Case study: Applying PFNS templates to ^{252}Cf PFNS of Kornilov or when to apply templates versus investigating bias

D. Neudecker (speaker)[1], D. Brown[2], A.D. Carlson[2,3], M.J. Grosskopf[1], R.C. Haight[1], K.J. Kelly[1], Tom Massey[4], B. Pritychenko[2], S. Vander Wiel[1], Noah Walton[1,5]
[1]LANL, [2]BNL, [3]NIST, [4]Ohio University, [5]UTK

Mini-CSEWG August 15, 2024

Thanks to Roberto Capote for connecting us to T. Massey and to N. Kornilov, who died too early, for his work on the ^{252}Cf PFNS.

LA-UR-24-28683

What is the aim of this session?

Aim: Establishing uncertainty standards for experimental UQ, discussing evaluation techniques and model UQ.

- One aspect of better UQ is quantifying all pertinent exp. uncertainties. Templates is one way of addressing that.
- Improved evaluation techniques are needed to explore biases in exp. data, design future experiments and deal with stiff models. Formats for evaluated data need also be explored.
- We need good model UQ to get towards medium-fidelity covariances.

A. Khatiwada
F. Diaby
C. Fritsch
D. Neudecker
Y. Danon
M. Grosskopf
V. Sobes
R. Capote
C. Thompson
D. Brown
A. Lovell
V. Sobes

Aim of this talk: start discussion on best practices on experimental UQ and needs on evaluation techniques

This is the AIACHNE story of Kornilov experimental UQ:

1) To demonstrate how to apply PFNS templates.

2) Show an example at the limits of what can be reached with good experimental UQ and at the start of uncovering biases (USU) in the data.

Simply said, we cannot stop at just doing good experimental UQ, we also need to get to the bottom of experimental biases.

Story part 1: We did our chosen best-practice UQ procedure for Kornilov ^{252}Cf PFNS and got nowhere …

Our chosen standardized UQ procedure for the ^{252}Cf PFNS standards evaluation

1) Get ALL literature and data from EXFOR.
2) Judge if you trust data based on literature and plotting. Are all important corrections addressed (background, detector response, multiple scattering, anisotropy, sample decay)?
3) Find all pertinent uncertainties from above sources and author if available. Are sufficient experimental unc. provided for good UQ?
4) Estimate unc. you cannot find otherwise with templates (and this should be little) and do UQ with ARIADNE.
5) (Bonus steps) See if there are still unexplained biases in the data via ML.

For identifying missing corrections and uncertainties, we used templates of expected PFNS measurement unc.

D. Neudecker et al.: EPJ Nuclear Sci. Technol. **9**, 32 (2023) 5

Table 1. Typical uncertainty sources encountered in PFNS measurements are listed dependent on their specific measurement type. Also, estimates of typical uncertainty ranges are provided in case this information cannot be derived otherwise for uncertainty-quantification purposes. "ND" was used as an abbreviation for nuclear data.

Unc.	Shape (%)	Clean-ratio shape (%)	Ratio-calibration shape (%)
δc	Must be provided	Must be provided (δc_s & δc_m)	Must be provided (δc_s & δc_m)
δb	0.2–3	0.2–2	0.2–3 for both
δm	1–20 (not corrected)	0.1–5 (not corrected)	1–20 (not corrected, both)
	0.1–3 (corrected)	0–0.8 (corrected)	1–3 (corrected, both)
$\delta \varepsilon$	2–7 (efficiency)	Cancels	Unc. in determining χ_m
	0–10 (response not folded)	–	0–10 both (response not folded)
δa	0.1	0.1	0.1
$\delta \tau$	0.1	0.1	0.1 for both
ND	0.1–5 (simulations)	0–0.5 (simulations)	0.1–5 both (simulations)
	–	From libraries (reference)	From libraries (reference)
δt	2.5 ns	2.5 ns both	2.5 ns both
ΔL	2 mm	2 mm both	2 mm both
$\delta \omega$	Impurity-level dependent	Both samples	Both samples

From PFNS templates DN, EPJ-N 9, 32 (2023).

There were open questions on Kornilov data regarding the light curve, backgrounds, and multiple scattering.

1) Get ALL literature and data from EXFOR. ✓
2) Are all important corrections addressed? ✗

Correction	Questions
Background	• Unclear if random coincidences were corrected (effect > 10 MeV). • Unclear if alpha background was corrected. • Unclear how good gamma separation was (effect > 10 MeV).
Multiple scattering	• Simplified modeling of detector and surrounding. Could impact wings.
Detector response	• Question on light curve above 12 MeV.
Decay of sample	✓
Anisotropy	✓

Kornilov, Report INDC(USA)-108 (2015).
List of expected corrections from PFNS templates DN, EPJ-N 9, 32 (2023).

