Using ML to find root causes for discrepancies in experimental data underlying the new ^{252}Cf PFNS Standard

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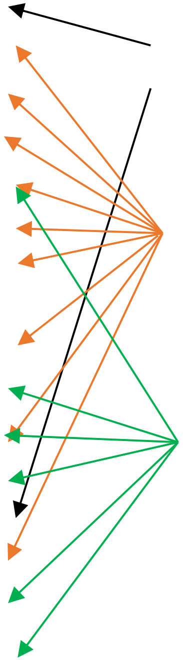
Introduction: the covariance session focuses on improved UQ methods, testing and new covariance types

Jesson Hutchinson
Georg Schnabel
Denise Neudecker
Vlad Sobes
Cole Fritsch and Noah Walton
Daniel Philips
Kyle Beyer
Break
Marc Salinas
Andre Sievering
Ajeeta Khatiwada
Noah Walton
Rike Bostelmann
Goran Arbanas
Chris Chapman
Amanda Lewis



Covariance testing

UQ methodology

New covariance types

Two major comments:

- The Neutron Data Standards will be released in 2026. Please, implement them in your evaluations!
- There is an increased push for AI/ML that we can leverage for better UQ.

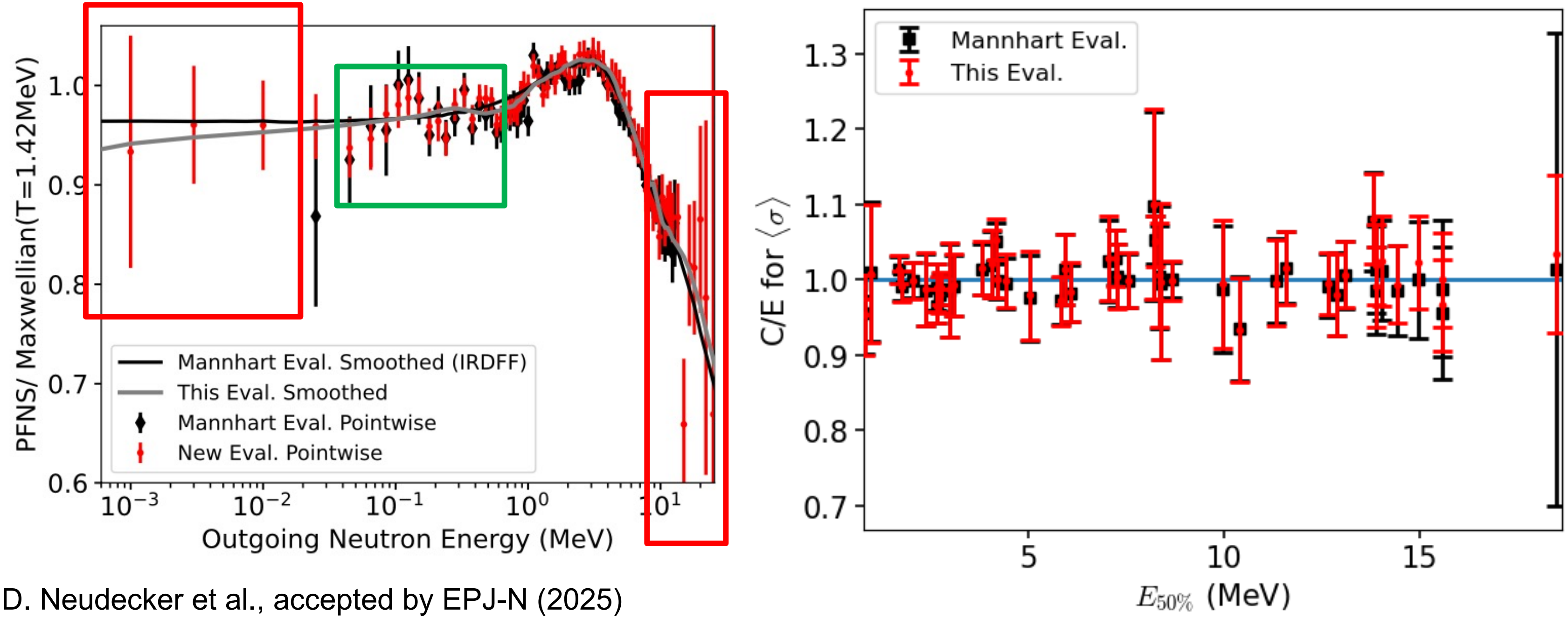
Two take-home messages:

