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**Title:** AIACHNE work towards a new 252Cf(sf) PFNS evaluation

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Web

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# AIACHNE work towards a new $^{252}\text{Cf}(\text{sf})$ PFNS evaluation

AIACHNE (AI/ML Informed cAlifornium CHi Nuclear data Experiment) team: D. Neudecker (speaker)<sup>3</sup>, D. Brown<sup>1</sup>, A.D. Carlson<sup>2</sup>, M.J. Grosskopf<sup>3</sup>, R.C. Haight<sup>3</sup>, K.J. Kelly<sup>3</sup>, B. Pritychenko<sup>1</sup>, S. Vander Wiel<sup>3</sup>, Noah Walton<sup>3,4</sup>  
<sup>1</sup>BNL, <sup>2</sup>NIST, <sup>3</sup>LANL, <sup>4</sup>UTK

Neutron Data Standards meeting

10/9-13/2023

LA-UR-

# AIACHNE has a team from BNL, LANL, NIST and UTK. It covers experiment, evaluation and AI/ ML specialists.



D. Brown  
ND expert



B. Pritychenko  
EXFOR



M. Grosskopf  
AI/ ML



R. Haight  
Experiment



K. Kelly  
Experiment



D. Neudecker  
ND evaluation



S. Vander Wiel  
AI/ ML

EXFOR database and literature database  
ENDF/B libraries

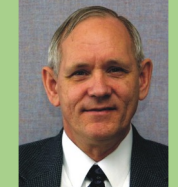
Chi-Nu array  $^{252}\text{Cf(sf)}$  PPAC  
ML tool to find features related to outliers  
EUCLID AI/ML experiment design  
ARIADNE UQ evaluation tool

Neutron Data Standards database

GMA evaluation code

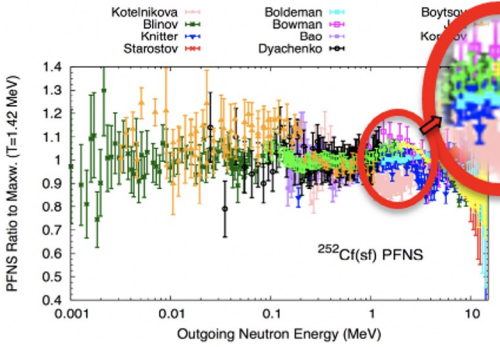


N. Walton  
Student



A. Carlson  
Standards lead

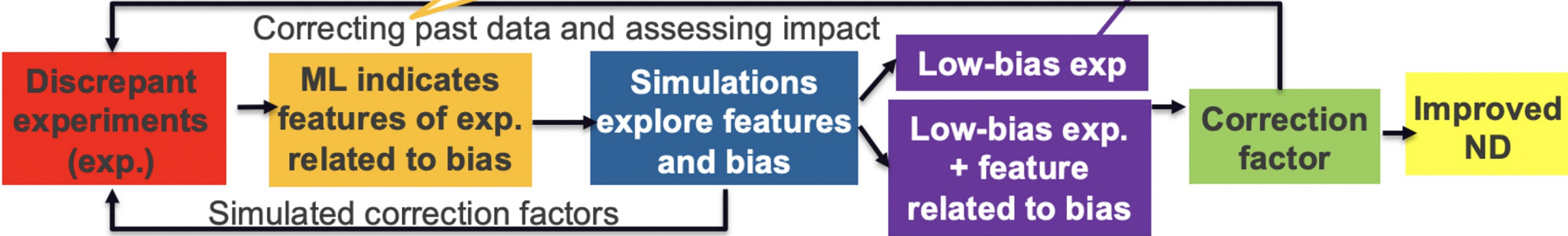
# We will create and validate a ML capability to design $^{252}\text{Cf}(\text{sf})$ PFNS exp. maximally reducing discrepancies in past exp.



Developing advanced ML



Using state-of-the-art LANSCE equipment

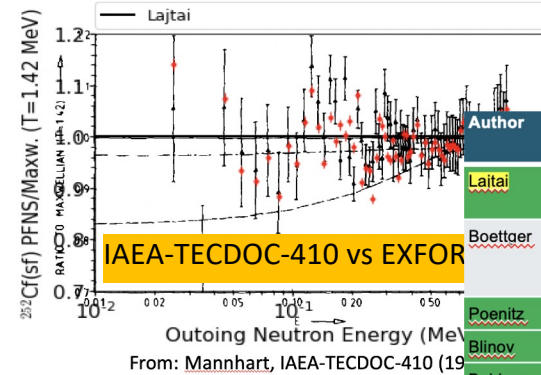


We use ML capability to pin-point measurement features likely related to bias (USU) and select experiments based on MCNP studies. Incidental output is a new  $^{252}\text{Cf}$  PFNS evaluation.

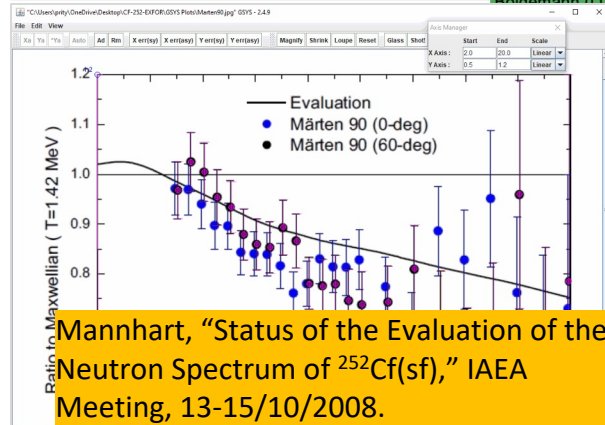
# Repeat from last time: Recovered input data for the current $^{252}\text{Cf}(\text{sf})$ PFNS Neutron Data Standard that was previously lost.

- Input data to **standard** was lost.
- Some of the data are not even in EXFOR.
- We recovered data for standard and added 2 data into EXFOR database
- **We are trying to make the current  $^{252}\text{Cf}(\text{sf})$  PFNS evaluation (more) reproducible again.**
- We will update EXFOR database with features for historic data that are not yet recorded, and provide curated data for standards & SG-50.

Lajtai: likely not the same data as in EXFOR.



Author	EXFOR-Accession number
Lajtai	41158.003; or Dyachenko 40875003
Boettaer	Not in EXFOR, Naohiko submitted request for inclusion to NEA.
Poenitz	14278.002
Blinov	40418.007
Baldemann (L)	30775.003
stic)	30775.002



Not in EXFOR, Naohiko has made a preliminary input deck.