There were MANY missing uncertainties, including major uncertainty sources …

1) Get ALL literature and data from EXFOR. ✓
2) Are all important corrections addressed? ✗
3) Are sufficient experimental unc. provided for good UQ? ✗

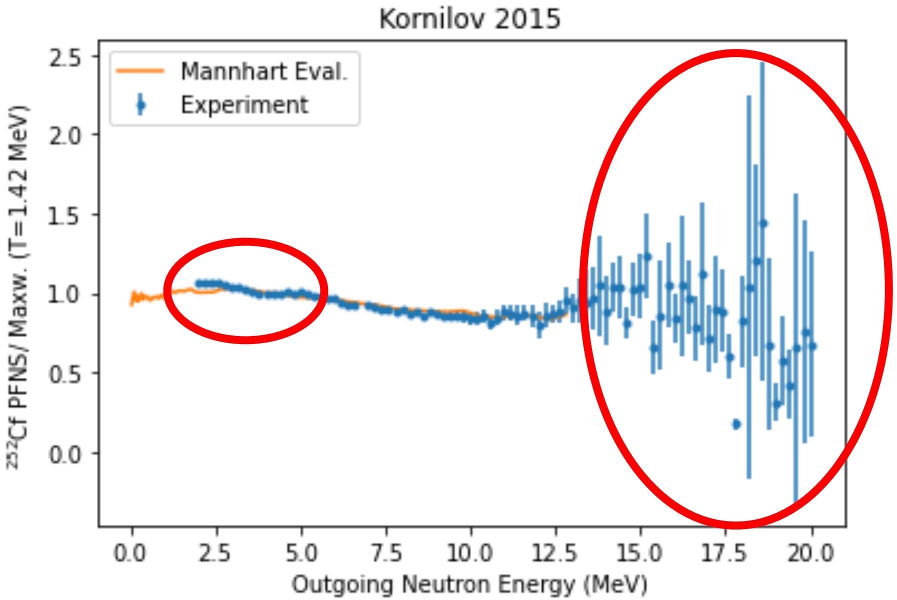
List of expected unc. from PFNS templates DN, EPJ-N 9, 32 (2023).

Uncertainty	y/n	Uncertainty	y/n
Statistical	✗	Background	✗
Time resolution	✗	Multiple scattering	✗
TOF length unc.	✓	Deadtime (small)	✗
Detector response	✓	Impurity (small)	✗
Anisotropy (small)	✗		

Uncertainties in EXFOR were somewhat unclear …?

There were structures in the data that we could not explain and uncertainties seem low compared to structures.

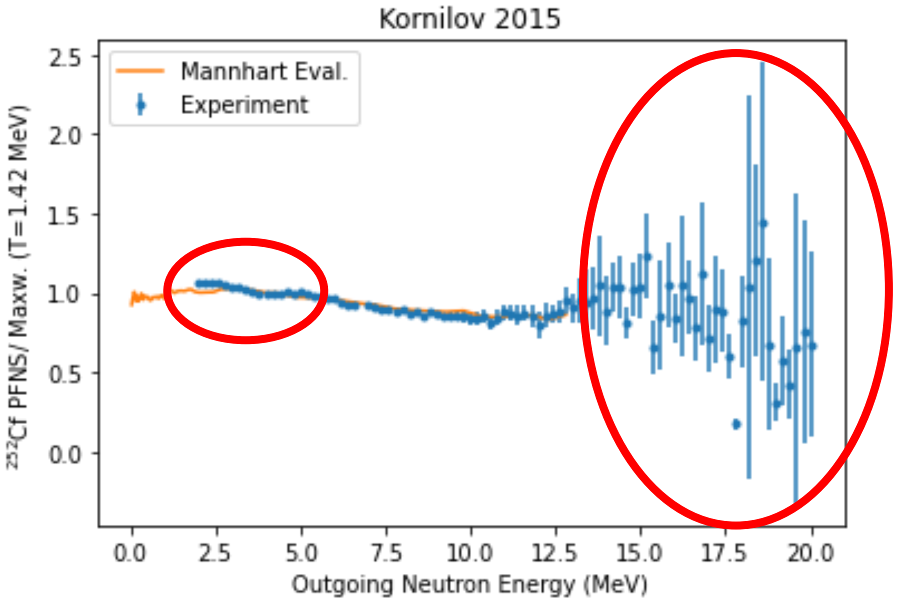
1) Get ALL literature and data from EXFOR. ✓
2) Are all important corrections addressed? ✗
3) Are sufficient experimental unc. provided for good UQ? ✗
4) Estimate unc. you cannot find otherwise with templates and do UQ with ARIADNE.