- After nearly 40 years, a new $^{252}Cf(sf)$ PFNS Standard will be released.
- AIACHNE developed a tool that allows you to study via ML what is the physics root cause of discrepancies (USU). This tool can be applied to nuclear data evaluations with good experimental coverage but discrepancies.

Why does $^{252}Cf(sf)$ PFNS matter?

- >70% of PFNS measured using that observable.
- Important for IRDFF community for neutron dosimetry.
- Important for fission applications ranging from global security, detector development, etc., to nuclear medicine.

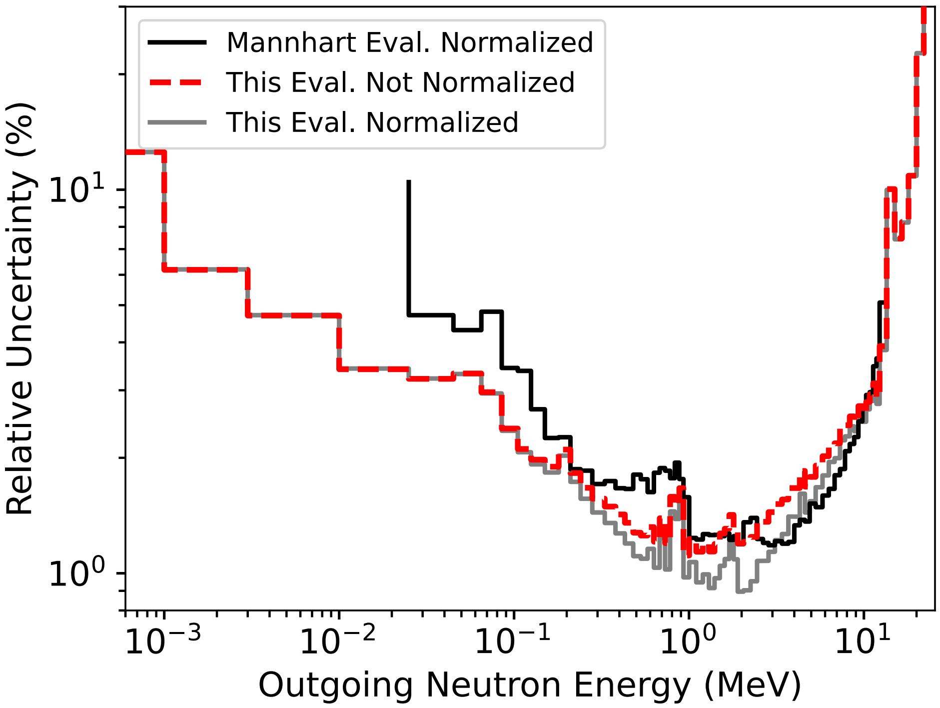
The AIACHNE project produced a new, fully reproducible ^{252}Cf(sf) PFNS evaluation that agrees with SACS.

