Towards a new ^{252}Cf(sf) PFNS evaluation: A multi-chapter story.

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Neutron Data Standards Meeting 2025 Jan 27-31, 25

LA-UR-25-20638

Thank you to Roberto Capote for feedback throughout!

We would like to show today:

- Our new $^{252}Cf(sf)$ PFNS evaluation and discuss the stages needed for the standards committee to accept this new evaluation.
- A new experiment coming up for the $^{252}Cf(sf)$ PFNS.
- A technique to pin down physical root causes of unknown systematic experimental discrepancies.

The topics will be covered in slightly different order:

1. A technique to pin down physical root causes of unknown systematic experimental discrepancies.
2. Our new ^{252}Cf(sf) PFNS evaluation and discuss the stages needed for the standards committee to accept this new evaluation.
3. A new experiment coming up for the ^{252}Cf(sf) PFNS.

From last standards meetings: We replace 2 data sets accepted by Mannhart, reject 1 and accept 10 new data sets.

Mannhart standard evaluation

Author & year	EXFOR-number
Dyachenko 1989	41158.003.
Boettger 1990	Not in EXFOR.
Poenitz 1983	14278.002
Blinov 1973	40418.007
Boldemann (Li) 1986	30775.003
Boldemann (Plastic)	30775.002
Maerten 1984	Not in EXFOR.

Proposed input for new standard

Author + Year	Author + Year
Lajtai 1990	~~2xBlain 2017~~
Boettger 1990	3xBoytsov 1983
Poenitz 1983	2xChalupka 1990
Blinov 1973	4xBlinov 1980
X	*Kornilov, 2015*
Boldemann (Plastic)	
X	2xMaerten 1990

At the last standards meeting, the committee rejected Blain, 2017 because of large scatter in the data. Deeper study of Kornilov, 2015 data was recommended.

We show a technique to pin down physical root causes of unknown systematic experimental discrepancies.

We are applying machine learning (ML) to uncover the physics root cause of experimental unrecognized sources of unc. (USU).

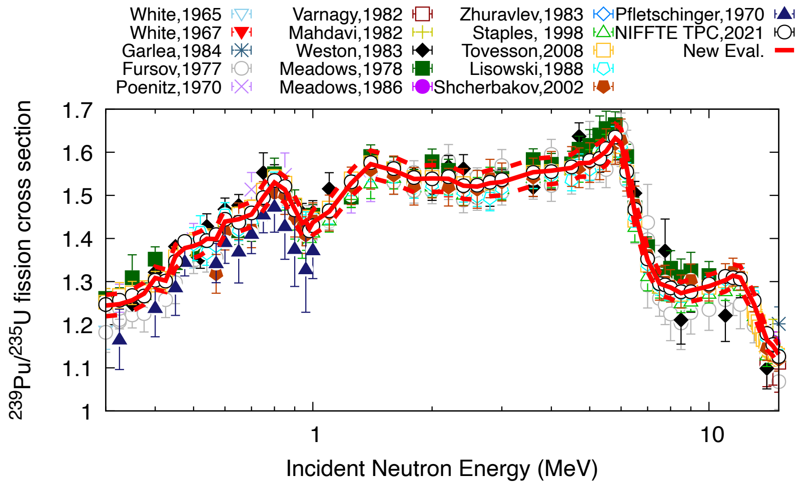
The big questions we are after:

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

Benefit of answering questions:

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

Background: Neutron Data Standards introduced 2018 USU to account for discrepancies in data with unknown source.



Carlson, NDS 148 (2018); Capote, NDS 163 (2020).

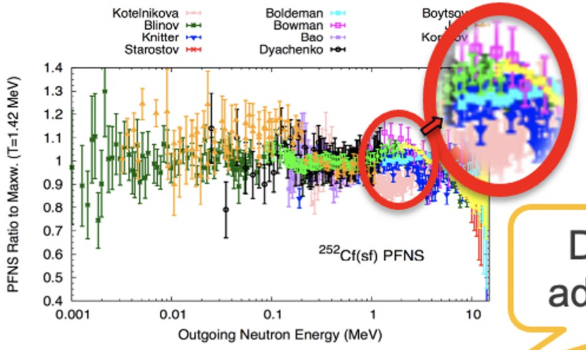
<u>The good</u>: we are quantifying obviously missing uncertainties in data.

<u>The ugly:</u> unc. based on the spread of data covering up our missing understanding physics root causes of discrepancies.

<u>The bad:</u> large unc. on quantities depending on standards with no way forward to reduce unc. if defined based on the spread of data.

<u>The solution:</u> We try to uncover physics root causes driving discrepancies and either reject data with justification or correct them.

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

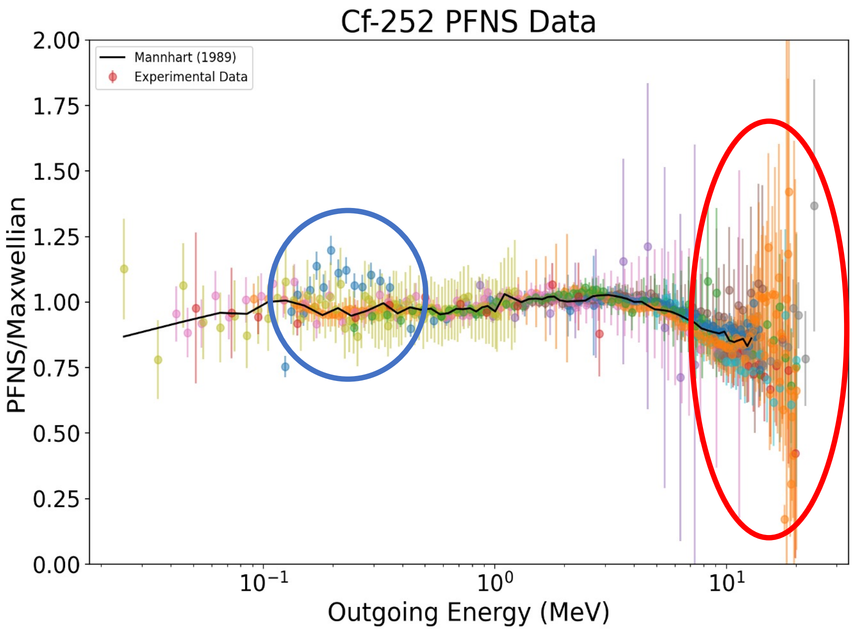
Correcting past data and assessing impact

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.



<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?

We included those data into ML study that had a reasonable degree of documentation, unc. & were (somewhat) physical.

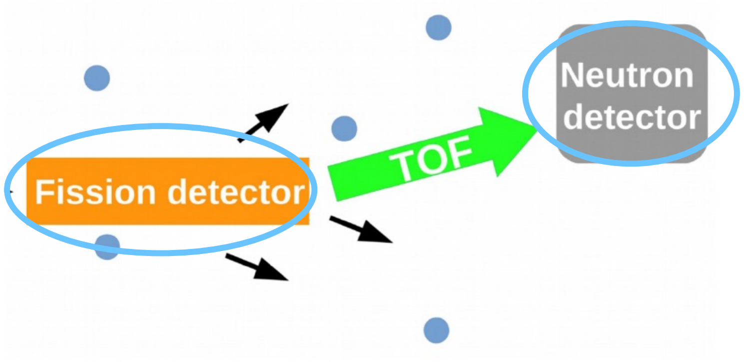
Author + Year	Author + Year	Author + Year	Author + Year
Bao 1989	~~Bowman 1985~~	~~6xGreen 1973~~	2xMaerten 1990
~~Bentsch 1979~~	3xBoytsov 1983	~~2xJeki 1971~~	~~Meadows 1965~~
2xBlain 2017	1xChalupka 1990	Knitter 1973	~~Nefedov 1983~~
1xBlinov 1973	~~Coelho 1989~~	Kornilov 2015	Poenitz 1982
4xBlinov 1980	~~Conde 1965~~	~~Kotelnikova 1975~~	~~2xStarostov 1983~~
Boettger 1990	~~Dyachenko 1989~~	Lajtai 1990	
2xBoldeman 1986	~~Goeoek 2014~~	~~2xMaerten 1984~~	

Taken into account by Mannhart (green)   ~~X~~ Not taken into account for ML

Dyachenko and Maerten, 1984 were preliminary data that were replaced by Lajtai and Maerten, 1990 final data.

We included also measurement metadata into analysis as biases must be tied to set-up issue or analysis technique.

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!!!