Structures at lowest and high energies led to data outside Mannhart evaluation at low energies and larger scatter than uncertainties at high energies.

Judgment at last standards meeting: REJECT and only use for validation of evaluation given lack of unc. and bias.

1) Get ALL literature and data from EXFOR. ✓
2) Are all important corrections addressed? ✗
3) Are sufficient experimental unc. provided for good UQ? ✗
4) Estimate unc. you cannot find otherwise with templates and do UQ with ARIADNE.

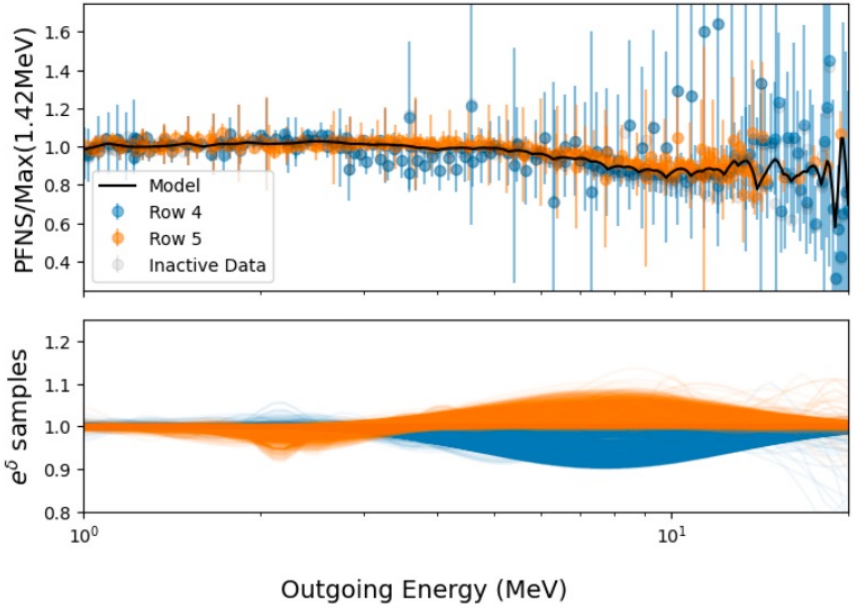


RC: But that is what templates are for?

DN: These are Kornilov mean values with Neudecker uncertainties … Not good for standard.

In the background was also information from ML saying that Kornilov data at high energies were biased!

5) (Bonus steps) See if there are still unexplained biases in the data via ML. ❌



Bias is found by ML in Kornilov data (mostly “Row 4”) at high energies. Related to either background or detector response ...

N. Walton et al., “Machine-learning assisted identification of potential sources of bias in prompt-fission neutron spectra (PFNS) measurements”, in preparation.

More in the talk of Mike Grosskopf.

Story part 2:

- R. Capote contacts Prof. T. Massey.
- We get more information on experiment corrections and uncertainty information.
- We have more unbiased data.
- WE CAN SALVAGE PART OF THE DATA!!! 

We could answer many open questions with Tom Massey based on digging through Kornilov's back-ups and literature.

1) Get ALL literature and data from EXFOR. ✓
2) Are all important corrections addressed? ✓

Correction	Questions	Answers
Background	• Unclear if random coincidences were corrected. • Unclear if alpha background was corrected. • Unclear how good gamma separation was.	• Literature found on random coinc. cor. ✓ • Alpha background small. ✓ • 2D PSD spectrum shows good separation. ✓
Multiple scattering	• Simplified modeling of detector and surrounding. Could impact wings.	• Likely smaller effect. ✓
Detector response	• Question on light curve above 12 MeV.	• Questions on light curves remain. Cut data below ~4 MeV and above 13 MeV.
Decay of sample	✓	✓
Anisotropy	✓	✓

Could fill out many missing uncertainties based on related literature and additional information

