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Title: Templates of expected measurement uncertainties and machine learning to understand unknown sources of discrepancies

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Templates of expected measurement uncertainties and machine learning to understand unknown sources of discrepancies

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BAND Nuclear Data Workshop Dec. 18, 24

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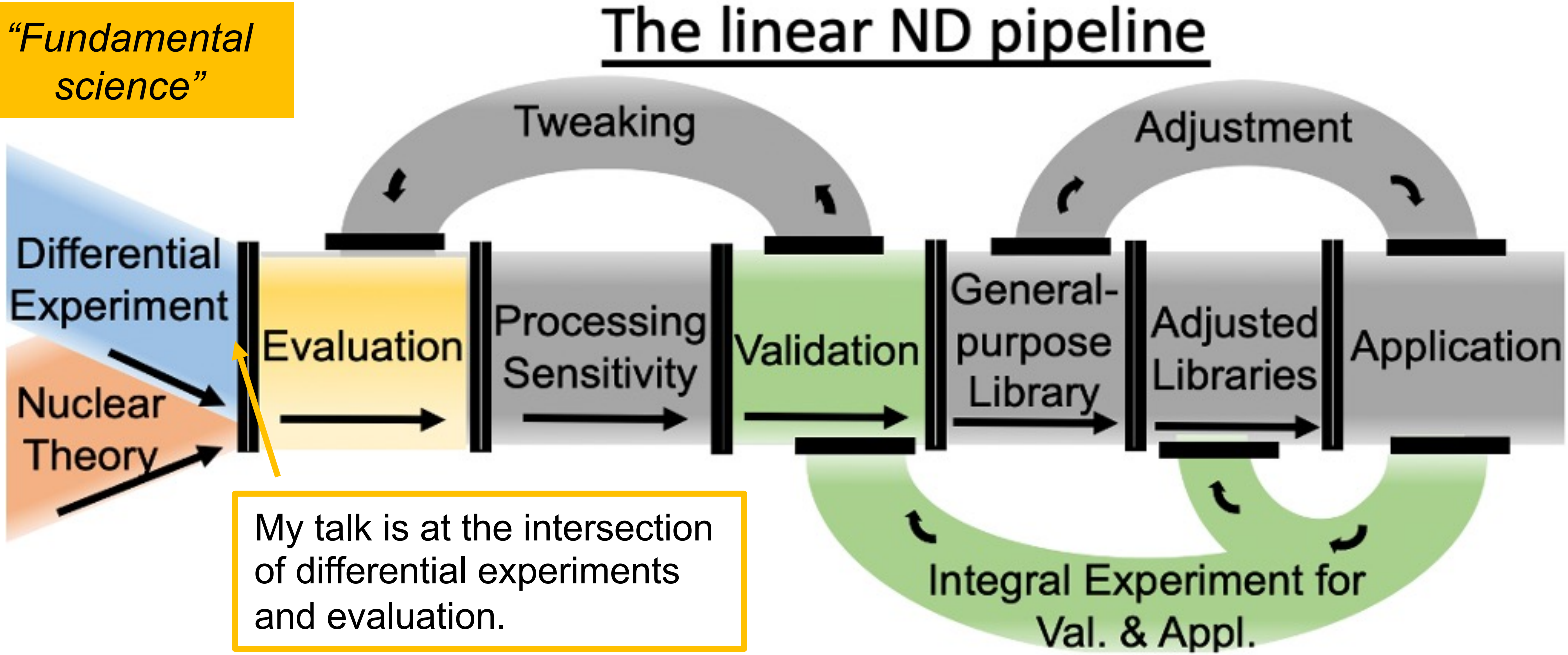
Experimental uncertainty quantification: key piece of creating nuclear data that connect "fundamental" to "applied" science.

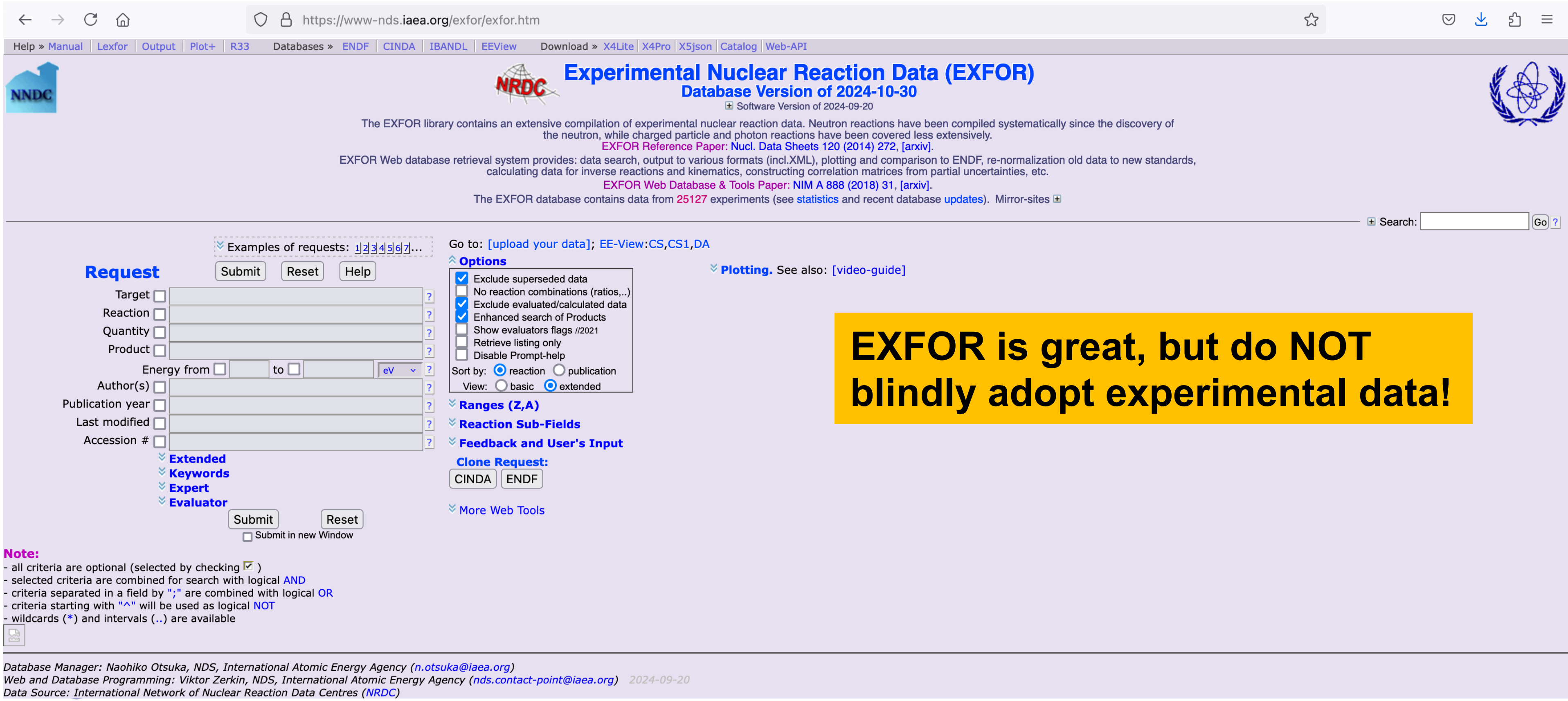
"Fundamental science"