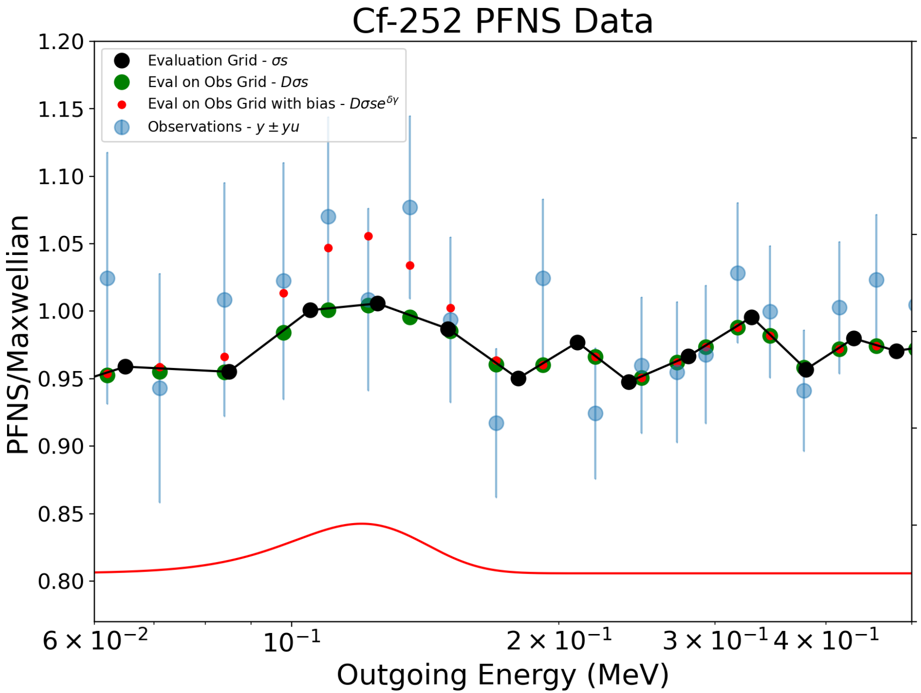
These metadata are retrieved from EXFOR in a by-hand process.

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.

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

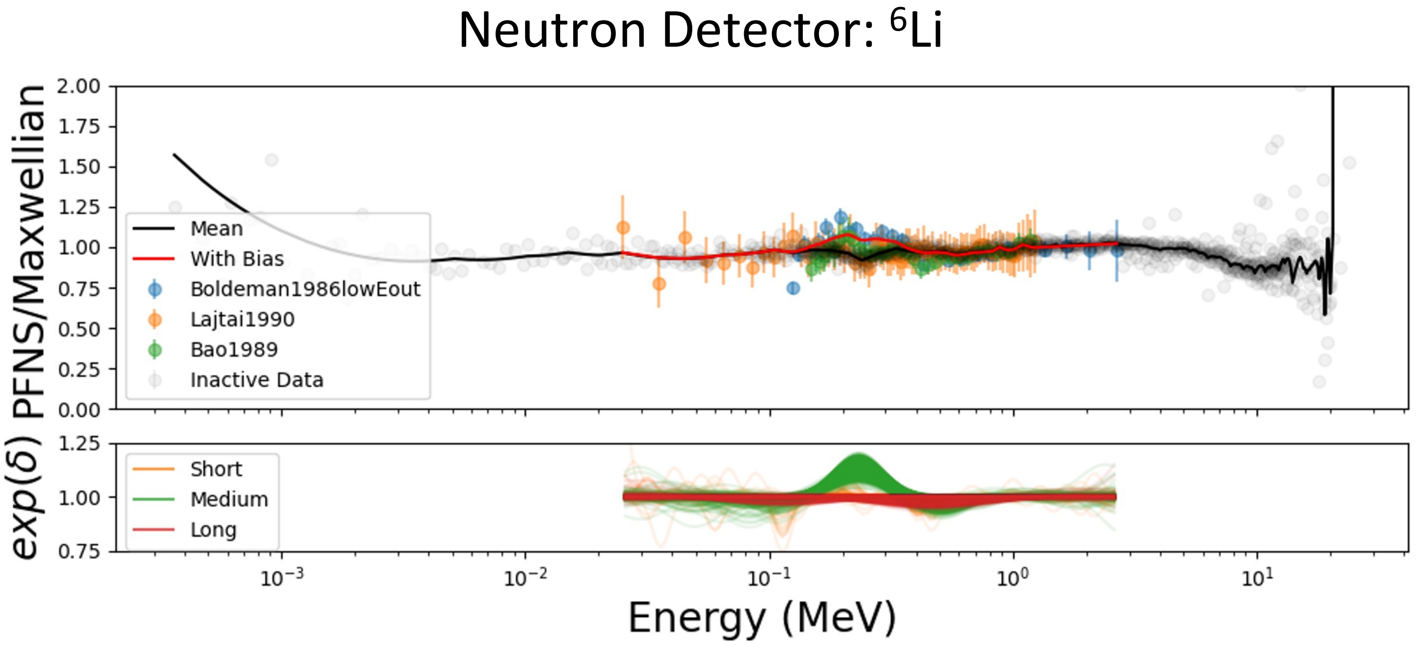
$\delta =$ $B\gamma =$ relative bias
$\mathbf{B} =$ bias basis matrix
$\gamma =$ bias coefficients
$\cdot =$ element-wise product



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

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

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

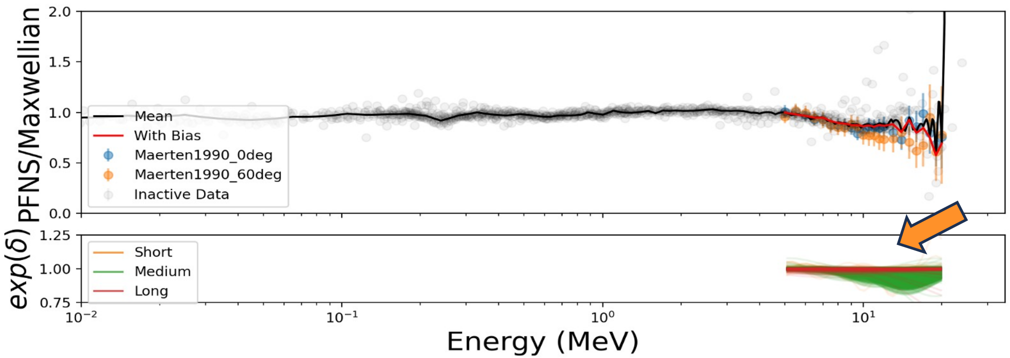


Advantage of algorithm: Enables to more quantitatively identify bias in exp. data as a function of energy to be included in evaluation algorithm.

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

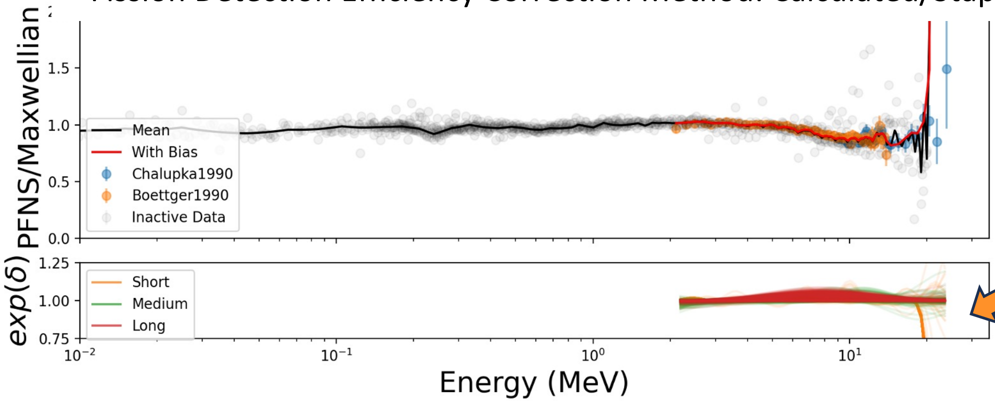
Effect at high energies was attributed to many features. Detailed expert discussion and analysis of data pointed to fission detection (angular dependence of fission fragments), especially in Marten data.