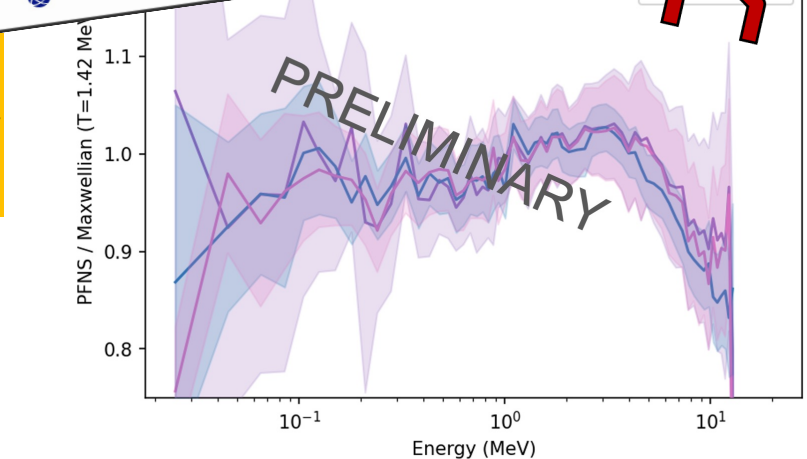
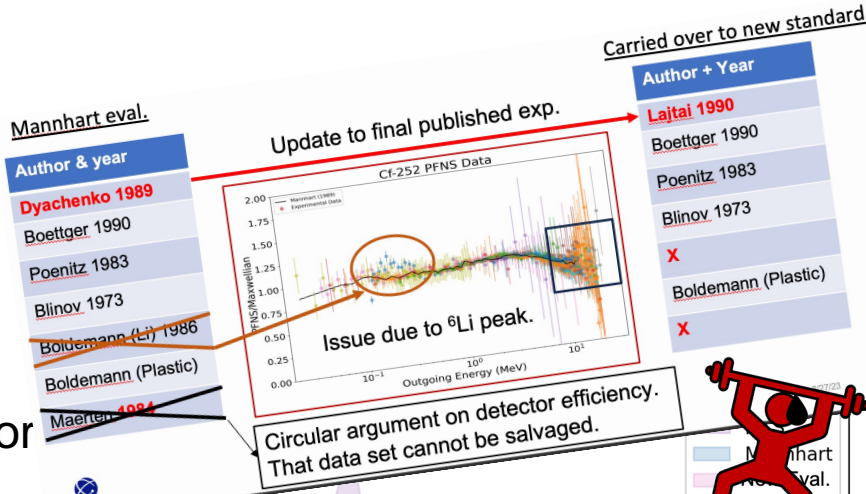
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# Date = 30.Sep.2022, 11:38:57
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# set yrange[0.5, 1.2]
# MD5Fig : 498118cb3fe19f586357e8
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# Axis_Y : 3fc6df18e0b3c3023fe8ed9
#
# x      y      dy
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5.548  1.025  0.059
6.061  1.005  0.059
6.554  0.954  0.056
7.087  0.934  0.051
7.560  0.879  0.051
8.054  0.860  0.051
8.567  0.853  0.052
9.062  0.894  0.055
9.575  0.866  0.054
10.048 0.780  0.051
10.561 0.775  0.054
11.055 0.779  0.057
11.548 0.747  0.062
12.062 0.738  0.067
13.050 0.743  0.071
14.059 0.810  0.088
```

# Critically reviewed past data as input for ML & new standard evaluation.

- Significant effort to review past experiments uncovered issues impacting current standard.
- Reviewed (and accepted) data that have been measured after current standard evaluation.
- Undertook detailed UQ and feature analysis; provided for ML analysis and will be provided for standards if interested.

**It would be great if this work could result in new standards evaluation impacting all major actinide PFNS.**

-> So, here we are going to show our reasoning towards updating the standard.



# Agenda of introduction and overview

- Which data sets are currently available
- Data used by Mannhart for his evaluation and which ones he likely rejected
- Which data accepted by Mannhart did we reject and why
- Which data could have been rejected by Mannhart and we accepted
- Which new data since Mannhart evaluation did we accept
- UQ procedure
- Preliminary results
- Discussion





**Which data sets are currently available  
and what did Mannhart use?**



# 26 data sets are currently available, some have sub-sets. We reviewed all of them in detail.

Author + Year	Author + Year	Author + Year	Author + Year
Bao 1989	Bowman 1985	6xGreen 1973	2xMaerten 1990
Bentsch 1979	3xBoytssov 1983	2xJeki 1971	Meadows 1965
2xBlain 2017	2xChalupka 1990	2xKnitter 1973	Nefedov 1983
7xBlinov 1973	Coelho 1989	Kornilov 2015	Poenitz 1982
4xBlinov 1980	Conde 1965	Kotelnikova 1975	2xStarostov 1983
Boettger 1983	Dyachenko 1989	Lajtai 1990	
2xBoldeman 1986	Goeoek 2014	2xMaerten 1984	



# Mannhart rejected data because of biases, poor UQ or doc., non-TOF exp., missing random coinc. / ang dist cor.

Author + Year	Author + Year	Author + Year	Author + Year