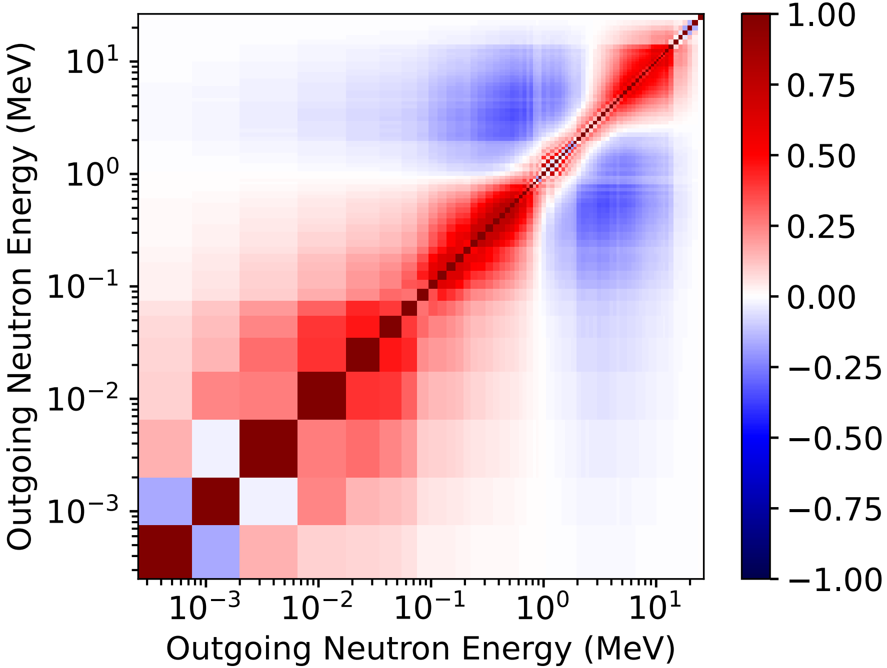


D. Neudecker et al., accepted by EPJ-N (2025)

Previous Standard (Mannhart, 1985) could not be reproduced because input data were lost. This one includes new experimental data & covers a broader energy range.

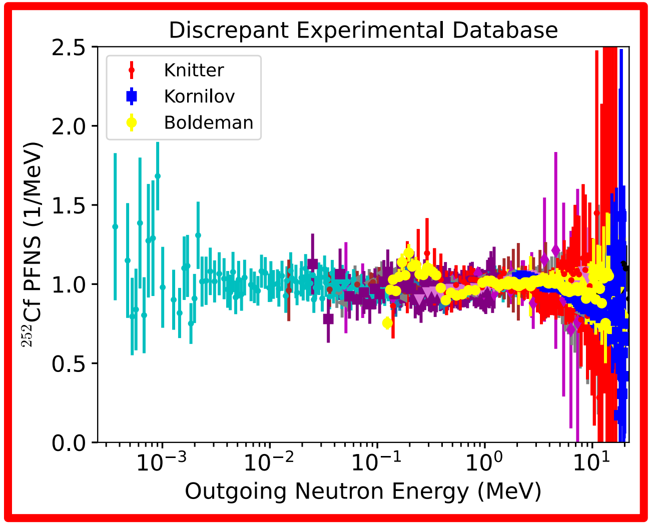
The evaluated uncertainties were reduced below 3 MeV and above 8 MeV due to new experimental data but also ….

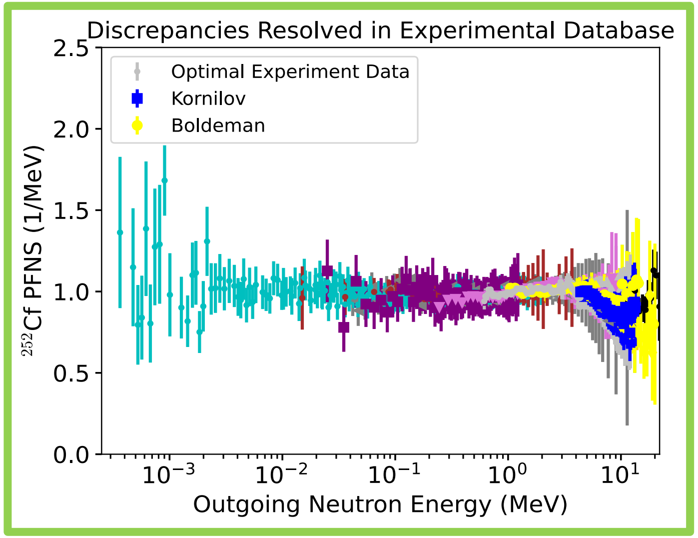




… AIACHNE performed a study on experimental discrepancies using ML!

An ML supported process resolved discrepancies in ^{252}Cf PFNS experiments on sound physics basis.