Fission Detection Efficiency Correction Method: Calculated/Measured



~30% of samples highlight Maerten data

Fission Detection Efficiency Correction Method: Calculated/Stapre



~10% of samples highlight Chalupka data

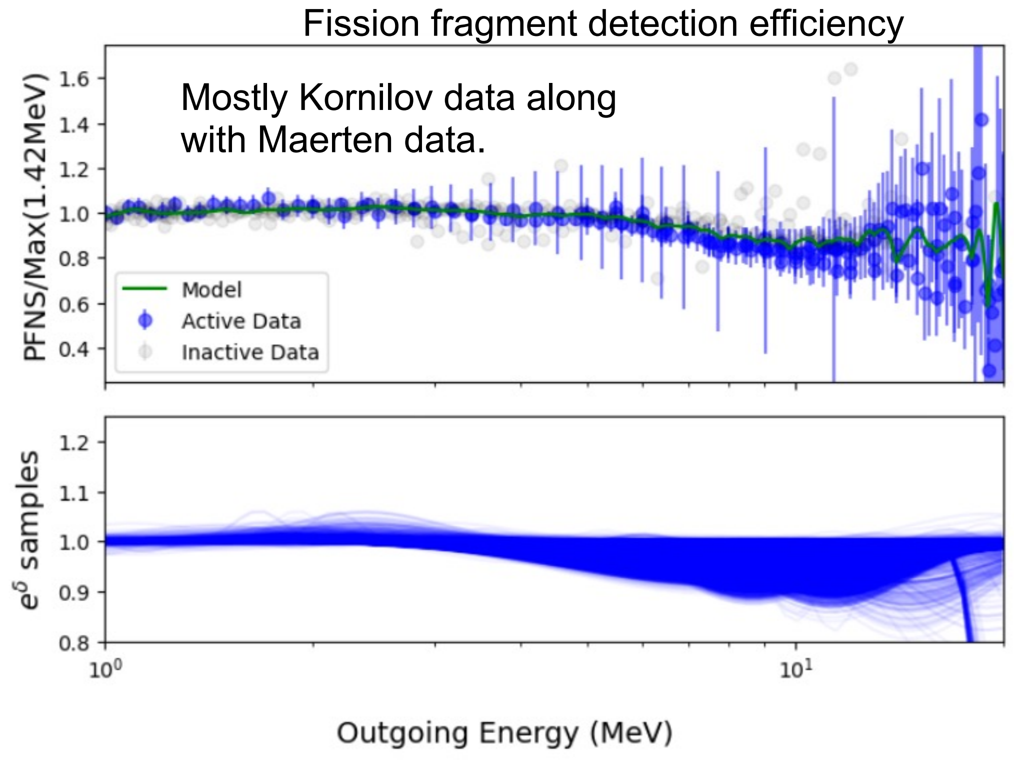
The algorithm finds features related to bias experts might have otherwise overlooked. The algorithm results require expert interpretation.

ML results also list in several categories Kornilov data.

Bias in Kornilov data related to:

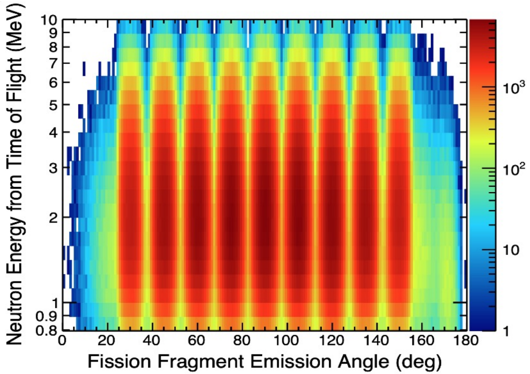
- Fission fragment efficiency,
- Various uncorrected background,
- Neutron detector components,
- ...

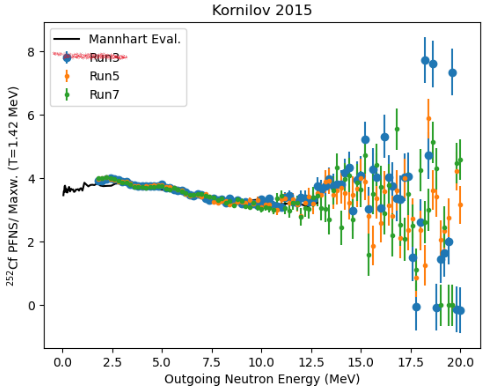
In essence, the algorithm told us to go and look more at the data. ☺

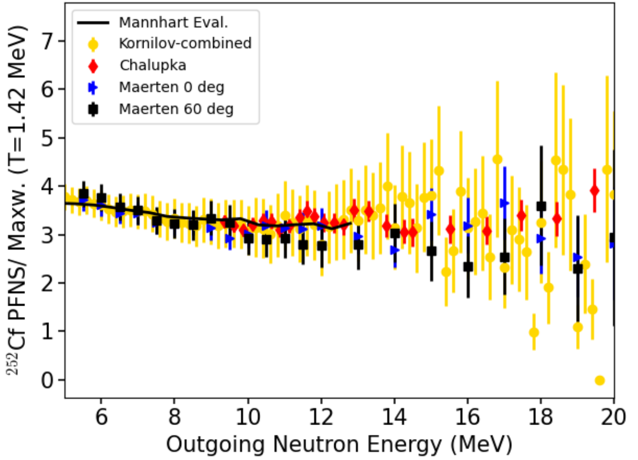


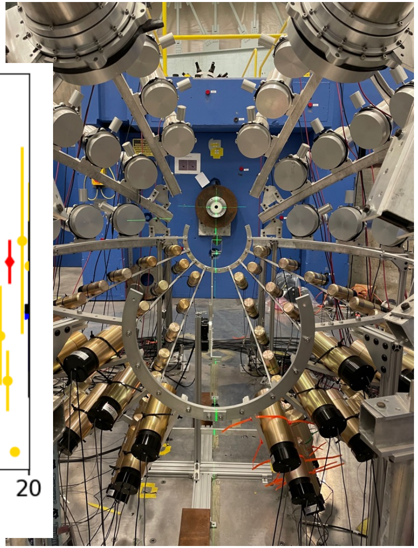
It is key for experts to take a second look at ML results. We are doing that via exp. and simulations.

- 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: Maerten's own and Chi-Nu fission fragment simulation studies point to data at 60° being unbiased. ***We rejected 0° data.***









*see Neudecker, mini-CSEWG 2024 talk for details.

You might why all of this work? Simply to get the best possible evaluation!!!

- 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*.***
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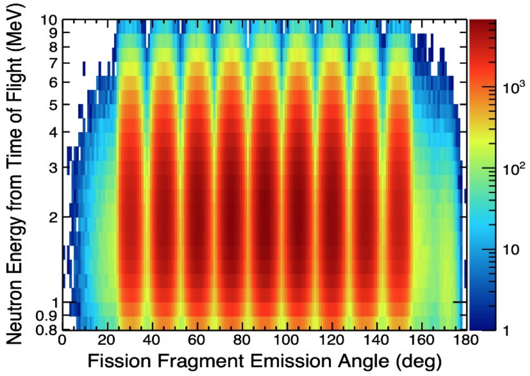

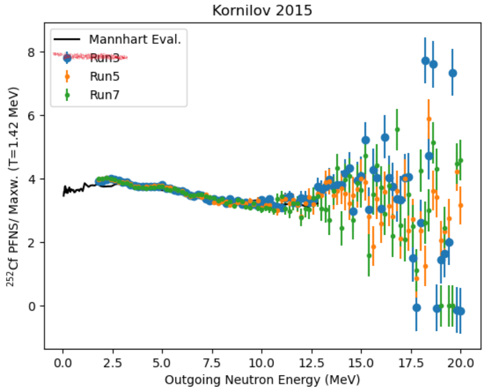

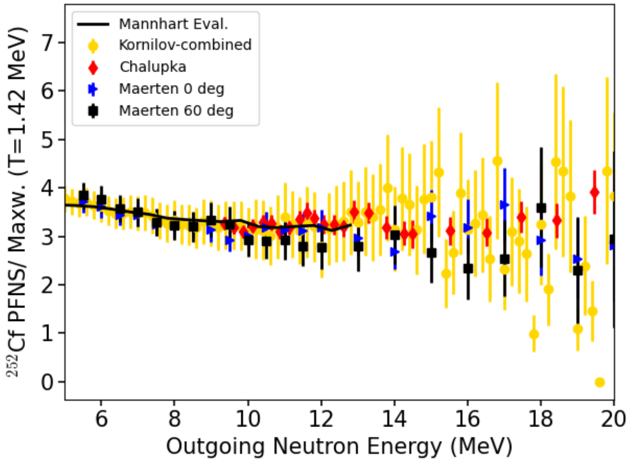

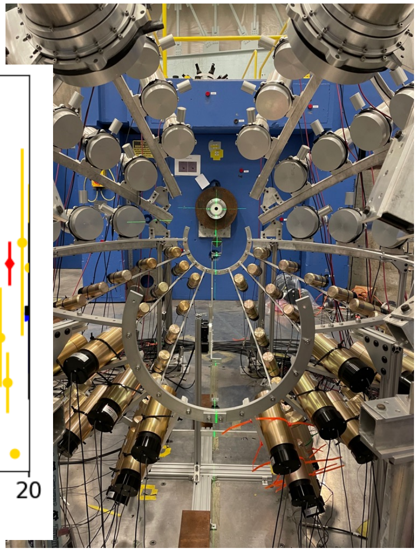

*see Neudecker, mini-CSEWG 2024 talk for details.

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We show our new ^{252}Cf(sf) PFNS evaluation and discuss the stages needed for the standards committee to accept this new evaluation.