<del>Bao 1989</del>	Bowman 1985	<del>6xGreen 1973</del>	2xMaerten 1990
<del>Bentsch 1979</del>	<del>3xBovisov 1983</del>	<del>2xJeki 1971</del>	<del>Meadows 1965</del>
2xBlain 2017	2xChalupka 1990	<del>2xKnitter 1973</del>	<del>Neredov 1985</del>
7xBlinov 1973	<del>Coelho 1989</del>	Kornilov 2015	Poenitz 1982
4xBlinov 1980 ?	<del>Conde 1965</del>	<del>Kotelnikova 1975</del>	<del>2xStarostov 1983</del>
Boettger 1983	Dyachenko 1989	Lajtai 1990	
2xBoldeman 1986	Goeoek 2014	2xMaerten 1984	

■ Taken into account  
■ Would be accepted

✗ Taken into account  
■ New



# Which data accepted by Mannhart did we reject and why



# Found issues in past data that could impact validity of Mannhart (current) standard evaluation.

Mannhart eval.

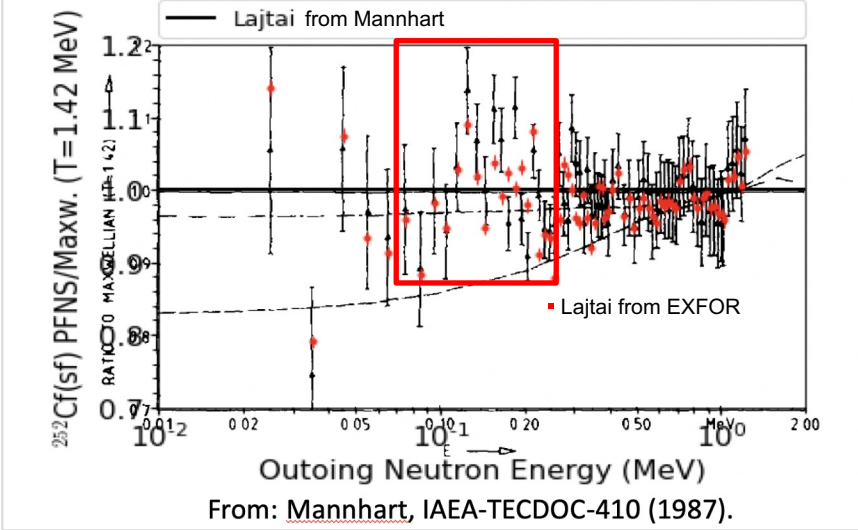
Carried over to new standard

Author & year
Dyachenko 1989
Boettger 1990
Poenitz 1983
Blinov 1973
Boldemann (Li) 1986
Boldemann (Plastic)
Maerten 1984

Update to final published exp.

Author + Year
Lajtai 1990
Boettger 1990
Poenitz 1983
Blinov 1973
X
Boldemann (Plastic)
X

**Lajtai: likely not the same data as in EXFOR.**



Dyachenko noted issue in detector efficiency that was fixed in final publication



# Lajtai (1990): ${}^6\text{Li}$ feature not present in final results

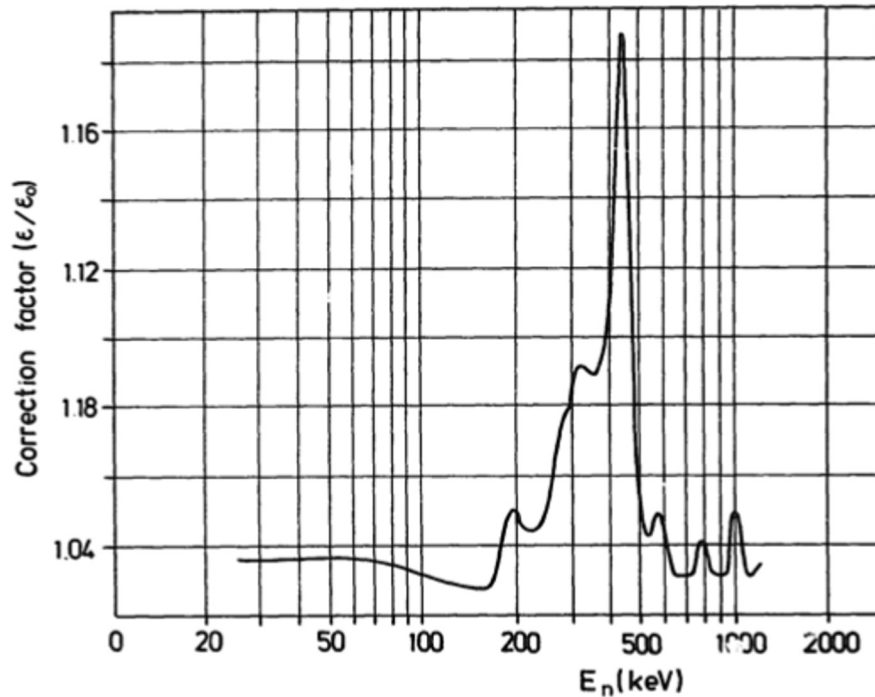


Fig. 1. Efficiency correction factor for the thin  ${}^6\text{Li}$  glass detector (Monte Carlo calculation).

- Observed increase in efficiency at energies above the resonance
- Attributed to resonances in other materials of the glass (mainly Si and O), but conceptually from short-time scatters into  ${}^6\text{Li}$  resonance
- Performed separate measurements of efficiency, and benchmarked against Monte Carlo Calculations
- Also, one of the only experiments to explicitly mention and quantify the response matrix of the experiment environment.



# Lajtai (1990): ${}^6\text{Li}$ feature not present in final results

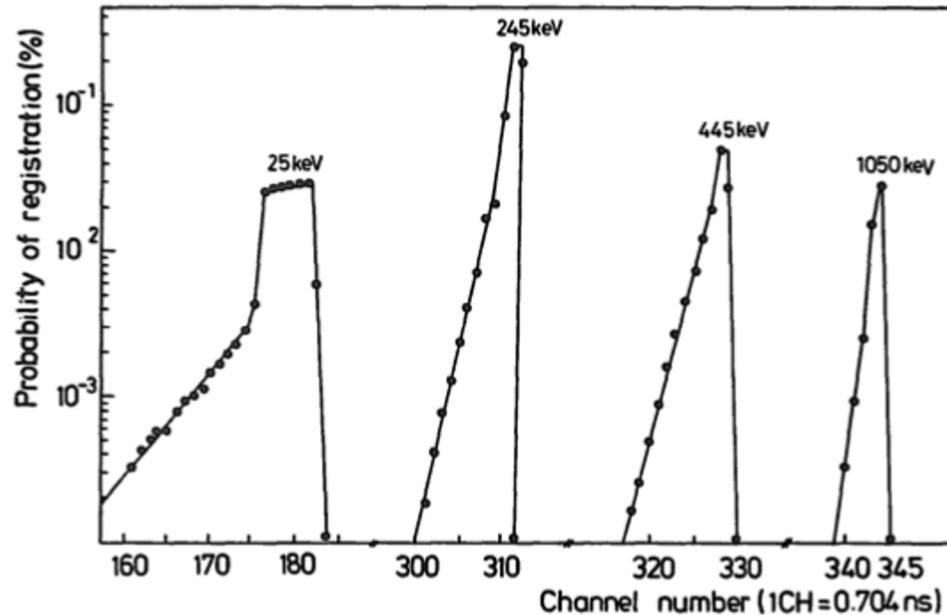


Fig. 2. Response functions of the thick  ${}^6\text{Li}$  glass detector.

- Response functions are coarse, and not up to today's standards, but this approach combined with their background subtraction appears to have removed this feature from their data.
- Lajtai data were heavily impacted by these resonance features, but seem to have accurately accounted for it in their final results.

Preliminary Lajtai data (first author Dyachenko in EXFOR) used by Mannhart are biased. Mannhart removed worst affected data points but biases were seen at several  $E_{\text{out}}$ .