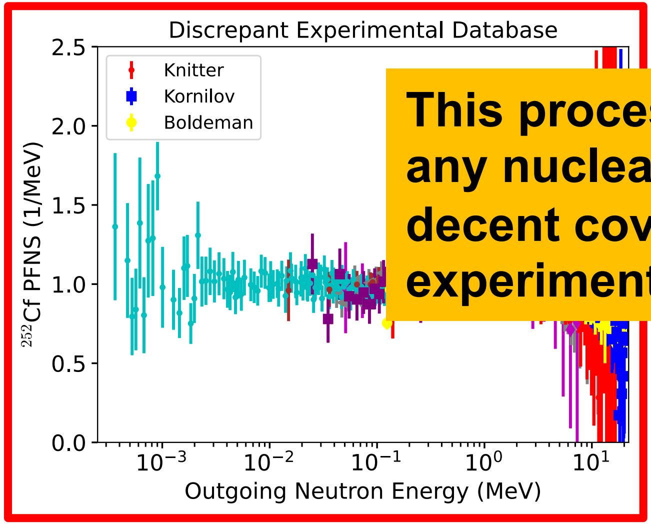


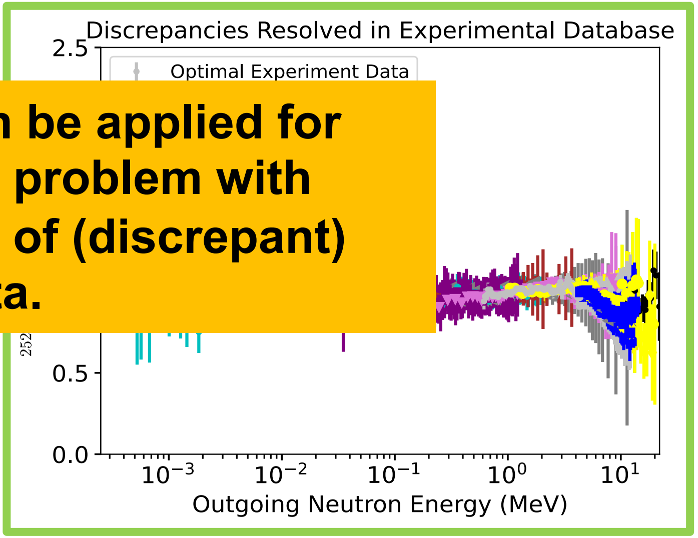
D. Neudecker et al., in preparation.

Our key questions:

- What is the root cause for discrepancies between trustworthy experiments?
- What experiments/ simulations can we perform to best reduce scatter in experimental data to reduce evaluated nuclear data uncertainties?

An ML supported process resolved discrepancies in ^{252}Cf PFNS experiments on sound physics basis.





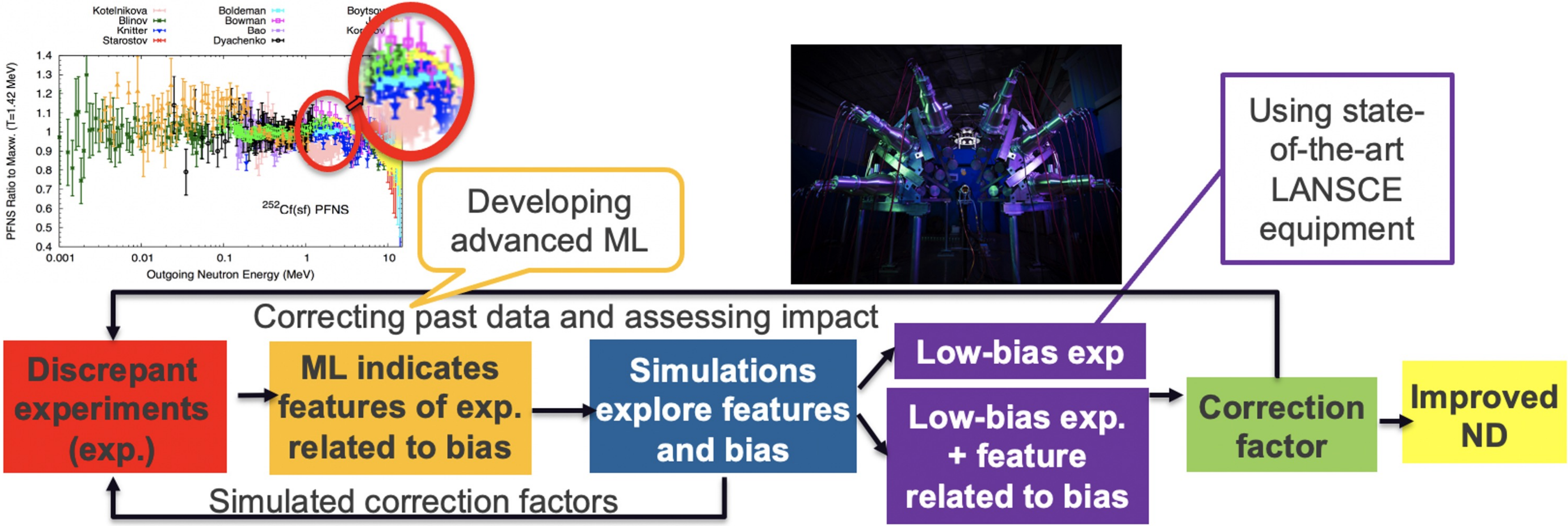
This process can be applied for any nuclear data problem with decent coverage of (discrepant) experimental data.