Stages of the evaluation:

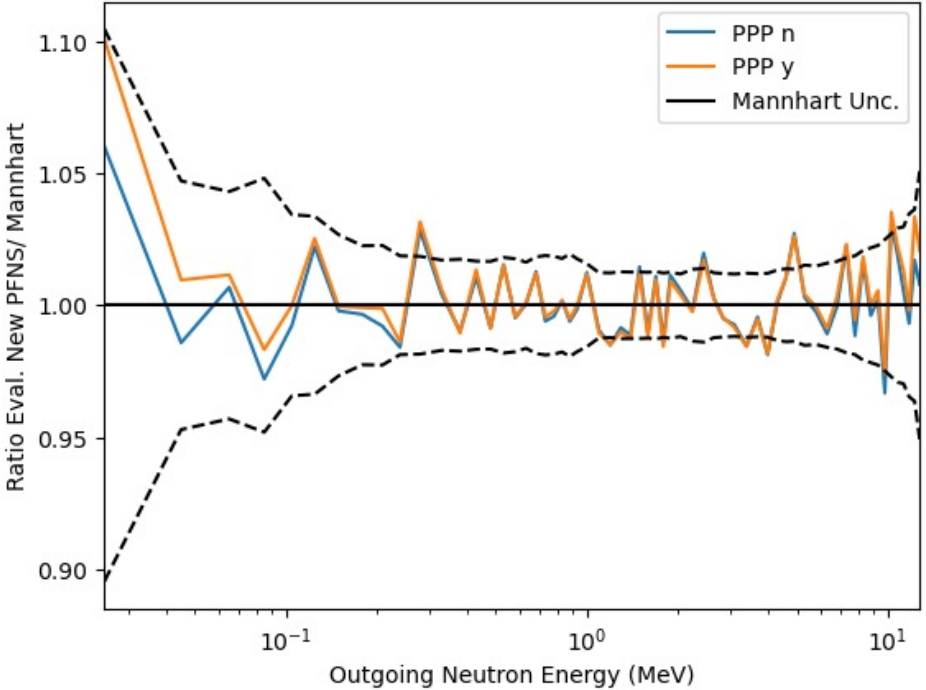
1. Survey the experimental data and find issues. DONE (see before).
2. Reproduce Mannhart’s evaluation to the best ability to see if our methods are correct.
3. Do new evaluation.
4. Calculate spectrum-averaged cross sections.

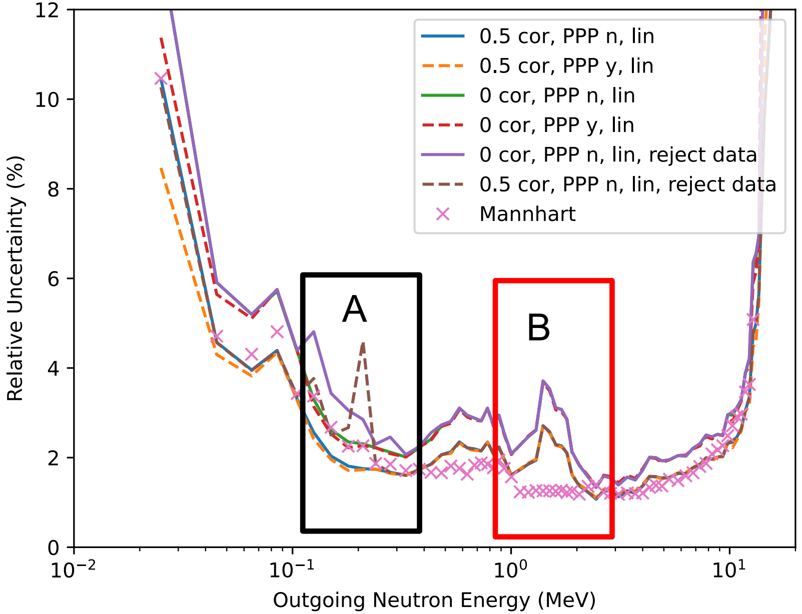
2. There is a lot we know and a lot we don't know about Mannhart's evaluation, unfortunately.

We know	***We don't know***
GLS algorithm *without PPP correction was used*	Prior mean values and covariances (minor)
We read experimental mean values and uncertainties from plots.	**We do NOT have experimental correlation coefficients! (major)**
How many data points were rejected.	**Which exact experimental data points were rejected! (big)**
Experimental data were transformed to evaluation grid before evaluation.	We cannot reproduce Mannhart's fit results, there is likely a mistake. (minor)

Mannhart evaluation is well documented in: Mannhart, IAEA-TECDOC-410 (1987).

2. We can still reproduce Mannhart mv within his evaluated uncertainties, but open questions remain:





Final judgment: We are missing information on exp. correlation (B) and which data were rejected (A) to fully reproduce Mannhart's evaluation, but PPP effect likely small.

3. New: Updated database, use IRLS (=GLS with Chiba-Smith correction for PPP), detailed new UQ for all data.

Mannhart standard evaluation

Author & year	EXFOR-number
Dyachenko 1989	41158.003.
Boettger 1990	Not in EXFOR.
Poenitz 1983	14278.002
Blinov 1973	40418.007
Boldemann (Li) 1986	30775.003
Boldemann (Plastic)	30775.002
Maerten 1984	Not in EXFOR.

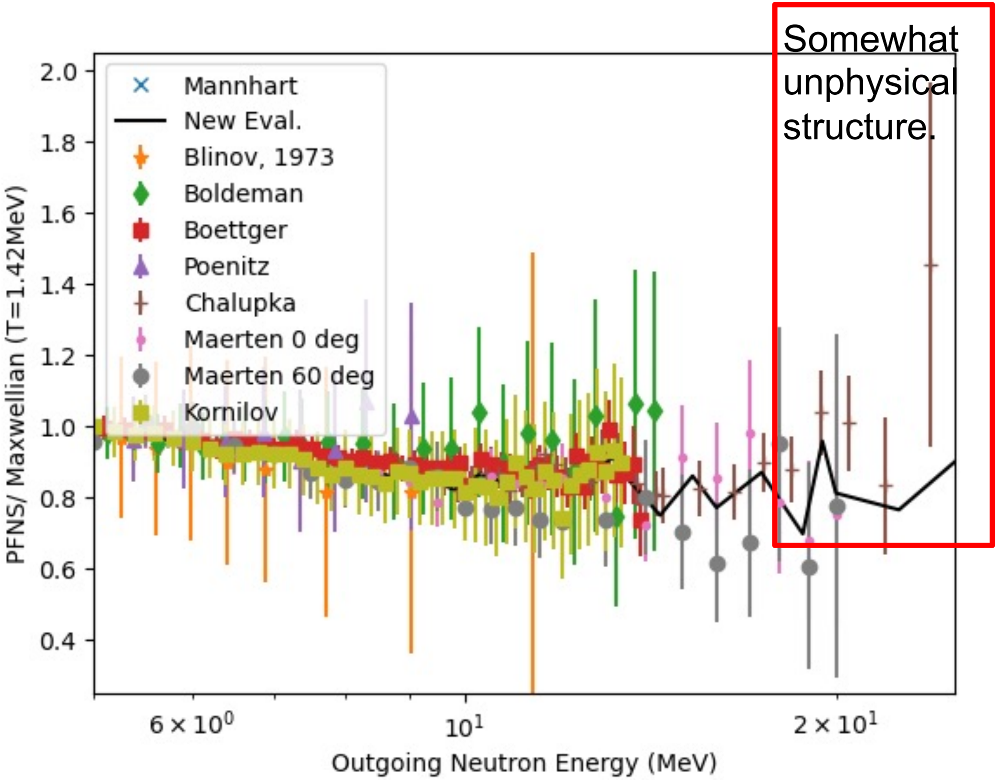
Proposed input for new standard

Author + Year	New Experiments
Lajtai 1990	Kornilov 2017
Boettger 1990	3xBoytsov 1983 (low energy)
Poenitz 1983	Chalupka 1990
Blinov 1973	4xBlinov 1980 (low energy extension)
X	
Boldemann (Plastic)	
X	Maerten, 60^o 1990

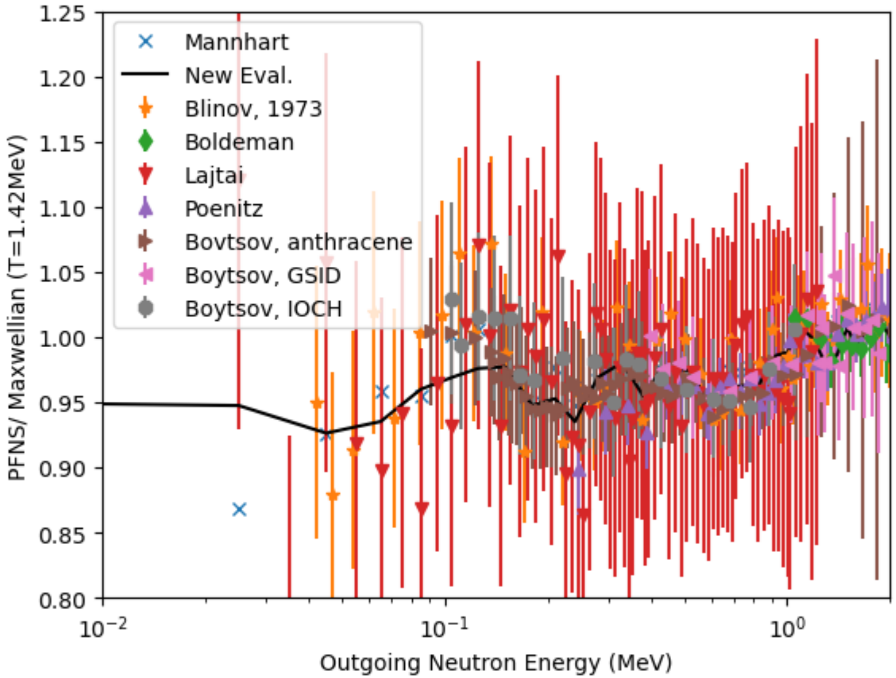
First evaluations presented at CSEWG and FIESTA.