# Found issues in past data that could impact validity of Mannhart (current) standard evaluation.

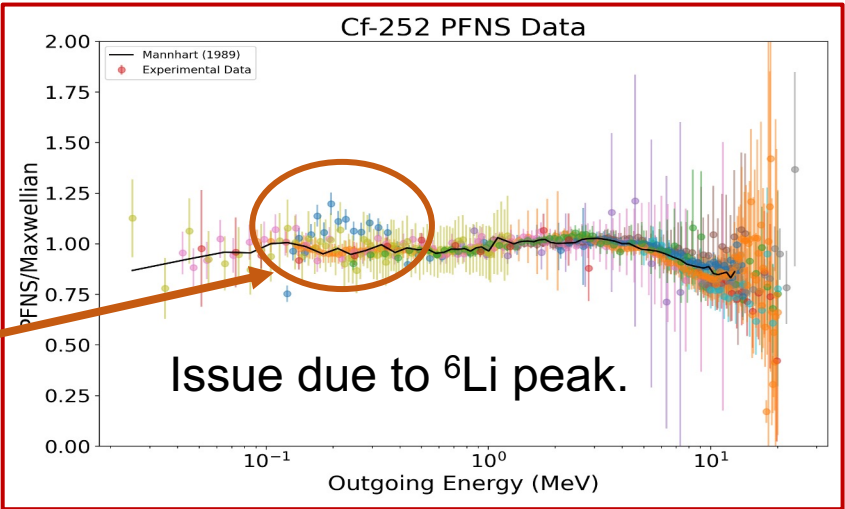
Mannhart eval.

Carried over to new standard

Author & year
Dyachenko 1989
Boettger 1990
Poenitz 1983
Blinov 1973
<del>Boldemann (Li) 1986</del>
<del>Boldemann (Plastic)</del>
Maerten 1984

Update to final published exp.

Author + Year
Lajtai 1990
Boettger 1990
Poenitz 1983
Blinov 1973
X
Boldemann (Plastic)
X





# Boldeman (1986): ${}^6\text{Li}$ feature shows an excess in results

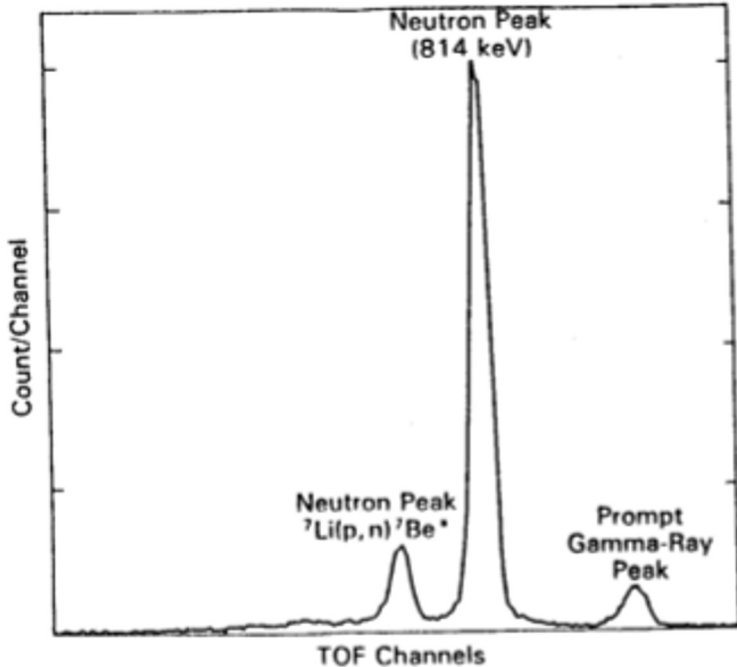


Fig. 6. The TOF response of  ${}^6\text{Li}$  glass scintillator to pulsed neutrons (2.9 ns full-width at half-maximum) of  $814 \pm 5$  keV. The prompt gamma-ray peak and the second peak due to the detection of neutrons from the  ${}^7\text{Li}(p,n){}^7\text{Be}^*$  reaction are identified.

- Used  ${}^6\text{Li}$ -glass detector
  - Seven measurements from 1.0-14.3 MeV with plastic scintillator, and one from 0.124-2.66 MeV with Li-glass
  - 2.0 mm thick, 5.08 cm diameter
- Separate measurements of  ${}^6\text{Li}$ -glass detector efficiency at Van de Graaff
  - Noted that the environment was maximally similar
    - Elevated floor, same FP and time cal., etc.
  - Initial attempts to calculate efficiency failed because of multiple scattering effects of phototube
  - Measured relative to a known reference counter for 0.124-1.400 MeV
  - Corrections applied for air attenuation, path length, etc., from reference detector to Li-glass.

# Boldeman (1986): ${}^6\text{Li}$ feature shows an excess in results

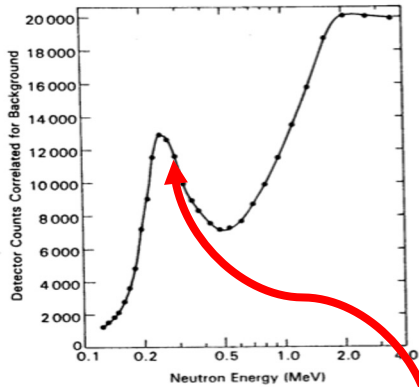


Fig. 12. Raw experimental data for  ${}^6\text{Li}$  experiment after background subtraction and correction for dead-time effects.

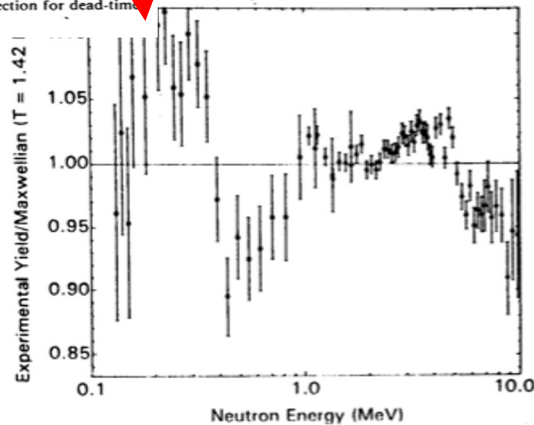


Fig. 13. Combined low- and high-energy data relative to a Maxwellian distribution with  $T = 1.42$  MeV:  $\circ$  = high-energy data and  $\square$  = low-energy data.

- There is still a visible excess in raw data and the final spectrum.
- Not the same level of care given to these data as in Lajtai in consideration of the 2D response effects.
- Mannhart removed 6 Boldeman-Li points around the resonance, but we visibly see more data points that are biased.
- Known  ${}^6\text{Li}$  biases and could adversely affect the evaluated PFNS.