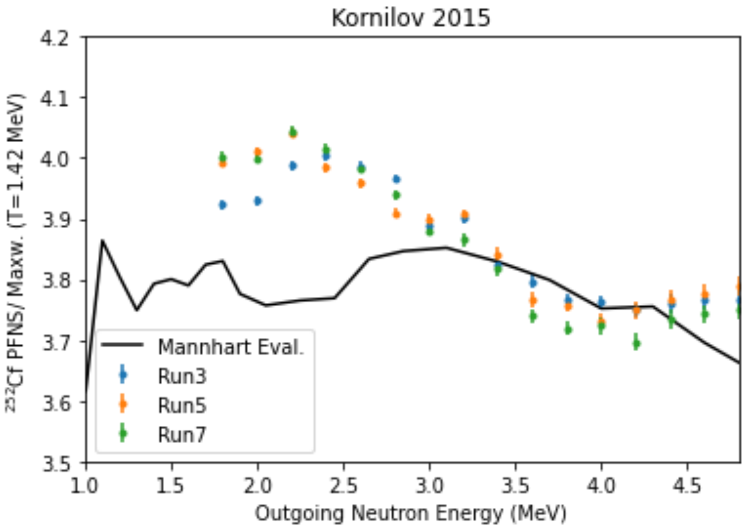
1) Get ALL literature and data from EXFOR. ✓
2) Are all important corrections addressed? ✓
3) Are sufficient experimental unc. provided for good UQ? ✓

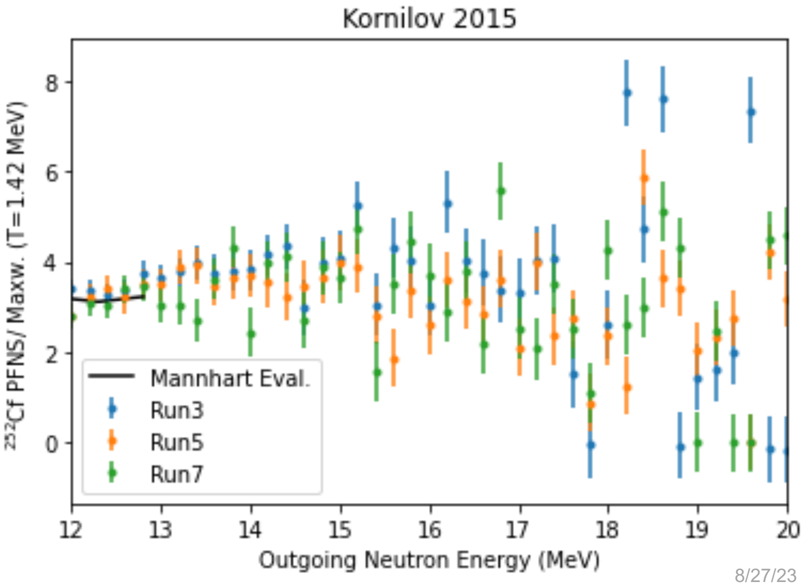
List of expected unc. from PFNS templates DN, EPJ-N 9, 32 (2023).

Uncertainty	y/n	Uncertainty	y/n
Statistical	✓ Found original data.	Background	✓ Based on now known correction.
Time resolution	✓ From informal docs.	Multiple scattering	✗ (small) after discussion.
TOF length unc.	✓ Needed correction	Deadtime	✗ (small)
Detector response	✓	Impurity	✗ (small)
Anisotropy	✗ (small)		

Lastly, because we had the original data, we could remove the biased Run 3 (issues with bias setting, lower statistics.)

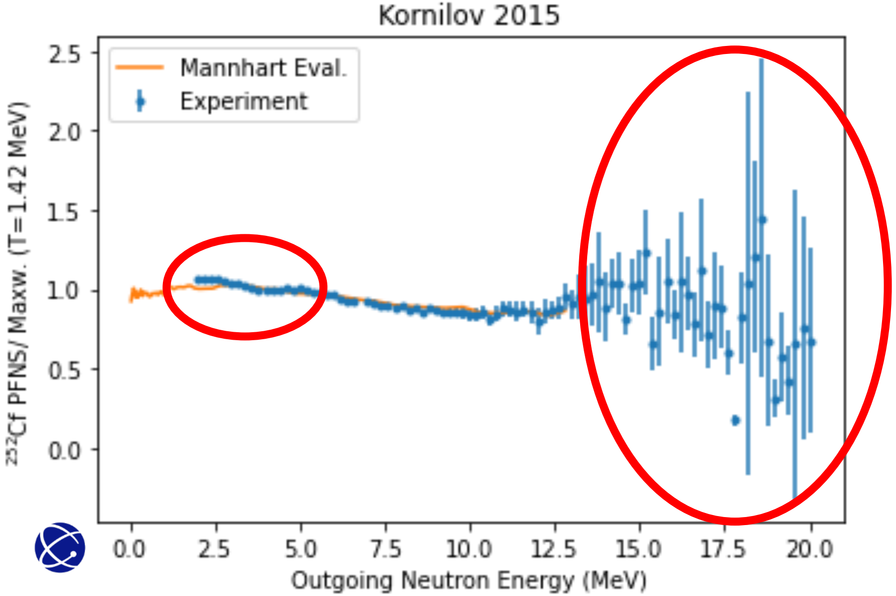
1) Get ALL literature and data from EXFOR. ✓
2) Are all important corrections addressed? ✓
3) Are sufficient experimental unc. provided for good UQ? ✓