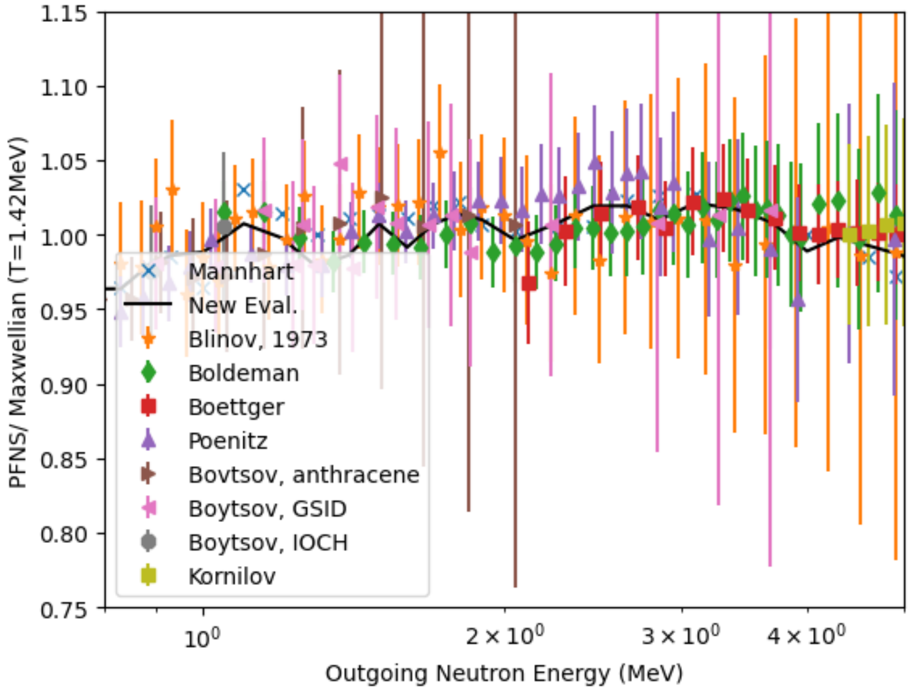
Discussions with Roberto at CSEWG & FIESTA about upturn in evaluated data caused by Chalupka and Maerten 0° data.

- Remove outlying points by Chalupka.
  - 1st variant: remove last point
  - 2nd variant: remove last four points
- Quantify unc. in Maerten data led to looking at what data might not be biased by detection angle and led to rejection of 0° data. Unbiased measurement angle is 60° per Chi-Nu and Maerten studies.



Evaluation rejecting 1 point of Chalupka and Maerten 0 degree data.





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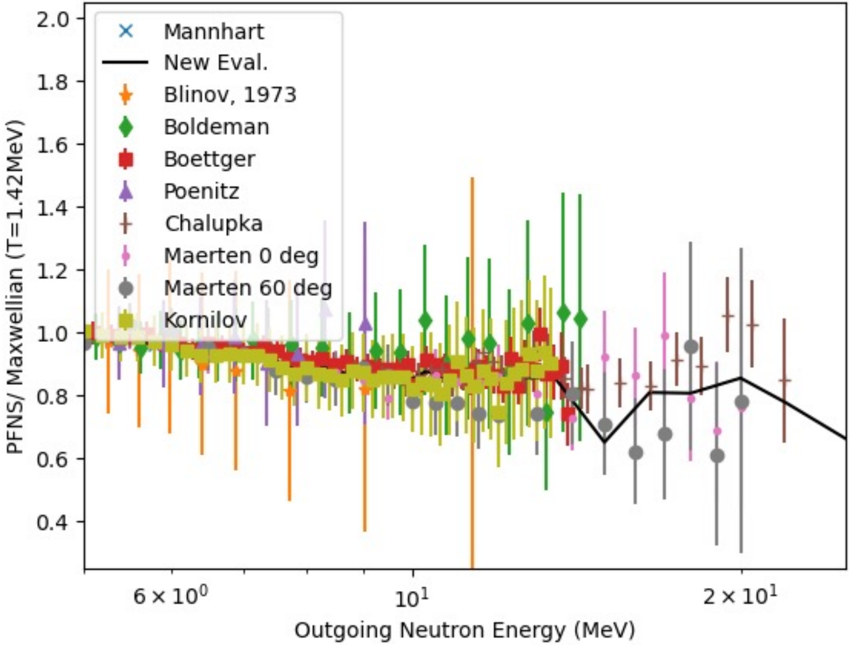
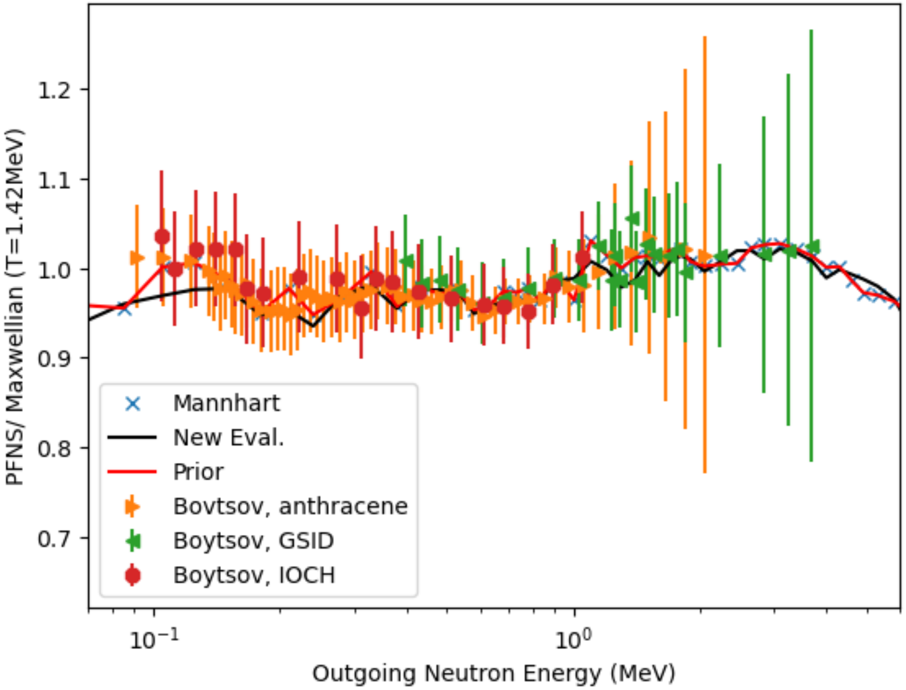
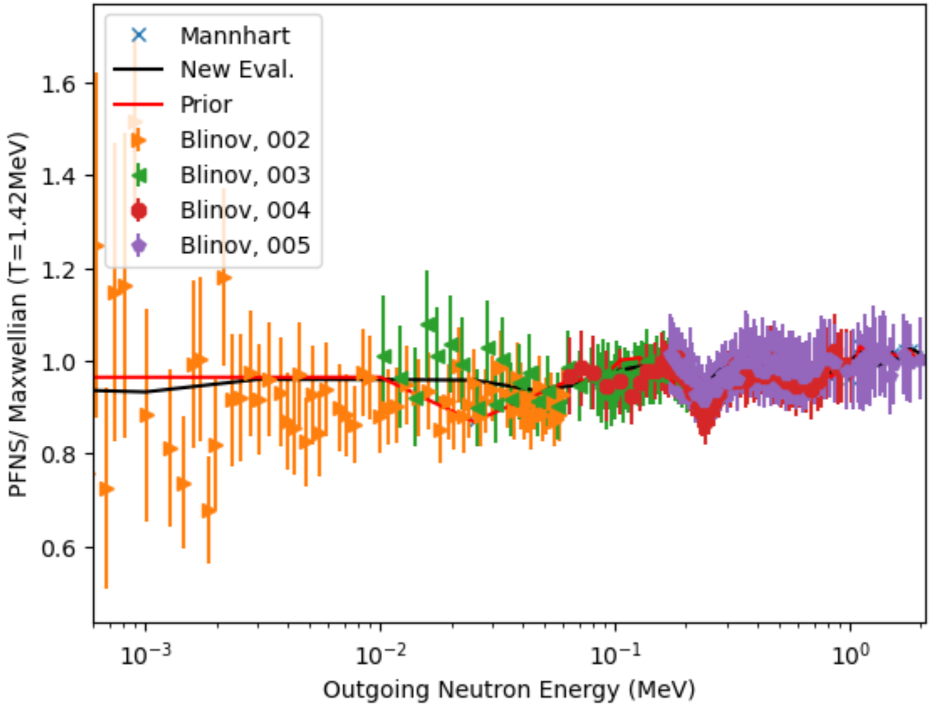
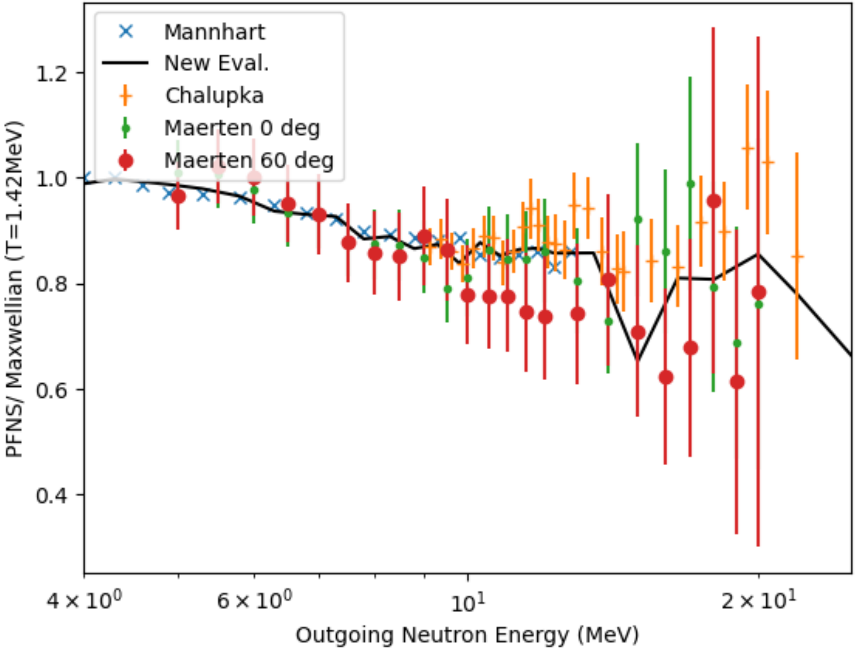