# Found issues in past data that could impact validity of Mannhart (current) standard evaluation.

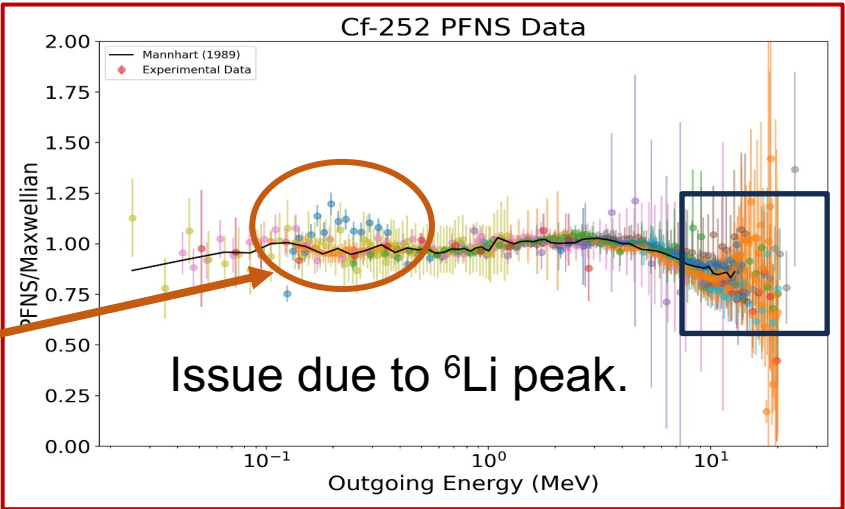
Mannhart eval.

Carried over to new standard

Author & year
<b>Dyachenko 1989</b>
Boettger 1990
Poenitz 1983
Blinov 1973
<del>Boldemann (Li) 1986</del>
<del>Boldemann (Plastic)</del>
<del>Maerten 1984</del>

Author + Year
<b>Lajtai 1990</b>
Boettger 1990
Poenitz 1983
Blinov 1973
<b>X</b>
Boldemann (Plastic)
<b>X</b>

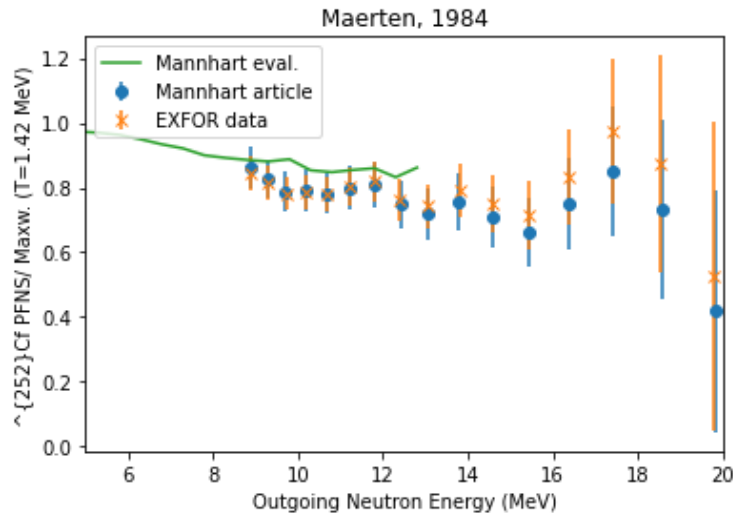
Update to final published exp.



Circular argument on detector efficiency. That data set cannot be salvaged.



# Maerten (1984) used $^{252}\text{Cf}$ NBS PFNS for calculating detector efficiency. Data seem preliminary.



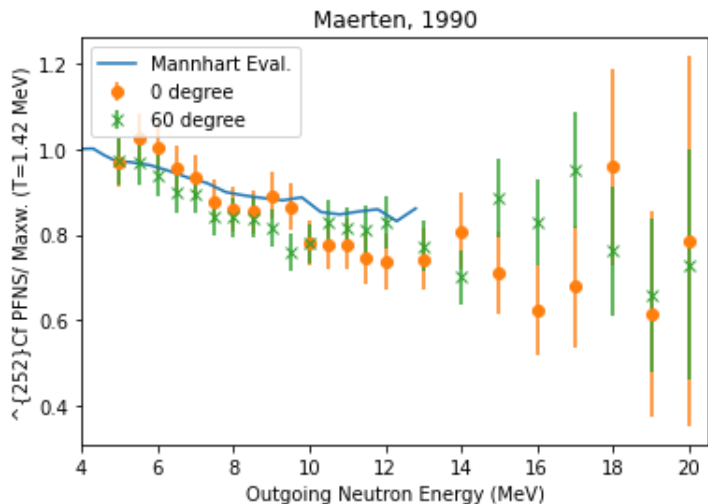
From INDC(GDR)-17/L: “We assumed the NBS evaluated spectrum for efficiency determination. [...] The [...] normalized energy spectra [...] were determined presuming the calculated efficiency data, [...] the efficiency functions [...] were determined for different threshold energies on the basis of the NBS evaluated spectrum.”

Determining the  $^{252}\text{Cf}$  PFNS via a detector efficiency calculated with an efficiency from a  $^{252}\text{Cf}$  PFNS evaluation is a circular argument.

This biases Mannhart PFNS towards NBS evaluation.



# We replaced Maerten (1984) with final published Maerten (1990) data that resolved the circular argument.



**These data will improve high  $E_{\text{out}}$  PFNS.**

From NSE 106, p. 353 (1990): “[...] the neutron detection efficiency [...] has to be known. This was calculated by use of a Monte Carlo code [...] were determined presuming the calculated efficiency data, [...] by measuring neutron response functions for monoenergetic neutrons at several energy points [...].”

We reached out to Maerten and he confirmed mono-energetic measurements for 1990 measurement.



# Märten (1990): Possibly Displays FF Efficiency Effects, Though a High Efficiency is Quoted...

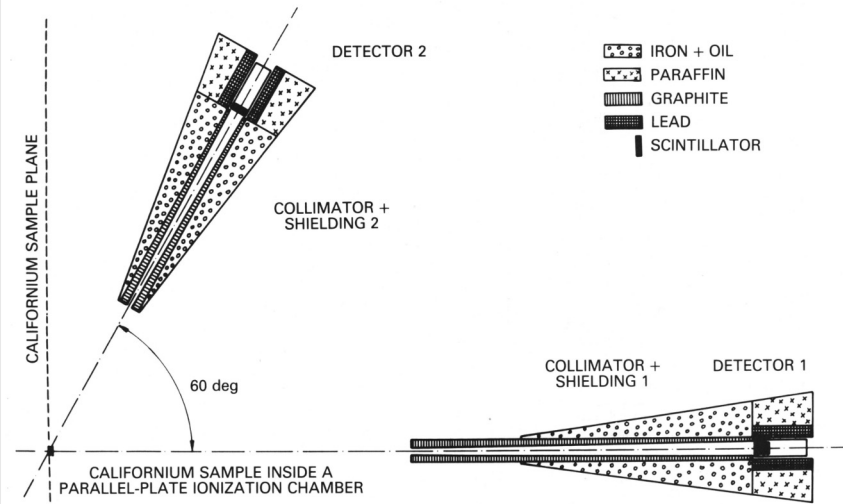


Fig. 1. The experimental setup.

- Märten papers are unique in that they measure two angles, and report both
  - Quote a 99.2(2)% efficiency from fission-neutron coincidence measurements
  - Small number of angles, but results are suggestive of an efficiency issue
  - Detector, path length, and shielding are also different, so there's potential for multiple effects.
- If there's an efficiency issue, expect higher average PFNS energy for detector 1 than detector 2.
  - Aligns with observations