My talk is at the intersection of differential experiments and evaluation.

"Applied science"

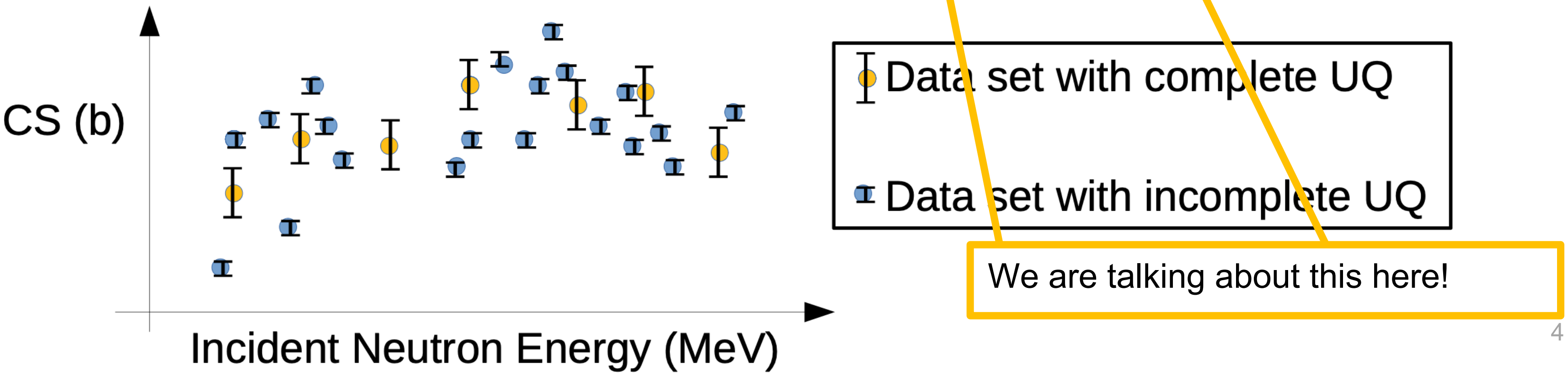
EXFOR (https://www-nds.iaea.org/exfor/exfor.htm) gives easy access to experimental data for nuclear data evaluations.



EXFOR is great, but do NOT blindly adopt experimental data!

BUT, one cannot adopt data blindly from EXFOR. One needs to:

- Retrieve data from EXOFR, renormalize data to the newest standard & plot.
- Remove clear outliers from experimental database.
- Review literature and EXFOR entries of each data set.
- Undertake detailed uncertainty quantification ***for each dataset in the database*** using EXFOR data, literature review & templates.
- Critically assess database & study physics causes of discrepancies.



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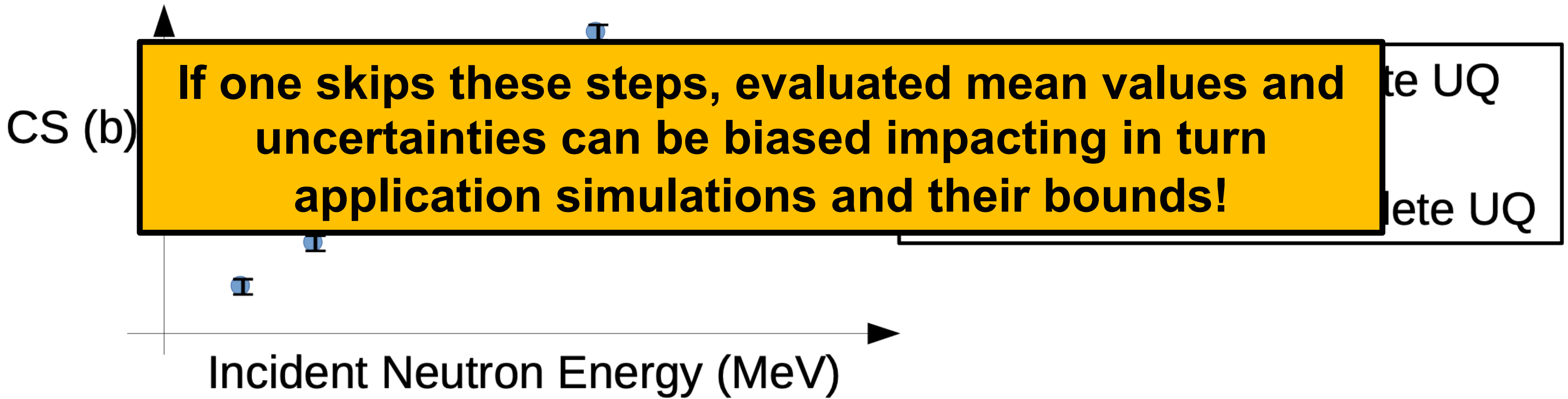
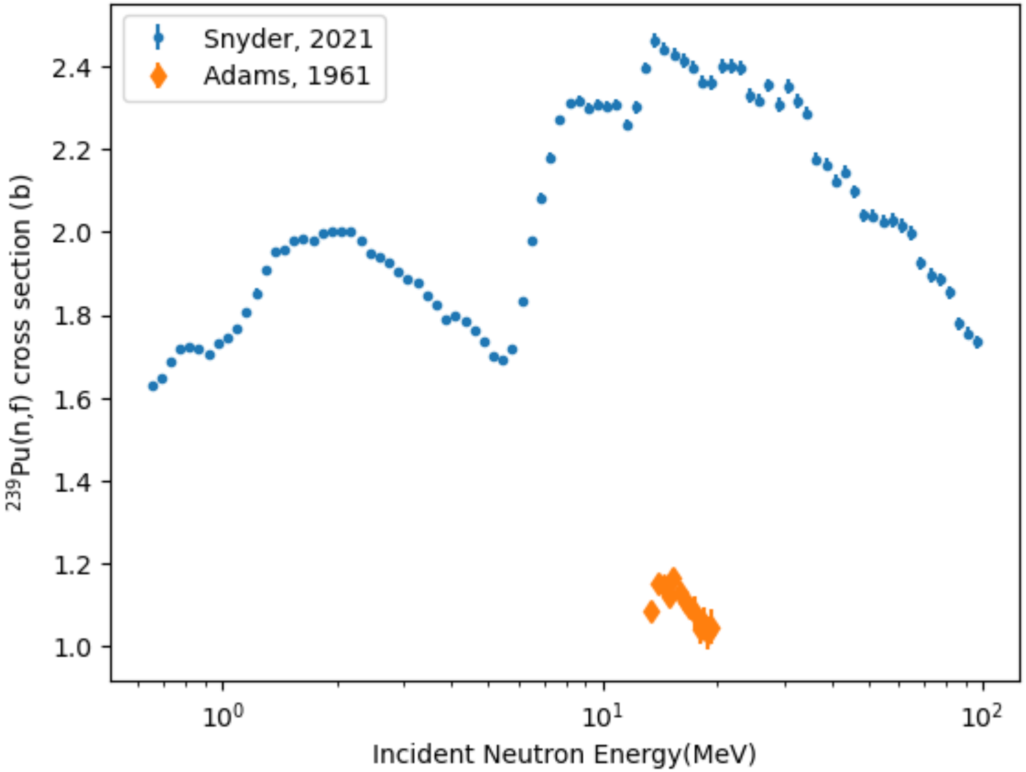