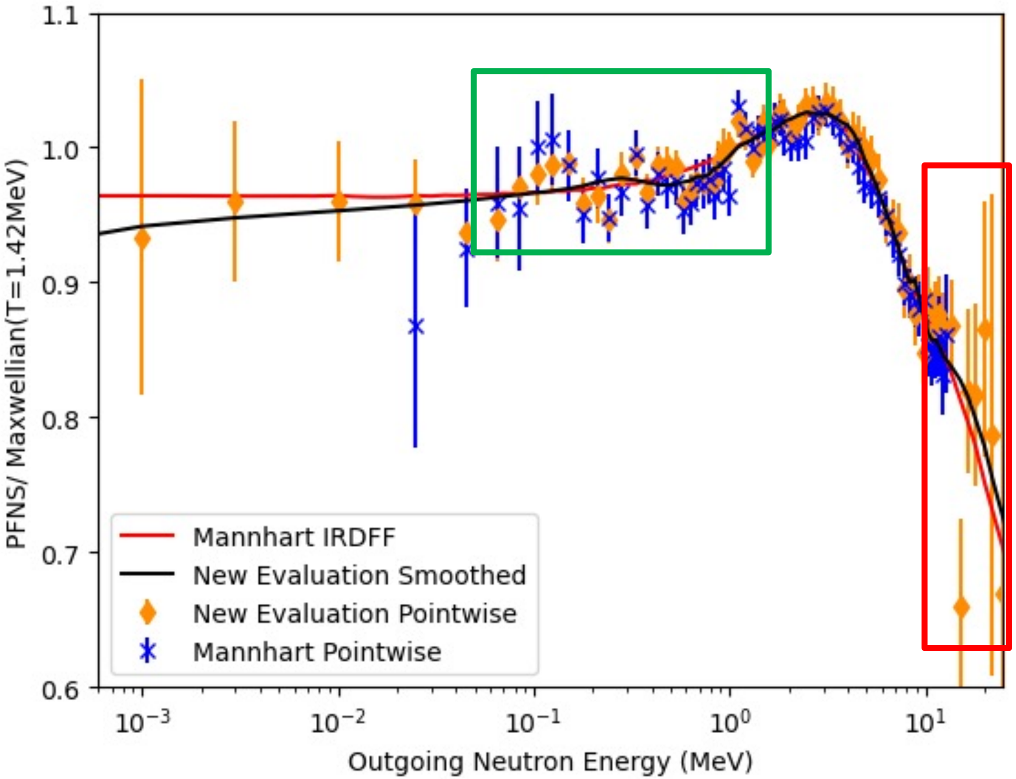


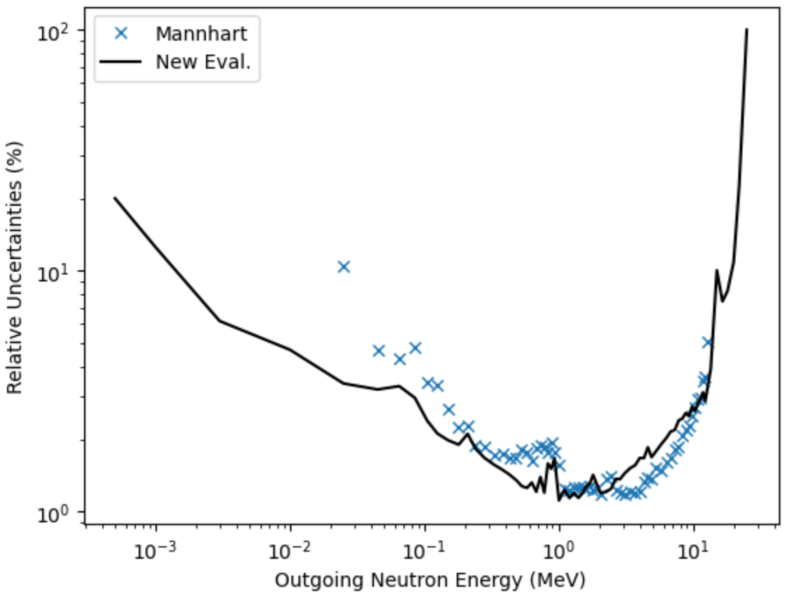
Evaluation rejecting 1 point of Chalupka and Maerten 0 degree data.



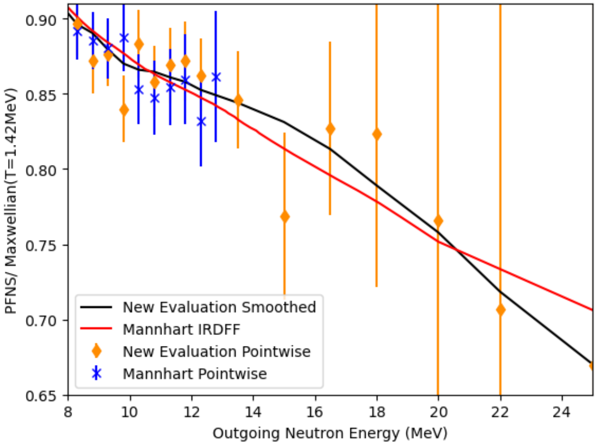


New evaluation reduces ^{6}Li peak and extends energy range. Maybe, more discussion needed at higher E_{out}?



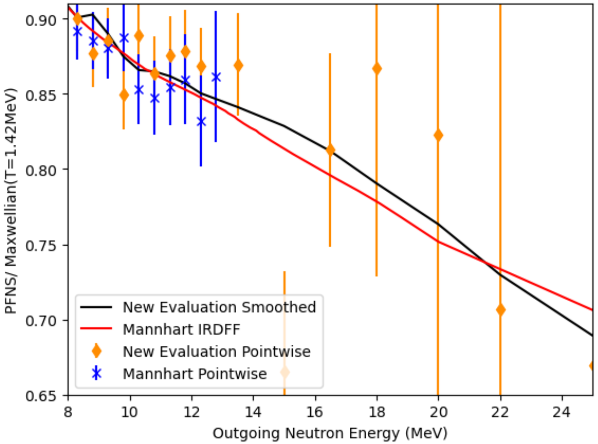


Chalupka 4 points versus 1 point removed versus considering Maerten at 0 deg.