  - What range of efficiency curves can reproduce the 99.2% efficiency *and* this  $\langle E \rangle$  mismatch?



**Which data that could have been rejected by Mannhart  
did we accept?**



# Data by Blinov (4 sets) and Boytsov (3 sets) not considered by Mannhart but we don't know why and he doesn't cite them?

## Mannhart standard evaluation

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

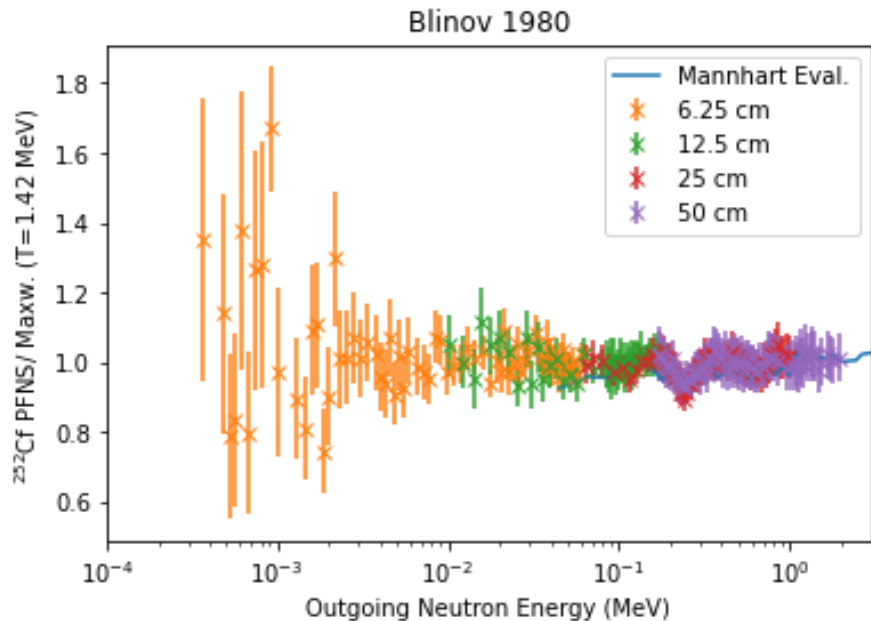
## Proposed input for new standard

Author + Year	Author + Year
<b>Lajtai 1990</b>	2xBlain <b>2017</b>
Boettger 1990	3xBoytsov 1983
Poenitz 1983	2xChalupka <b>1990</b>
Blinov 1973	4xBlinov 1980
X	
Boldemann (Plastic)	
X	2xMaerten <b>1990</b>





# Blinov data extends energy range of experimental data to low $E_{\text{out}}$ . Unclear if angular distribution was corrected.

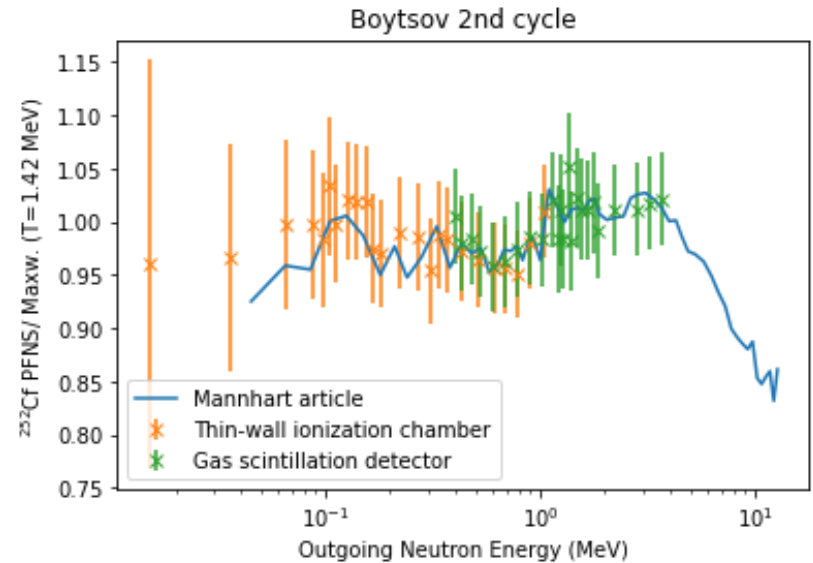
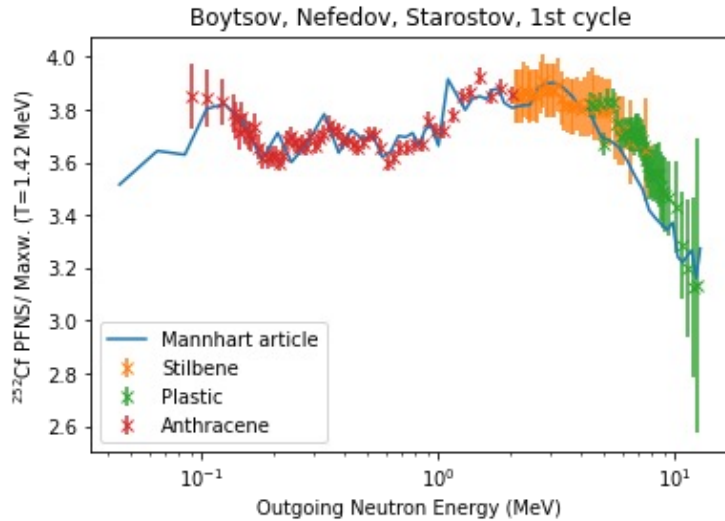


These data will improve low  $E_{\text{out}}$  PFNS evaluation.

- Measured with four flight path-lengths.
- Neutrons measured with  $^6\text{Li}(\text{Eu})$  crystal, response was MC simulated (ENDF/B-V.0  $^6\text{Li}(n,\alpha)$  cross sections).
- FF measured with gas scintillation counter.
- Time resolution: 1.5 ns.
- Backgrd./ mult. scatt. MC simulated and measured.
- Nearly all corrections done, unknown if ang. Dist. corrected but was the case for Blinov 1973.



# We use Boytsov data (anthracene, 2<sup>nd</sup> cycle) of Starostov series.



- Rejected plastic and stilbene data as they use eval.  $^{252}\text{Cf}$  PFNS to define det. eff. → circular argument.
- Anthracene n det. & miniaturized ionization chamber with 4.2 ns and 51 cm, det. Eff. Simulated with  $^1\text{H}/^{12}\text{C}$  ND.
- Corrections and unc. for many effects provided.

- Rejected ion. Chamber data below 150 MeV as  $^{235}\text{U}(n,f)$  cs has structures.
- Both n det. use  $^{235}\text{U}(n,f)$  cs to define eff.,
- FF detected with gas scint. Det.
- Trsl: 4.8 ns & 5.2 ns
- Corrections and unc. for many effects provided.

**Which new data since Mannhart evaluation did we accept?**



# Data by Lajtai and Maerten are final published versions of data accepted by Mannhart, he approved of Chalupka, Blain new.

## Mannhart standard evaluation

Author & year	EXFOR-number
<b>Dyachenko 1989</b>	41158.003.
Boettger 1990	<b>Not in EXFOR.</b>
Poenitz 1983	14278.002
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Maerten <b>1984</b>	<b>Not in EXFOR.</b>

## Proposed input for new standard

Author + Year	Author + Year