If one skips these steps, evaluated mean values and uncertainties can be biased impacting in turn application simulations and their bounds!

Example: data of Adams and Snyder read blindly from EXFOR are clearly discrepant!

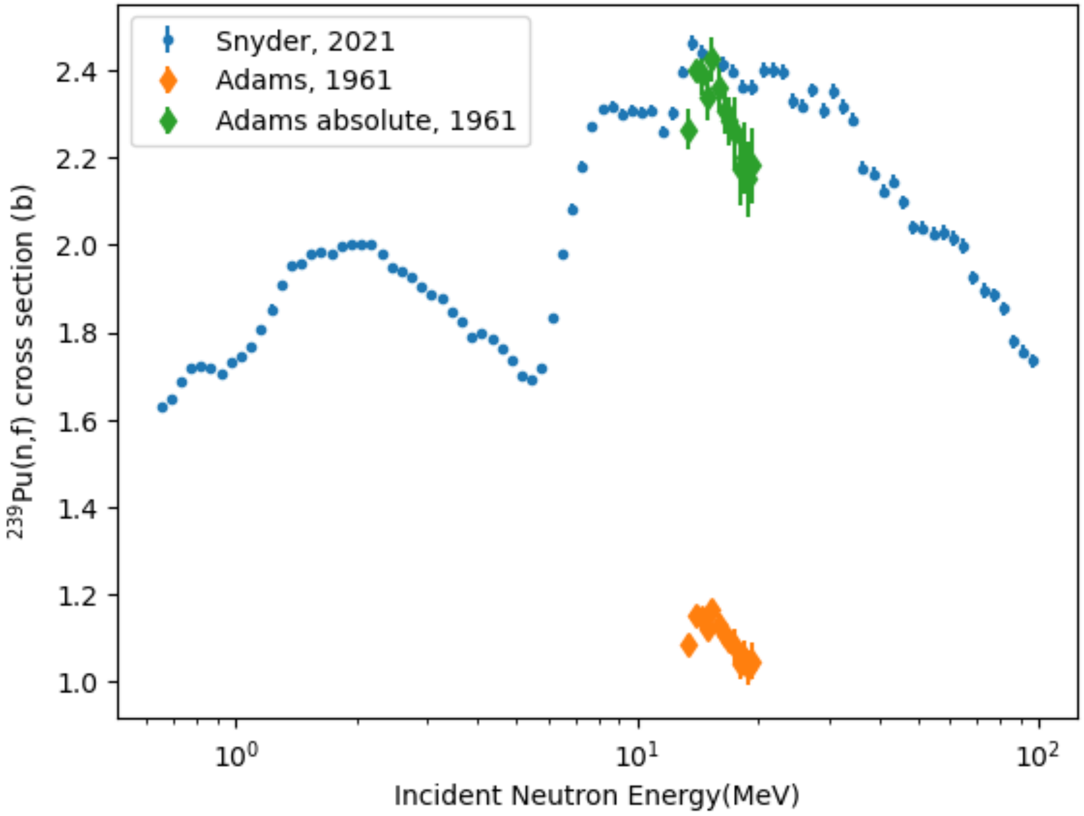


Adams data are shape data and need re-normalization, but only clear if you read the EXFOR entry in detail:

"REACTION 1((94-PU-239(N,F),,SIG,,REL)/(92-U-238(N,F),,SIG,,REL))
Normalized to unity at 14 MeV."

Accession #: 21209004 (Adams)
14721002 (Snyder)

Solution: Adams data are shape data. Ratio data are set to 1.0 at 14.0 MeV. Re-normalize to current evaluation.



- Renormalizing ratio data with factor 2.4/1.151 as this aligns the cross section with the VIII.1 ^{239}Pu(n,f) cs.
- We still see distinct discrepancies.
- Maybe, some uncertainties are missing?

Templates of expected measurement uncertainties

Templates of expected measurement uncertainties can help complete uncertainties for curated database.

Templates:

- Document what experiment information and uncertainty sources are needed for evaluators to make most use of experimental data stored in EXFOR.
- Provide stand-in values for uncertainty sources that are not provided by experimenters.

Template's benefit:

- Evaluators can make **more informed choices to fill in missing uncertainty** and correlation information.
- Leads to a **more balanced uncertainty quantification across different data sets.**

Applying templates for UQ leads to more realistic evaluated uncertainties for nuclear data libraries.