D. Neudecker et al., in preparation.

<u>Our key questions:</u>

- What is the root cause for discrepancies between trustworthy experiments?
- What experiments/ simulations can we perform to best reduce scatter in experimental data to reduce evaluated nuclear data uncertainties?

The general process requires as input experimental means & covariances and metadata features as input for ML.



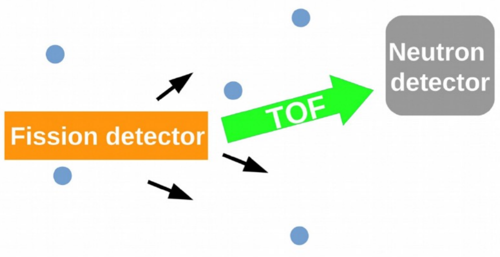
The ML output gives you clues what could be root causes of experimental discrepancies that can be followed up by simulations of historical data and new experiments.

Experimental metadata should encapsulate the key information on the measurement that could be related to bias.

I want to know if the following corrections were undertaken. Give a 'y', 'n', 'unclear' answer: Background, Multiple Scattering, Foil Thickness, Angular Distribution Fission Fragments, Forward Boost, Deadtime, Impurities, Geometry, Neutron Flux Variation, Delayed Gammas, PFNS, Neutron Detection Efficiency, Displacement of Sample, False Fission

Based on the document DeVroeyData:

- Background: **y**
- Multiple Scattering: **y** (neutrons scattered from fission chamber corrected)
- Foil Thickness: **y**
- Angular Distribution Fission Fragments: **y**
- Forward Boost: **unclear**
- Deadtime: **unclear**
- Impurities: **y** (Pu-239, Pu-241)
- Geometry: **unclear**
- Neutron Flux Variation: **unclear**
- Delayed Gammas: **n**



see also D. Brown talk.

	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		

These metadata were retrieved 2023 from EXFOR and literature in a **very long** by-hand process. LLMs can ingest EXFOR and speed up metadata retrieval by hours/ entry!

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.