<b>Lajtai 1990</b>	2xBlain <b>2017</b>
Boettger 1990	3xBoytssov 1983
Poenitz 1983	2xChalupka <b>1990</b>
Blinov 1973	4xBlinov 1980
X	
Boldemann (Plastic)	
X	2xMaerten <b>1990</b>



We would include 4 more measurement series in a new evaluation that were published after Mannhart's. Previously not possible as evaluation input lost.

# Data by Lajtai and Maerten are final published versions of data accepted by Mannhart, he approved of Chalupka, Blain new.

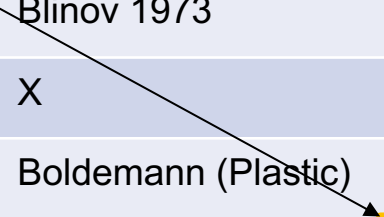
Mannhart standard evaluation

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Proposed input for new standard

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Boettger 1990	3xBoytssov 1983
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Blinov 1973	4xBlinov 1980
X	
Boldemann (Plastic)	
X	2xMaerten <b>1990</b>

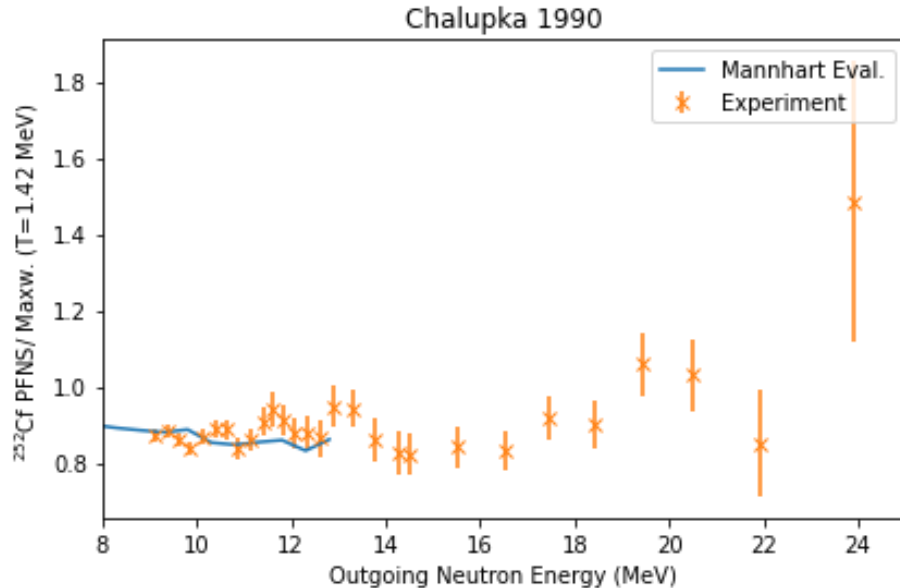
Discussed before.



We would include 4 more measurement series in a new evaluation that were published after Mannhart's. Previously not possible as evaluation input lost.



# Chalupka data was recommended by Mannhart for the evaluation.

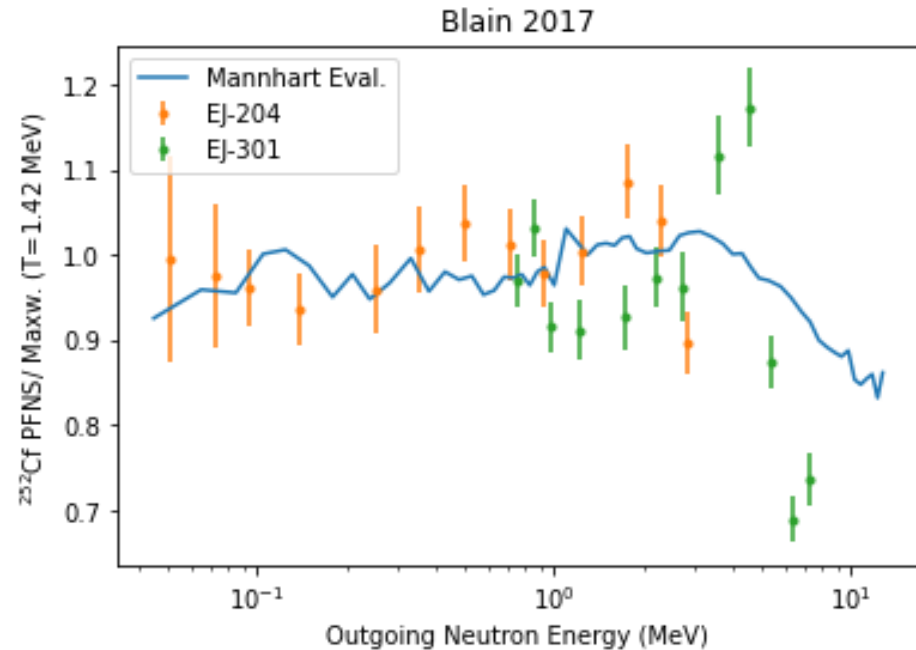


These data will improve high  $E_{\text{out}}$  PFNS.

- Measured in a mine in Bad Bleiberg, Austria (1000 m below mountain containing natural Pb) to reduce cosmic radiation.
- Neutrons measured with NE213 scintillator, response was MC simulated with 1 ns trsl.
- FF measured with 99.5% efficient fission chamber.
- All corrections done, many unc. provided.
- Contacted authors on some questions but no more information.



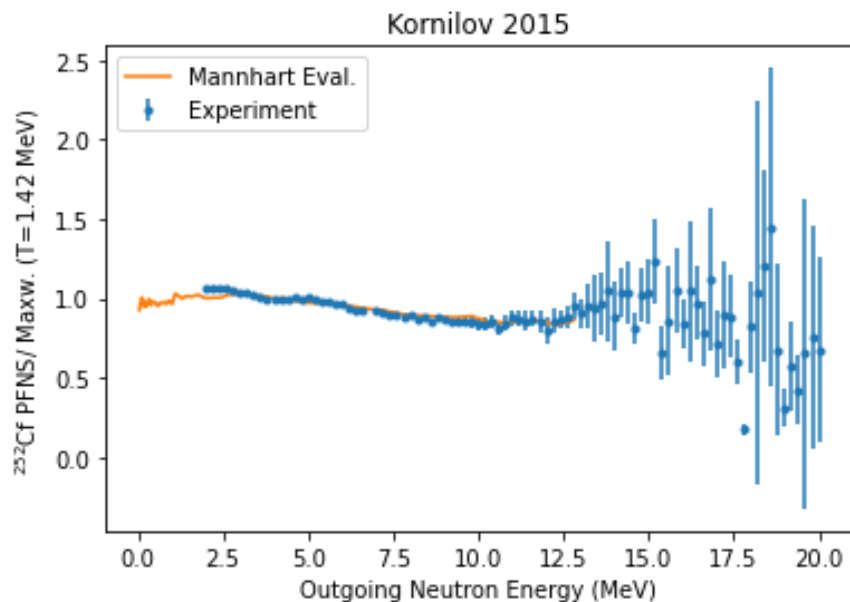
# Blain data for EJ-204 may be accepted if we get partial uncertainties.



- $^{252}\text{Cf}$  PFNS was measured as proof of principle for new FF detection technique.
- Neutrons measured with EJ-204/301 scintillators, EJ-301 was measured with LINAC  $+^{235}\text{U}(n,f)$  cs in dissimilar surrounding, both simulated with SCINFUL.
- Fission signal is if 2 out of 4 BaF2 gamma detectors fired.
- Time resolution: 3 ns.
- Concern: missing unc. (reached out to authors), detector eff. does not include surrounding for measurement, MCNP-Polimi calculations for gamma-tagging rely on poor gamma-fission data, g-background unc. seem low.



# Kornilov data will be used for validation until we have partial unc.



- Measured over a period of four years to get low statistical unc.
- Neutrons measured with (1 or 3) NE213 scintillator, efficiency was MC simulated.