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.

The example here shows the (n,f) cross section template.

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And here is the template:

Table 2: Typical uncertainty sources encountered in (n,f) measurements that involve detecting fission fragments are listed dependent on their specific measurement type. The amendments from the preliminary version of the template in Ref. [9] are highlighted in red.

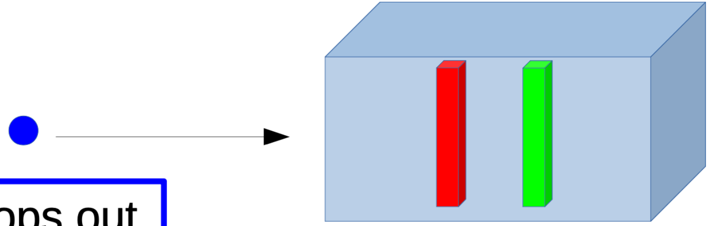
	Unc. source	Absolute	Absolute clean ratio	Absolute indirect ratio
Normalization	$\delta N_{(a/b\&c)}$	See Table 1	Both samples	Both samples
Counting	δc	Eqs. (3) and (5)	Both, combined	Both, combined
Statistics	$\delta\beta$ & δm; δm	0.2–2%	0.02–0.2%	0.2–2%
Multiple scattering	$\delta\beta$ & δm; $\delta\beta$	0.2–1%	Less than absolute	0.2–1%
	$\delta\varepsilon$ & $\delta\alpha$; $\delta\varepsilon$	1.1–4%	0.3–4%	1.1-4%, 0.5–1%
Efficiency	$\delta\varepsilon$ & $\delta\alpha$; $\delta\alpha$	Compare to nuclear data	Compare to nuclear data	Compare to nuclear data
Background	δb	0.2–>10%	0.2–>10%	0.2–>10%
Energy	δE	1%, 1-3 ns	Combined	Both detectors
Flux	$\delta\phi$	>1%	Cancels or small	Cancels or small
Impurity	$\delta\zeta$	See Table 3	See Table 3	See Table 3
Deadtime	δd	>0.1%	Both combined	Both detectors

The example covers this measurement type.

In clean ratio measurement, the (n,f) cs are measured relative to a reference cross section with the same detector.

Sample of interest with # of atoms N_1

Reference sample with # of atoms N_2



Φ drops out

ε reduces to a correction factor $\delta\varepsilon$ for the two samples.

$$\sigma(E)=\sigma_R^{ND}(E)\frac{C_1(E)\,N_2}{C_2(E)\,N_1}\delta\epsilon(E)\zeta(E)$$

The nuclear data of the reference data σ_R^{ND} is needed to get σ.

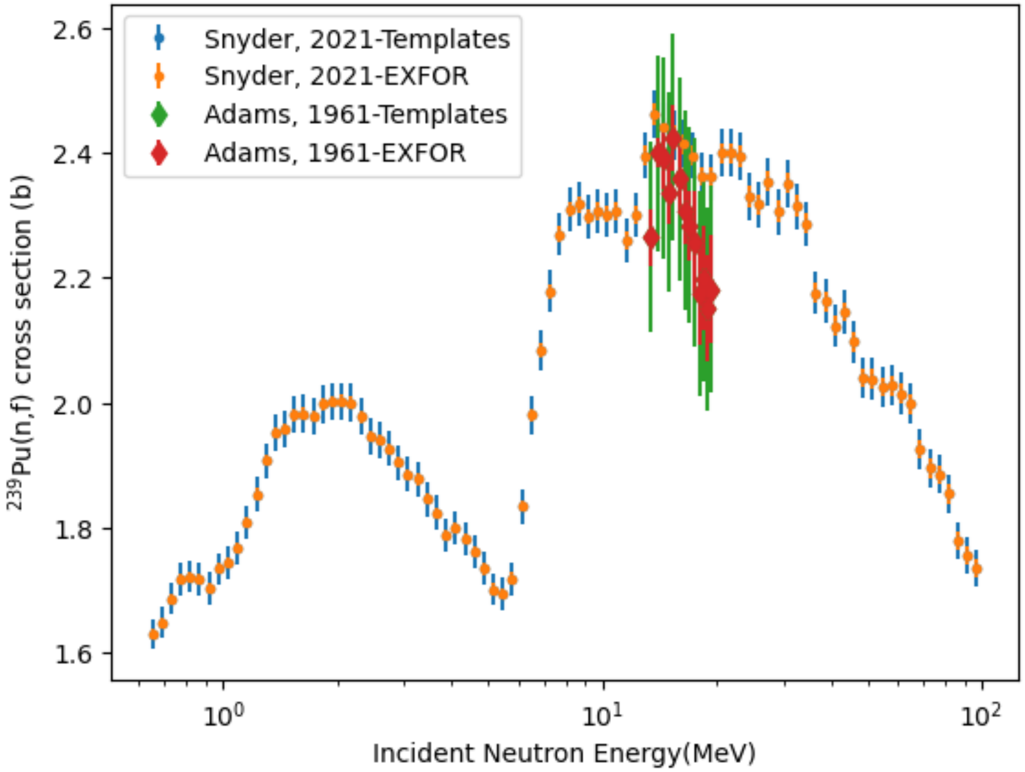
Our example: Adams misses a lot of uncertainty sources in EXFOR, Snyder only one (that is in another article).

Unc. source	Absolute	Absolute clean ratio
$\delta N_{(a/b\&c)}$	See Table 1	Both samples
δc	Eqs. (3) and (5)	Both, combined
$\delta\beta$ & δm; δm	0.2–2%	0.02–0.2%
$\delta\beta$ & δm; $\delta\beta$	0.2–1%	Less than absolute
$\delta\varepsilon$ & $\delta\alpha$; $\delta\varepsilon$	1.1–4%	0.3–4%
$\delta\varepsilon$ & $\delta\alpha$; $\delta\alpha$	Compare to nuclear data	Compare to nuclear data
δb	0.2–>10%	0.2–>10%
δE	1%, 1-3 ns	Combined
$\delta\phi$	>1%	Cancels or small
$\delta\zeta$	See Table 3	See Table 3
δd	>0.1%	Both combined

	Adams	Snyder
Normalization	N/A	×
Counting Statistics	✓	✓
Multiple scattering	×	✓
Efficiency	×	✓
Background	×	✓
Energy	×	✓
Flux	N/A	✓
Impurity	×	✓
Deadtime	×	✓

Missing uncertainties can be added via templates of uncertainties.