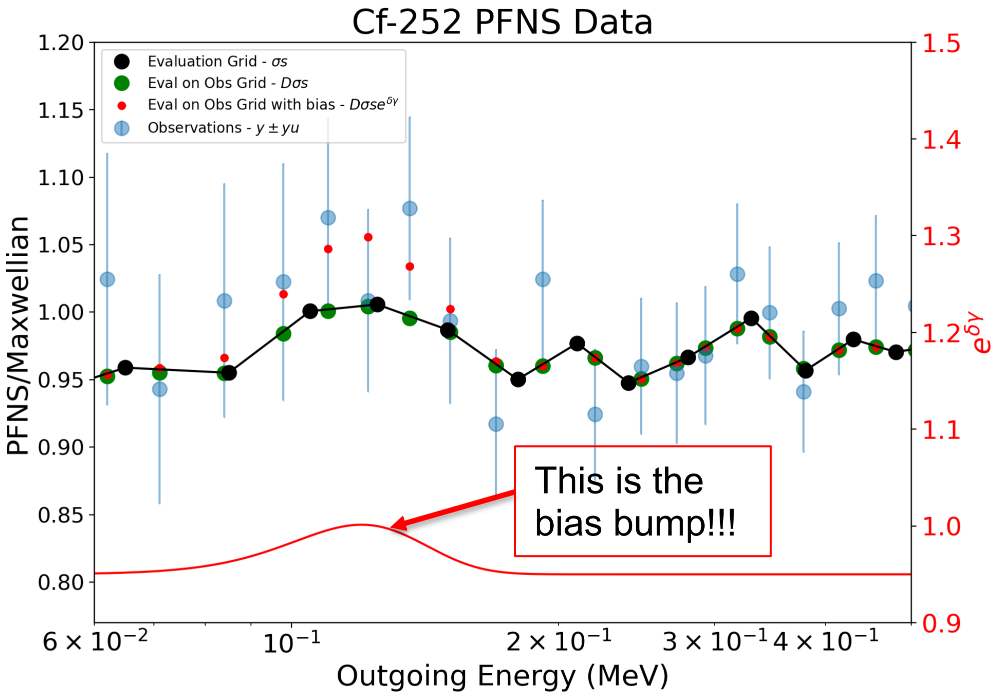
$$\boldsymbol{y} = \boldsymbol{D\sigma} \cdot \boldsymbol{e^{\delta}} + \boldsymbol{\varepsilon}$$

$\boldsymbol{\delta} =$ $\boldsymbol{B\gamma} =$ **relative bias**

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

$\boldsymbol{\gamma} =$ **bias coefficients**

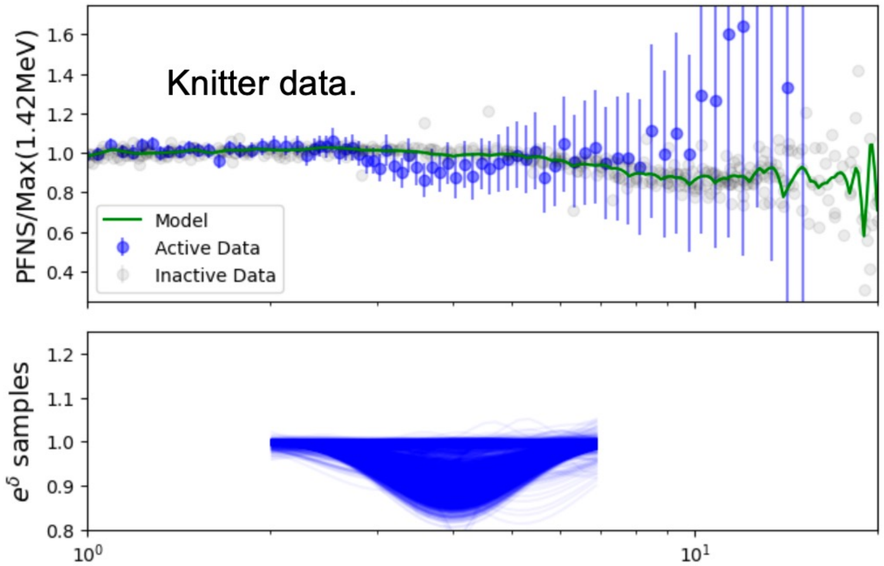
$\cdot =$ **element-wise product**



The code is open source: https://github.com/lanl/sparse_bias
N. Walton et al., Computer Physics Communications, 109698 (2025).

ML provides clues that help us (a) reject data with sound scientific basis & ...