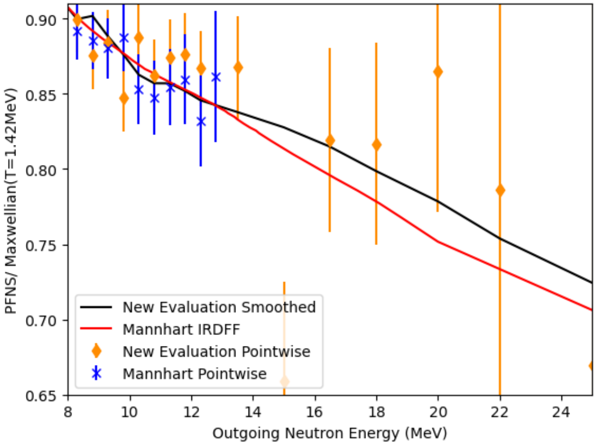
Chalupka 4 points removed.

2.131 MeV mean energy.



Chalupka 4 points removed & Maerten 0 deg removed.

2.132 MeV mean energy



Chalupka 1 points removed & Maerten 0 deg removed.

2.131 MeV mean energy

4. Calculating SACS: Boris and Dave calculated SACs with IRDFF data.

Dave's SACS

- Code used: FUDGE
- Experimental data used: IRDFF 2019, published in NDS 2020 (and REZ)
- Eval. Data: IRDFF group/ point-wise.

- Test-case: uses Mannhart spectrum to calculate SACS and compares to IRDFF calculated SACS → the same except for a few data points (under investigation).

AIACHNE:

- Used pointwise and smoothed spectrum (smoothed spectrum shown).
- Uses AIACHNE covariances.
- Lin-lin and log-log.

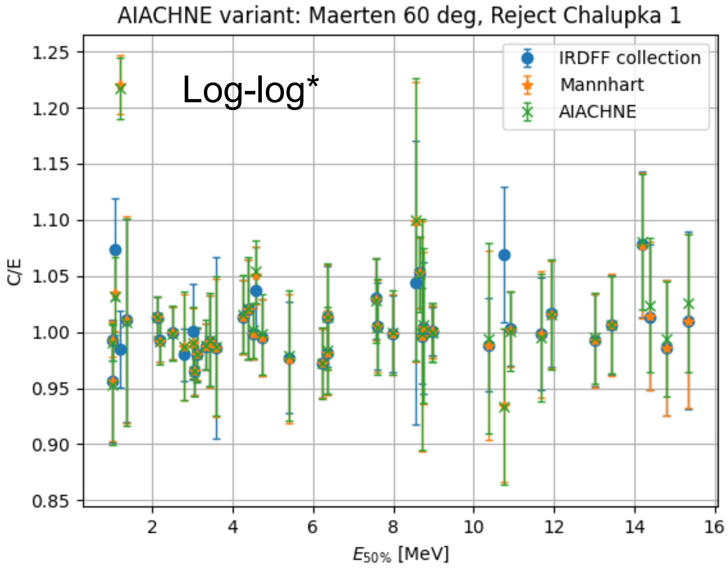
Boris' SACS

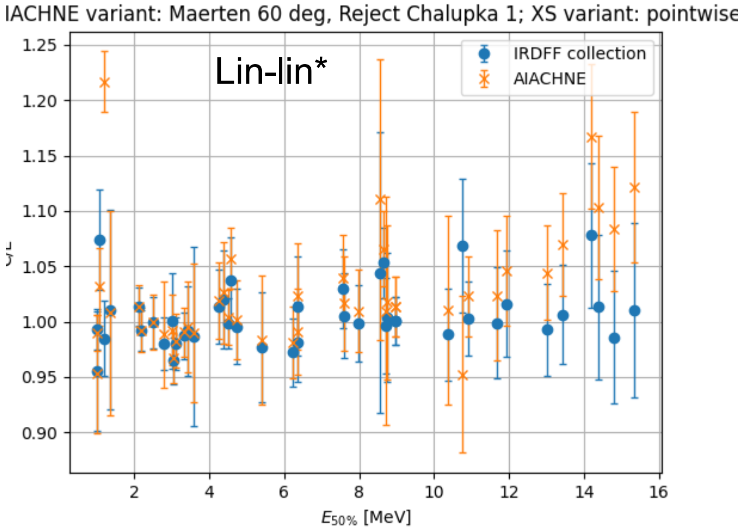
- Code used: Pritychenko, NDS 123, 2015, 119
- Experimental data used: IRDFF 2019, published in NDS 2020
- Eval. Data: IRDFF group/ point-wise, JENDL 5.0, VIII.1.
- Test-case: reproduces Mannhart.

AIACHNE:

- Used pointwise and smoothed spectrum (smoothed spectrum shown).
- Used relative uncertainties but not correlations.
- Lin-lin and log-log.

Calculating SACS: it matters if we require log-log versus lin-lin interpolation!! But we are close to Mannhart for log-log.

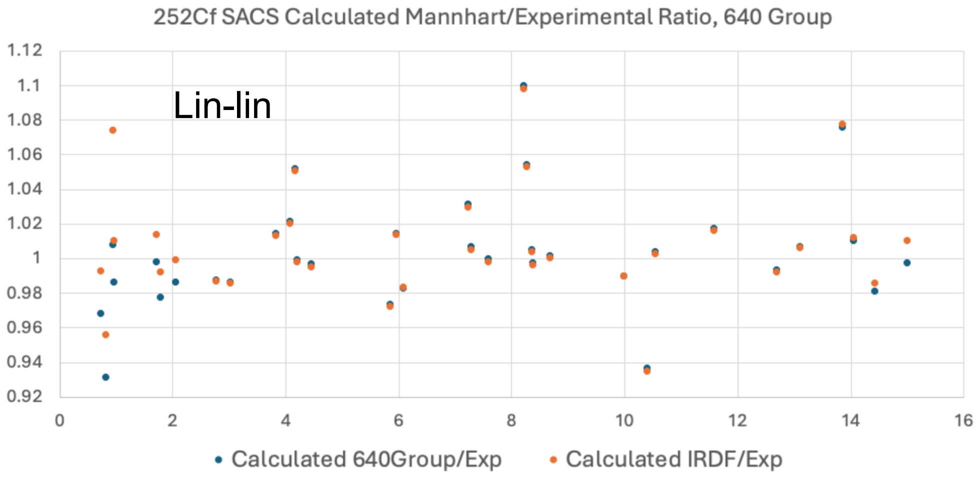


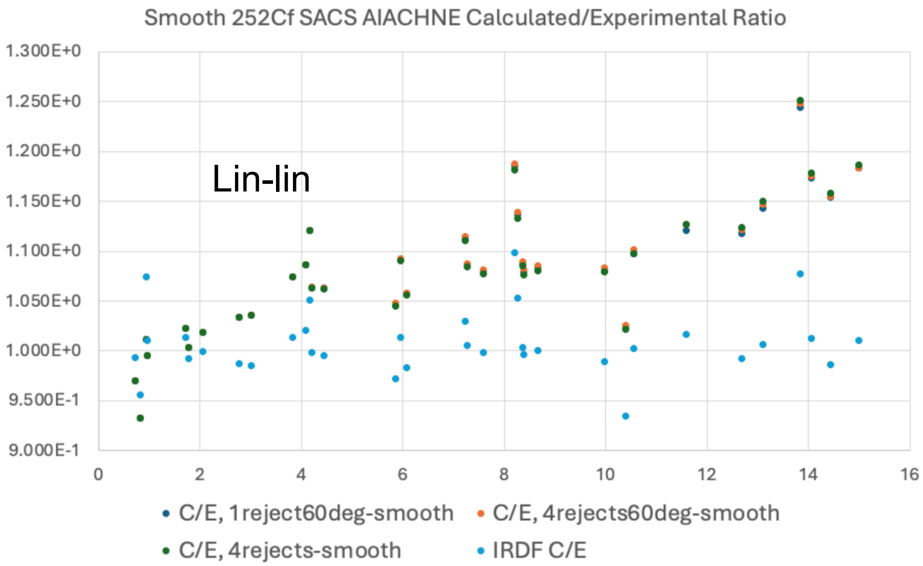


*for AIACHNE data.

Mike and Scott are working towards a denser grid with ML methods to make the lin-lin versus log-log less important.

It matters very little if we reject 1 or 4 Chalupka points or Maerten 0 degree data .