Adding template uncertainties results in data with overlapping uncertainties …



A word of caution:
While the uncertainties now overlap, I would still think twice before accepting Adams' data.

→ Templates help only report known systematic unc. Here, we need to explore physics root causes of experimental discrepancies.

Using ML to understand what are physics root causes of discrepancies between experimental datasets

We are applying machine learning to accelerate progress in understanding physics underlying nuclear data.

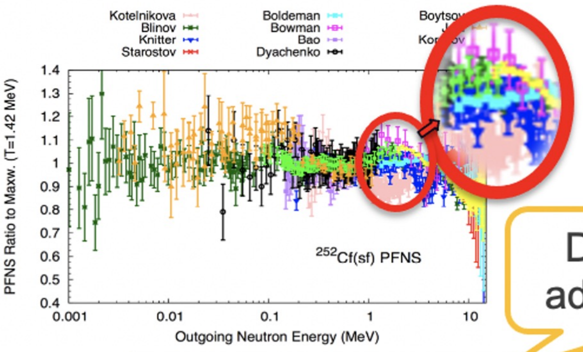
The <u>big questions</u> we are after:

- **What is the physical root cause for experimental discrepancies (despite complete experimental UQ)?**
- **What experiment can we perform to reduce scatter in experimental database?**

<u>Benefit</u> of answering questions:

- More targeted experiments reducing spread in an experimental data. This accelerates progress in understanding fission physics.
- Reduced uncertainties and better means for nuclear data that in turns lead to more reliable application simulation and better model fitting.

AIACHNE created a ML capability to explore discrepancies in past ^{252}Cf(sf) PFNS exp. & measures new data.



Developing advanced ML

Using state-of-the-art LANSCE equipment

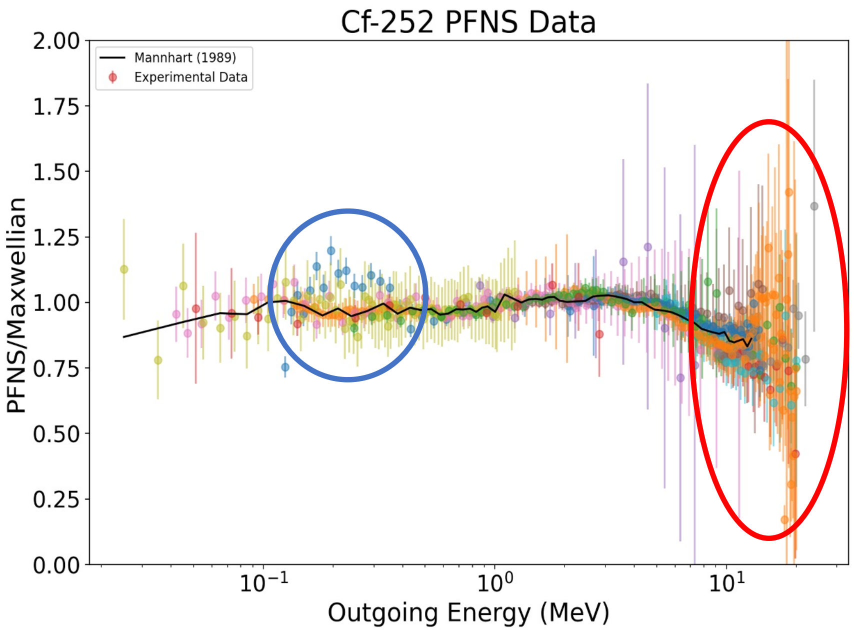
Correcting past data and assessing impact

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 → Improved ND

Simulated correction factors

To that end, we used a ML capability to pin-point measurement features likely related to bias and choose most impactful experiments based on MCNP studies.

The problem at hand: Experimental ^{252}Cf PFNS have a wide systematic scatter of data at low and high energies AFTER DETAILED EXPERIMENTAL UQ WITH TEMPLATES.



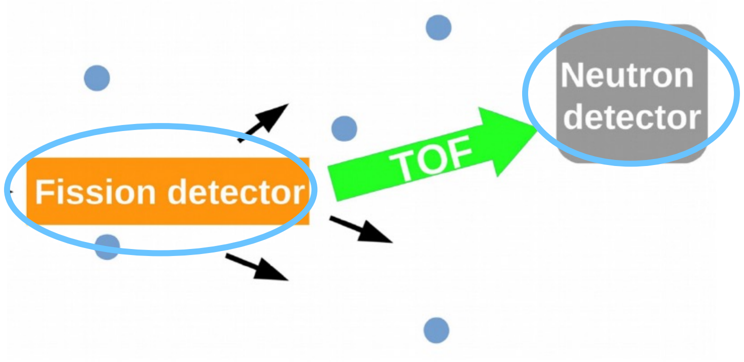
<u>Discrepancies at low E_{out} understood</u>: caused by incorrect resolution of ^{6}Li resonance for detector response.

<u>Discrepancies at high Eout **not** understood</u>:

- Background?
- Time resolution?
- Fission fragment issues?
- Neutron detector response?

Root cause of discrepancies must be tied to set-up issue or analysis technique encoded in measurement features.

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!!!

These metadata are retrieved from EXFOR in a by-hand process.

AIACHNE is using a sparse Bayesian model to identify potential sources of bias in ^{252}Cf PFNS data.

We are extending the Bayesian model with an energy-dependent, multiplicative bias. Sparsity ensures no bias for most energies but the term is active when the data indicate the need. A horseshoe prior reduces the number of potential biases.