- FF measured with 99% efficient ionization chamber.
- Only statistical unc. provided, no time resolution.
- Concerns: what about random coincidences (> 12 MeV)? Multiple scattering and detector response simulations were simplified.

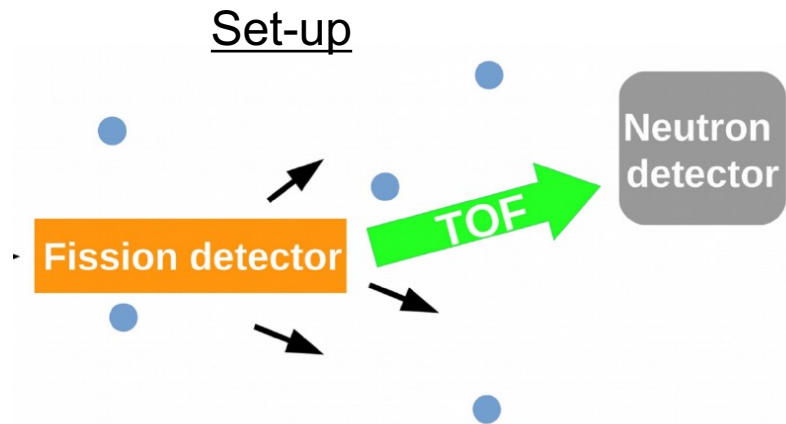




# UQ procedure and preliminary results



# We quantified uncertainties & collected features that hold clues to understand experimental biases for all 27 data sets.



## Analysis

$$PFNS(E) = \frac{C(E) - C_b(E)}{\epsilon(E)\tau(E)} m(E)\alpha(E)$$

$C$  ... counts;  $C_b$  ... background;  $m$  ... multiple scatt.  
 $\alpha$  ... angular distortion;  $\epsilon$  ... detector response  
 $\tau$  ... deadtime

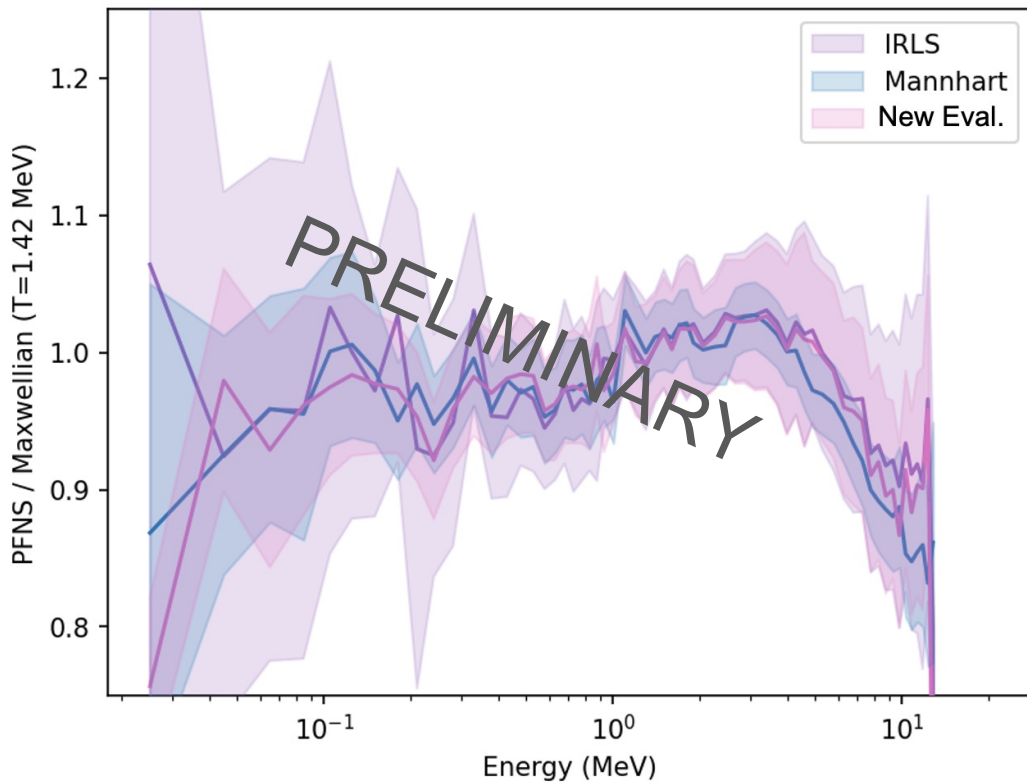
Uncertainty quantification: described in DN et al., "Templates of Expected Measurement Uncertainties for Prompt Fission Neutron Spectra," EPJ-N, accepted.

$$Cov^{exp} = Cov^{Count. Stat.} + Cov^{Backgd.} + Cov^{Mult. Scatt.} + Cov^{TOF} + Cov^{Det. Eff.} + \dots$$

**Metadata features for >130 categories** were collected from EXFOR/literature that encode set-up and analysis. **This was time-intensive!**



# Evaluation with new UQ leads to larger uncertainties. New data reduce unc., but we also see PPP effect at high $E_{\text{out}}$ .



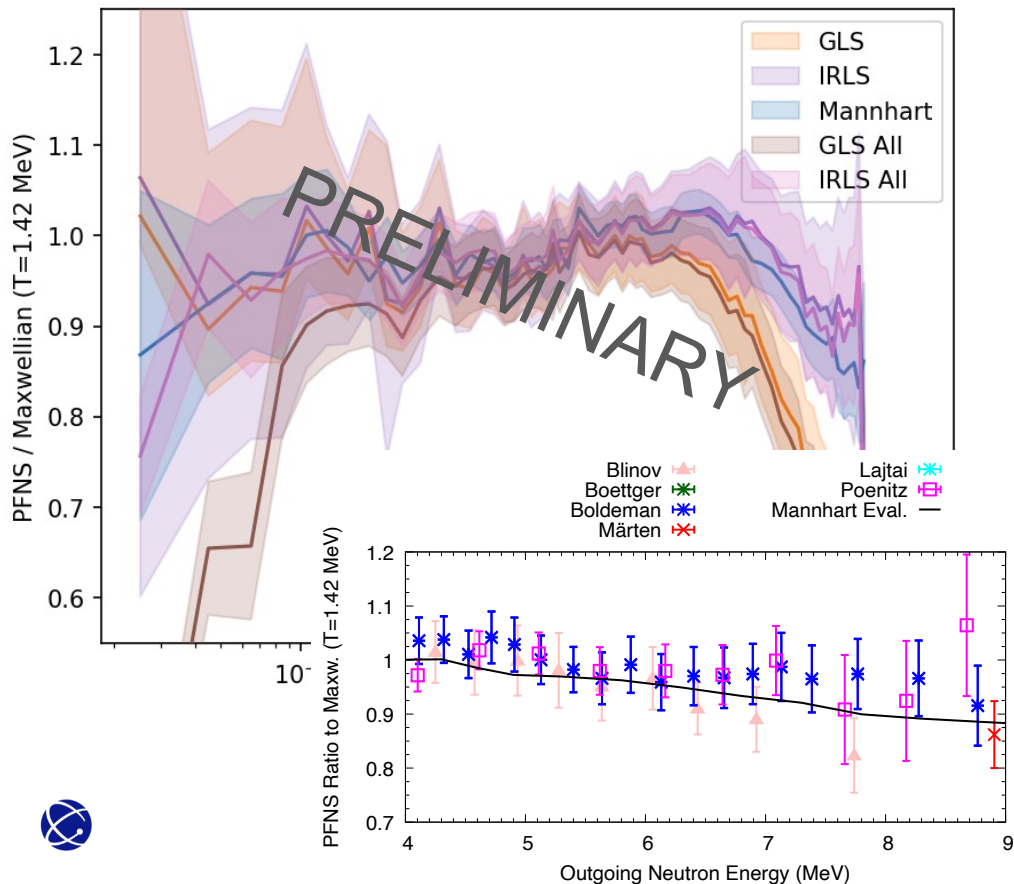
Mannhart ... Mannhart  
evaluation without smoothing

IRLS (=Chiba-Smith extended  
GLS) ... we use same data as  
Mannhart but nearly diagonal  
covariances → larger evaluated  
unc. & higher PFNS at high  $E_{\text{out}}$

New eval ... IRLS with new  
database.



# We wonder if Mannhart's evaluation could be affected by PPP at high $E_{\text{out}}$ where we have strong cor (trsl)



Observation:

- Mannhart eval. is on average slightly lower than bulk of exp. data from 5-9 MeV.
- GLS with our cov much lower due to PPP, IRLS pushes mean back up.

Tentative suspicion: Mannhart data could be affected by PPP > 5 MeV.

Problem: we don't have Mannhart's covariances to check, we don't know exactly which data were rejected.



# Discussion



# Discussion points

- How do you want data delivered? Total covariances or partial uncertainties with correlation coefficients (requires work in GMA due to time resolution → PFNS unc. conversion).
- Interested in features as well?
- Warning: right now we suspect a PPP effect in Mannhart data  $> 5$  MeV. Tread carefully with SACS!



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