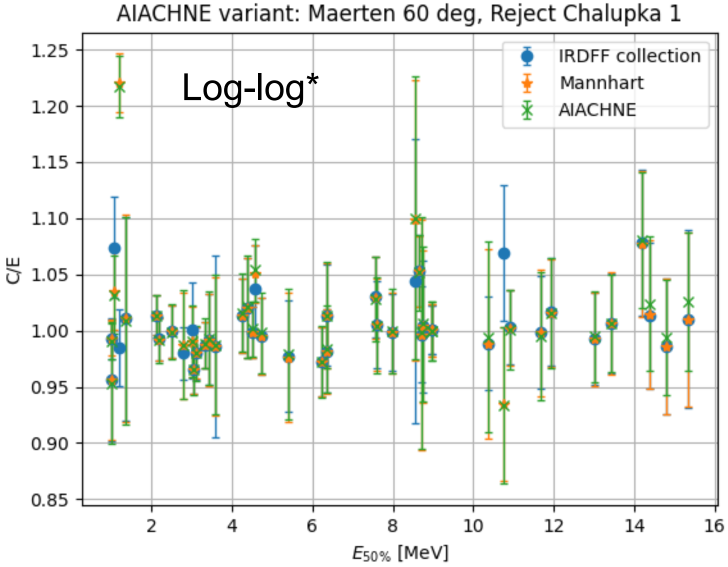


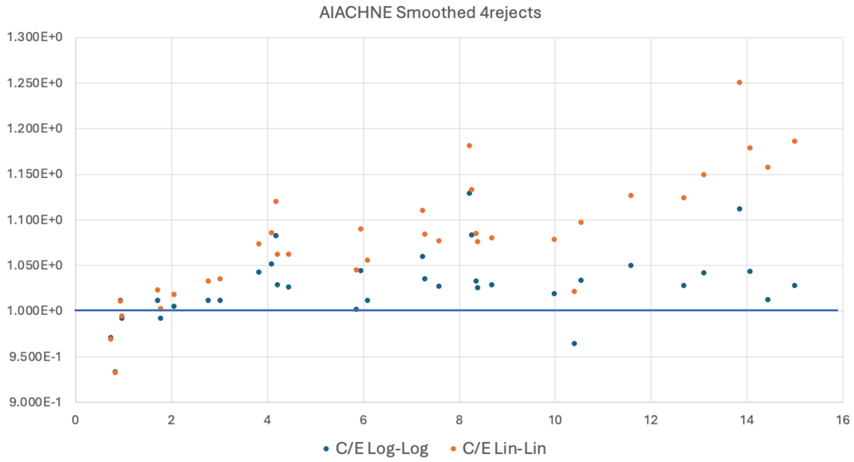


Boris is able to reproduce IRDFF data.

Rejecting Chalupka 1 versus 4 points or Maerten data does not really matter!

We still see differences in Boris' and Dave's SACS.





We are going to release data to Neutron Data Standards hoping that they will also test the data with SACS. Which version would you like of the evaluation??

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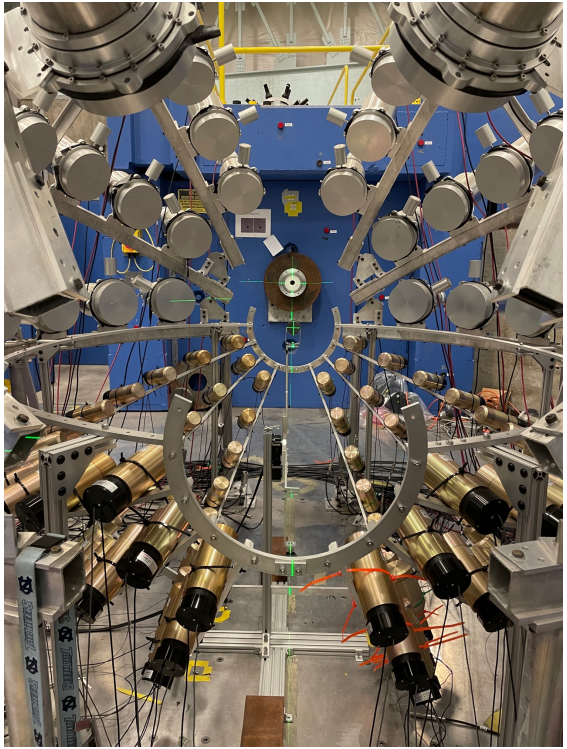
We show a new experiment coming up for the $^{252}Cf(sf)$ PFNS.

AIACHNE ^{252}Cf PFNS Measurement Employs New Techniques for Neutron Response Calibrations

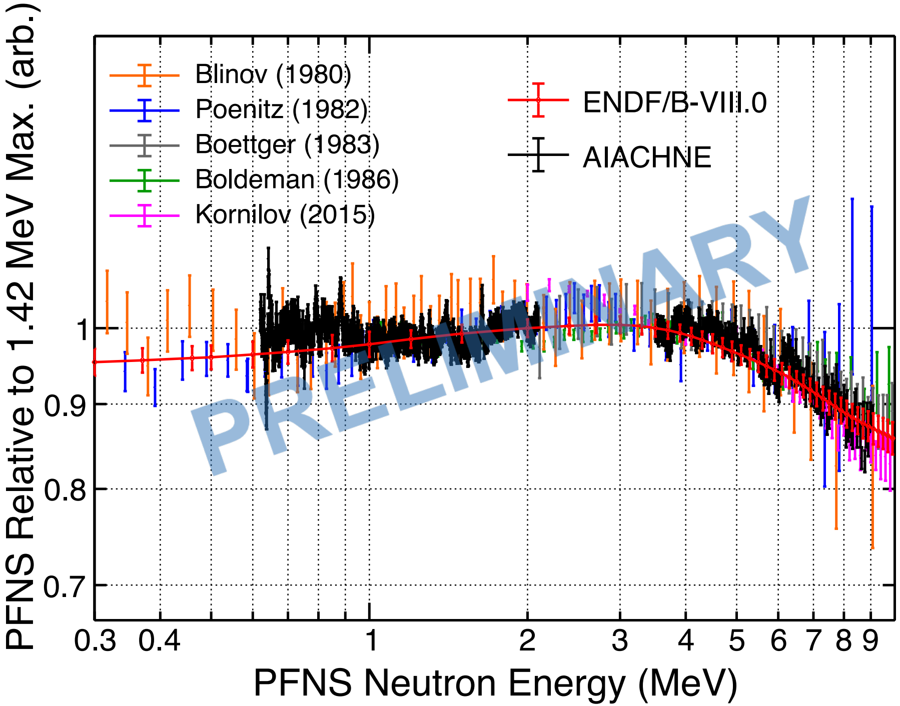


AIACHNE experiment:

- Utilize ^{9}Be and ^{12}C(n,n) elastic neutron scattering as a reference for ^{252}Cf PFNS
- As opposed to ^{1}H(n,n), ^{9}Be and ^{12}C scattering emit neutrons in all angles allowing for full spectrum integration
- Challenge: relativistically convert emitted neutron energies as a function of incident energy for laboratory angles from 30-150^{o} to an efficiency to be applied to ^{252}Cf fission data

CoGNAC array used by K.J. Kelly (LANL).

Method Reduces Systematic Errors, but Introduces Errors from Reference Nuclear Data Quantities



- High statistical precision allowed for high granularity of results
  - >800 data points shown
  - Compared with 313 points for other ^{252}Cf data shown here combined.
- Minor structures are indicative nuclear data discrepancies in the reference cross sections
- Improvements in analysis will yield continuous results (including 2-3.5 MeV range) and expanded energy range

Total uncertainties are shown for all datasets.

- <u>Summary:</u>

o Developed new ML technique to help pin down physical root causes of experimental discrepancies.

o New $^{252}Cf(sf)$ PFNS evaluation available.

o New $^{252}Cf(sf)$ PFNS measured & coming soon.

<u>Discussion:</u>

- o What else do you need to see for accepting the new evaluation?
- o What data do you want to have and when?
- o We will continue to collaborate on method development, sorry for being slow …

Thank you for listening!

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Abstract

The AIACHNE project presented on its method to pin-point physics root causes of systematic discrepancies between data sets, and new 252Cf PFNS evaluation, and a new 252Cf PFNS measurement. The new method to find physics root causes of systematic discrepancies between different experimental data sets uses a Bayes model to find biases tied to measurement features. It induces sparsity of systematic bias and features via a horseshoe prior. This method successfully identified known and previously unknown issues in data that prompted further analysis and improved the evaluation. We currently have a preliminary evaluation using a code that was able to reproduce Mannhart's evaluation within uncertainties (given that we don't know every detail of Mannhart's evaluation). This new evaluation shows less impact of the Li-6 peak seen in the detector response in some experiment and extends the energy range of the evaluation to lower and higher energies. Spectrum averaged cross sections (SACS) of IRDFF experiments calculated with our new evaluation are close to those calculated with Mannhart's spectrum except for the highest E-50% value if we use log-log interpolation. If we use lin-lin interpolation for the AIACHNE evaluation, we see a trend for too high calculated SACS compared to experimental SACS values stored in IRDFF. We are currently working on providing the data on a denser grid. At the same time, a new measurement of the 252Cf PFNS was undertaken using the CoGNAC array and several neutron-producing reactions to obtain a detector response. This new experiment will be included in the evaluation once the analysis is finalized and might help us to better understand the Li-6 response function of past measurements.