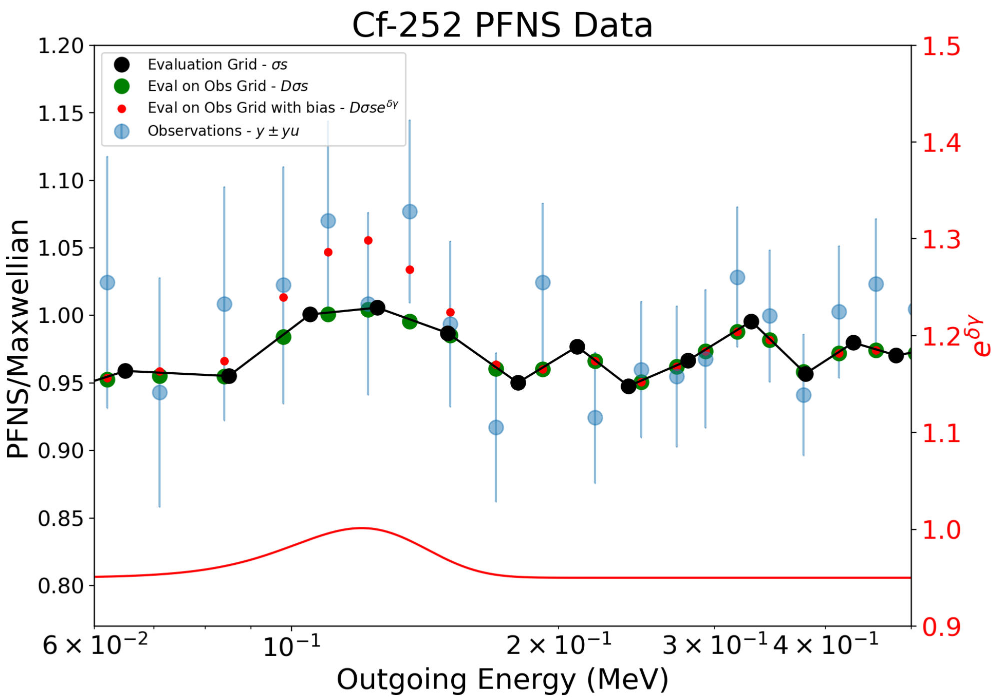
$$y = D\sigma \cdot e^{\delta} + \varepsilon$$

$\delta =$ $B\gamma =$ **relative bias**

$\mathbf{B} =$ **bias basis matrix**

$\gamma =$ **bias coefficients**

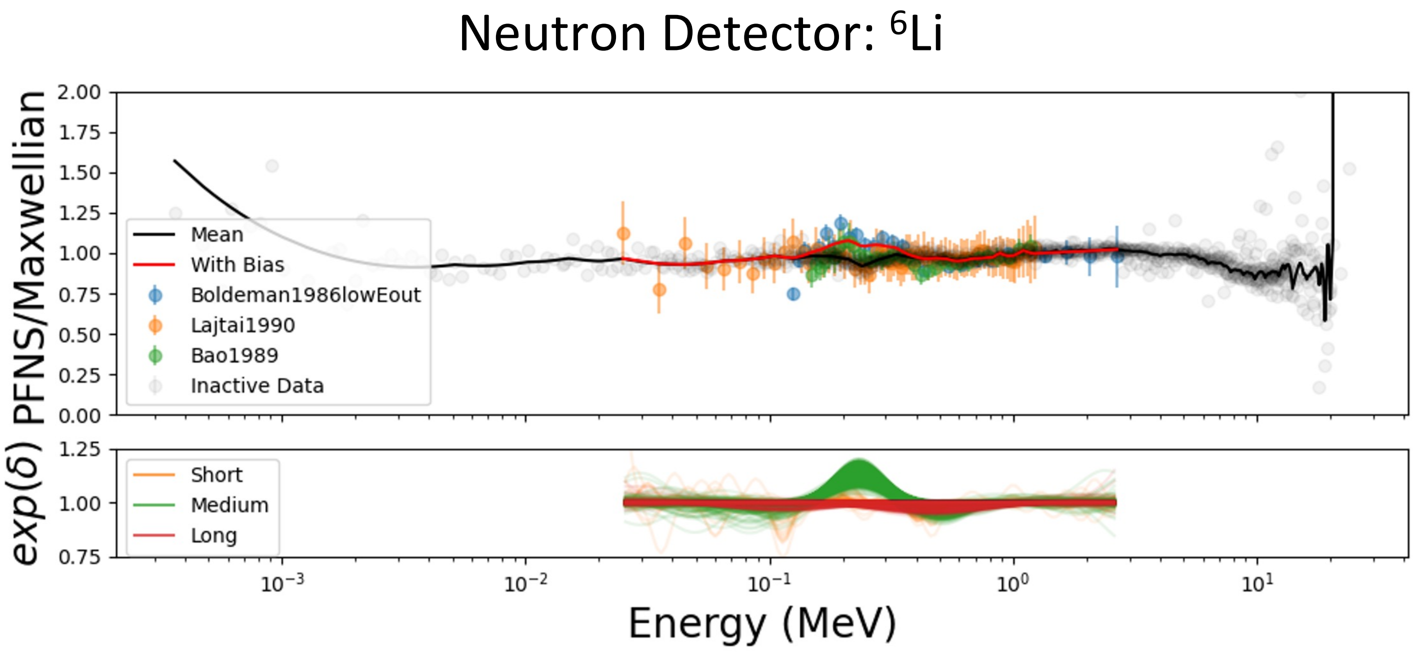
$\cdot =$ **element-wise product**



The algorithm deals well with a large number of correlated features compared to experimental data.

Validation example: does the algorithm correctly identify expected bias due to ^{6}Li peak? – Yes, it does!

Study is documented in paper: N. Walton, LA-UR-24-29607 (2024), submitted.



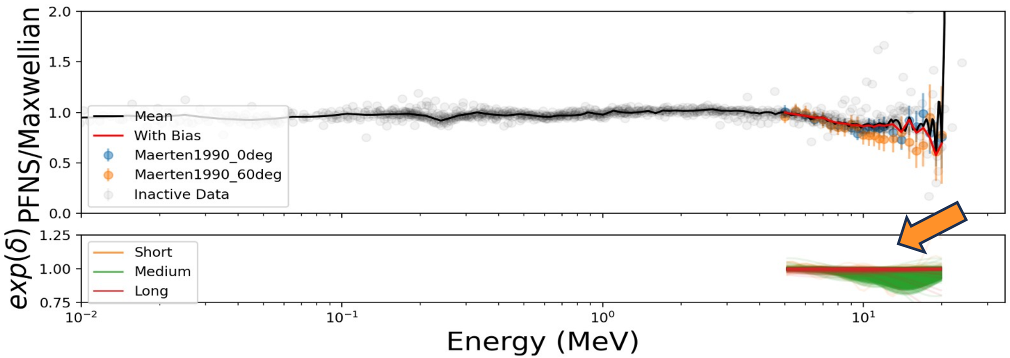
Advantage of algorithm: Enables to more quantitatively identify bias in exp. data as a function of energy to be included in evaluation algorithm.

