPEC SG-50 use cases

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”:

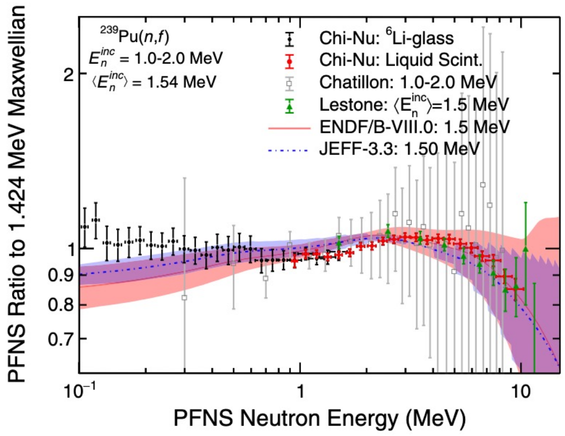
- Goal: evaluate one or more nuclear-data observable including the best understanding of experimental data and theory at the time.
- Use of retrieved data:
  - judges, corrects & re-normalizes data with new monitors,
  - estimates & adds missing unc., estimates cor, identifies outliers, builds a database 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":

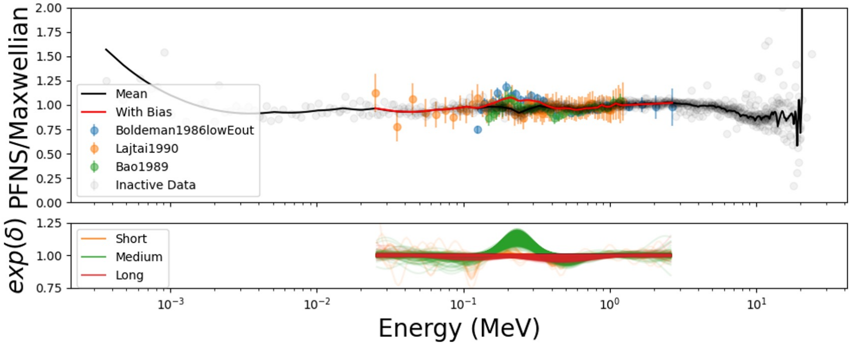
- Goal: model developer develops model to predict available exp. data accurately; model user fits parameters such that model values predict exp. data to its best ability.
- Use of retrieved data:
  - uses large amounts of EXFOR across many nuclides and observables;
  - compares model-predicted quantities 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.).

Data automatically retrieved 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.

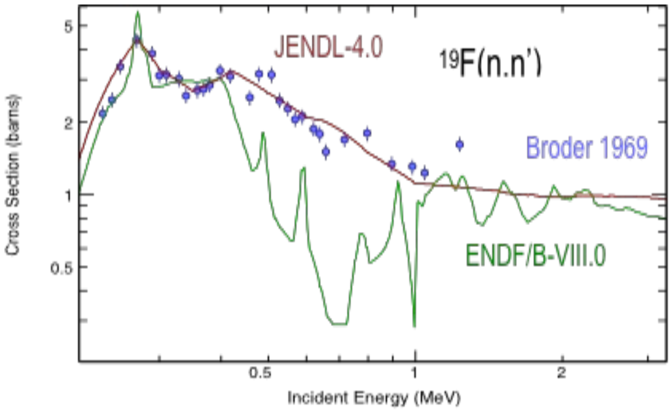
Neutron Detector: ^{6}Li*



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.

More on templates

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.

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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 $\bar{\nu}_p$ or $\bar{\nu}_t$ are used as a bare-minimum input for the evaluation. If $\bar{\nu}_p$ is evaluated and the measurement is of $\bar{\nu}_t$, 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) $\bar{\nu}$, 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 $\bar{\nu}_p$ 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 $\bar{\nu}_p$ and $\bar{\nu}_t$ can be measured to high precision. However, even small variations in $\bar{\nu}$ 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) $\bar{\nu}_t$ 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 $\bar{\nu}_p$ and

$\bar{\nu}_t$ 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.

Knowing measurement type informs what:
- Uncertainties
- Metadata
- Corrections

Are needed to be reported in the EXFOR entry.

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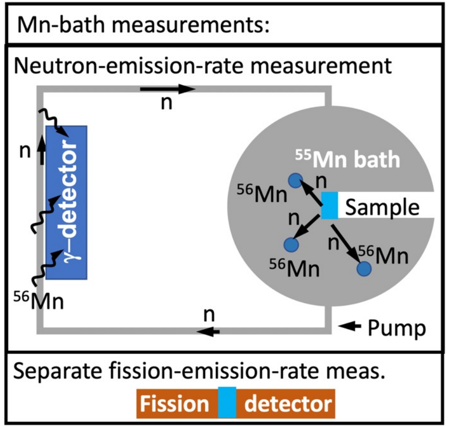

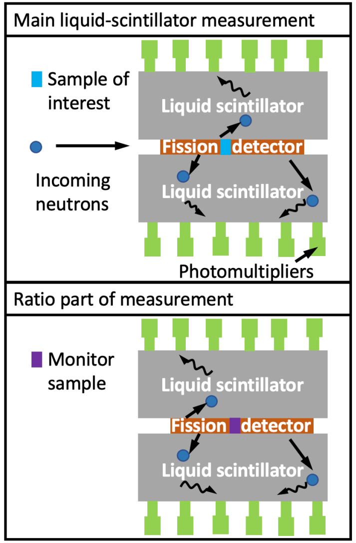

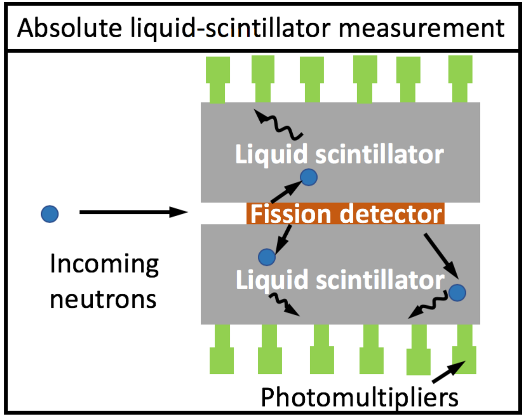

Templates document what uncertainties should be provided per measurement type.

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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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]

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) 0.15 (low α-activity sample)	Gaussian	0.2
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 0.5 (2$^{\mathrm{nd}}$-chance fission)	Gaussian	Full (same E_{inc}) Gaussian (different E_{inc})
δL_n	0.2	N/A	Full	0.5
δa	N/A (isotropic)	0.01–0.3 0.5 at 2$^{\mathrm{nd}}$ c.f. and >10 MeV	0.8–1.0	0.6
$\delta\overline{\nu}^m$	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!

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For this example, corrections would be:

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

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.