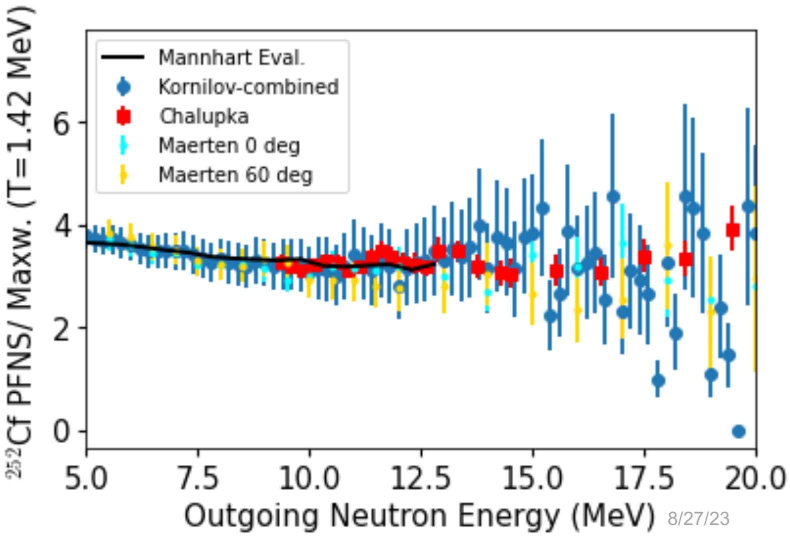




There were structures in the data that we could not explain and uncertainties seem low compared to structures.

1) Get ALL literature and data from EXFOR. ✓
2) Are all important corrections addressed? ✓
3) Are sufficient experimental unc. provided for good UQ? ✓
4) Estimate unc. you cannot find otherwise with templates and do UQ with ARIADNE.





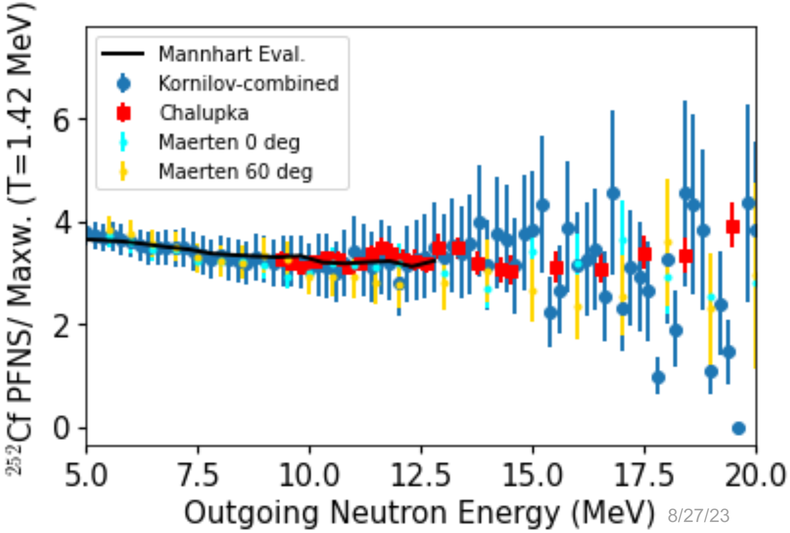
There were structures in the data that we could not explain and uncertainties seem low compared to structures.

1) Get ALL literature and data from EXFOR. ✓
2) Are all important corrections addressed? ✓
3) Are sufficient experimental unc. provided for good UQ? ✓
4) Estimate unc. you cannot find otherwise with templates and do UQ with ARIADNE.

Better agreement because of:

- Removing outlying Run 3.
- More realistic uncertainties. I assumed best-case time resolutions but unc. was actually higher.

We can adopt at least part of the data.



Discussion

Discussion

- Clearly, doing the best UQ is key to getting at what could be issues in the data. **Is there a(n exp.) UQ procedure we want to recommend as community? How do we cite properly shared databases established by evaluators and how to acknowledge people who did the UQ?**
- Also, clearly, there are limits where UQ can get you. ML-based evaluation techniques can help us uncover USU. We should make using these techniques a standard rather than a bonus step. **Let's discuss new evaluation techniques.**
- Lastly, how can we make sure that all pertinent uncertainties make it into our libraries?

Acknowledgements

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.