Another example: 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).

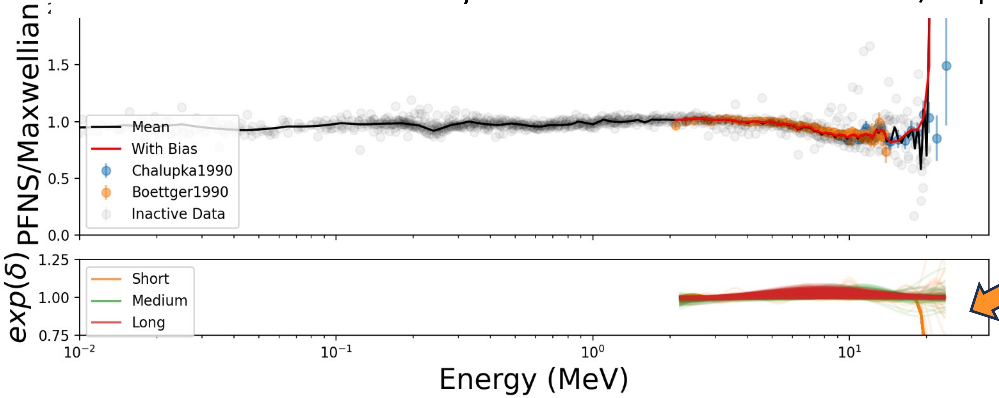
The algorithm finds features related to bias experts might have otherwise overlooked. The algorithm results require expert interpretation.

Fission Detection Efficiency Correction Method: Calculated/Measured



~30% of samples

Fission Detection Efficiency Correction Method: Calculated/Stapre



~10% of samples

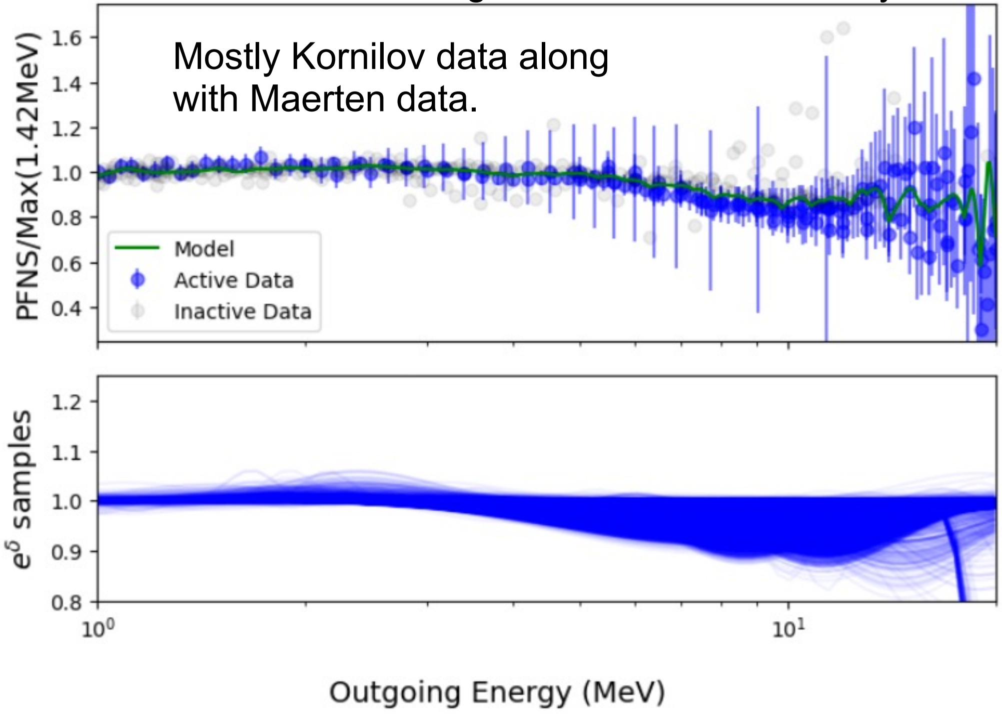
ML results also list in several categories Kornilov data.

Bias in Kornilov data related to:

- Fission fragment efficiency,
- Various uncorrected background,
- Neutron detector components,
- ...

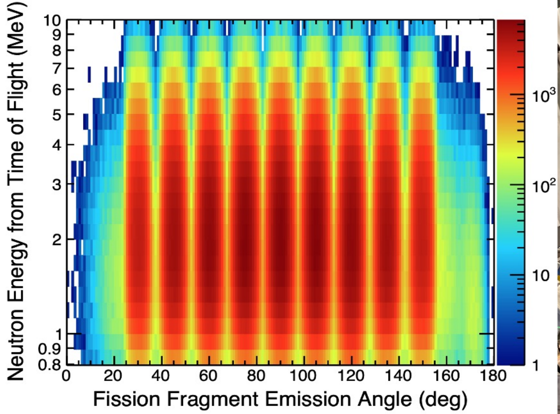
In essence, the algorithm told us to go and look more at the data. ☺

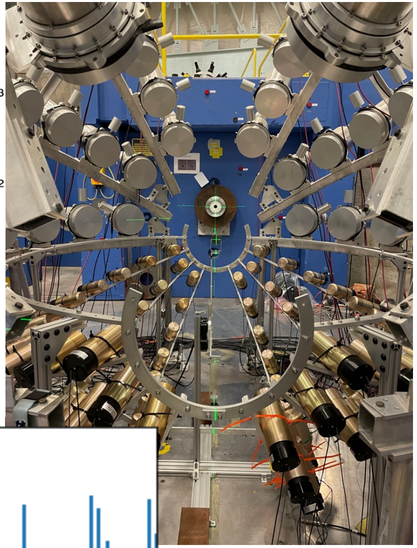
Fission fragment detection efficiency

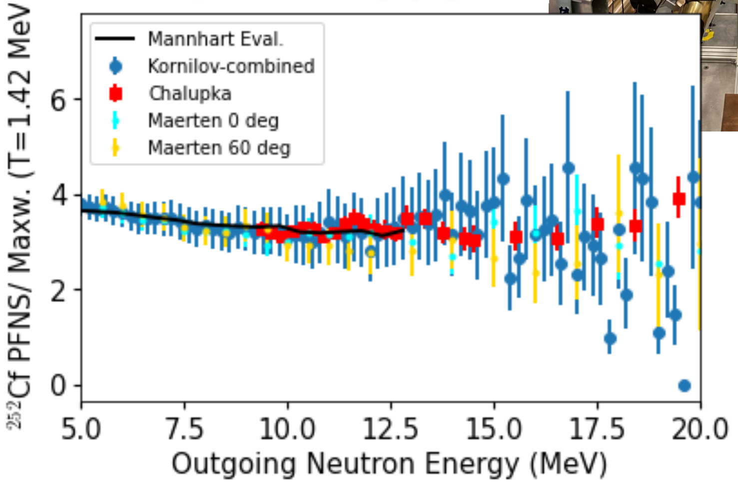


It is key for experts to take a second look at ML results. We are doing that via exp. and simulations.

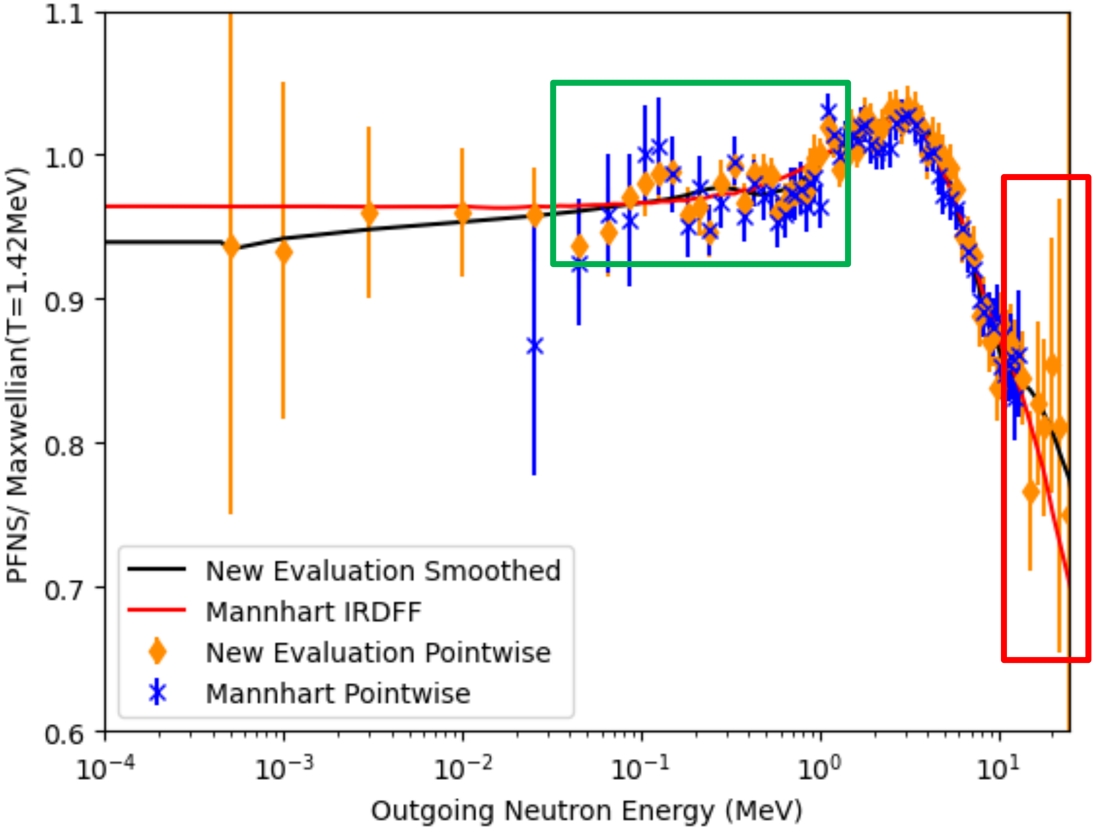
- Boldeman ^{6}Li bias: will be explored via CoGNAC ^{252}Cf PFNS experiment by K. Kelly.
- Kornilov bias: AIACHNE team worked with Tom Massey to identify issue (neutron detector response extrapolation) and removed biased run from data set.
- Maerten bias: will simulate fission fragment angular distribution for correction.

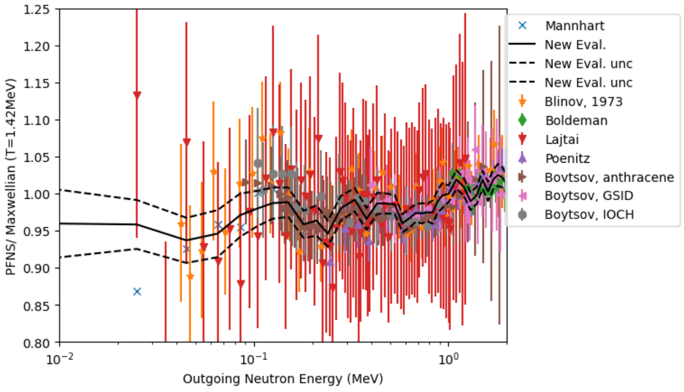


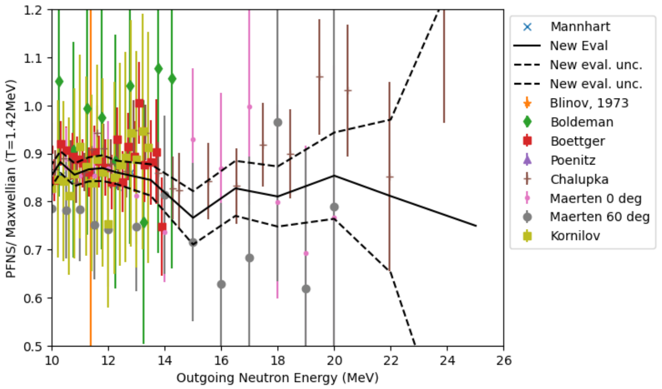




New evaluation reduces ^{6}Li peak but more work needed at high outgoing energies correcting data.







Conclusions

- o Don’t use data straight from EXFOR but do detailed experimental UQ & review of data,
- o Templates help us give realistic uncertainty estimates where uncertainties were missing.
- o If, despite good exp. UQ, one still observes discrepancies, question what is the physics root cause!
- o Interplay between expert judgment and ML results can be key to tease out more understanding of physics information than each on their own.

Thank you for listening!

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