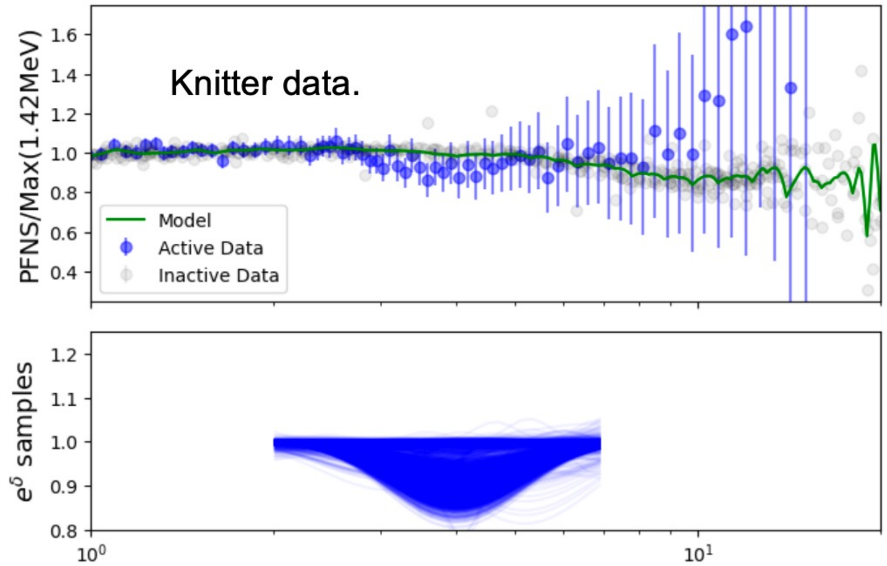
Multiple scattering & neutron detector response



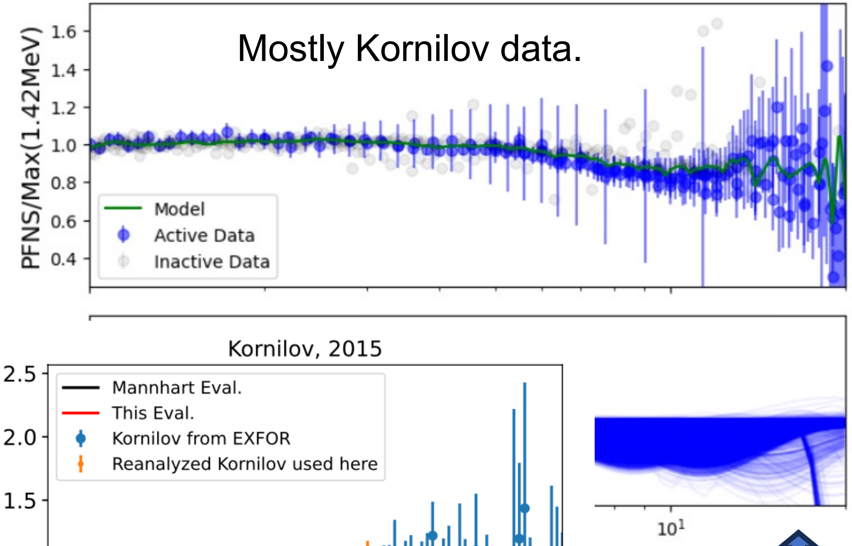
ML provided the clues to what is wrong with Knitter data substantiating decision for rejection.

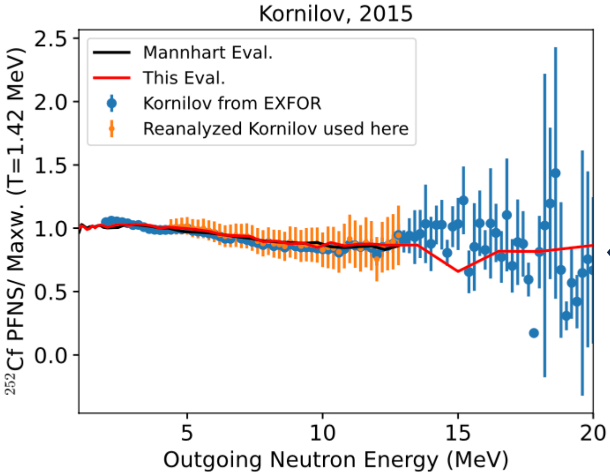
ML provides clues that help us (a) reject data with sound scientific basis & (b) correct them via targeted simulations.

Multiple scattering & neutron detector response



Fission fragment detection efficiency

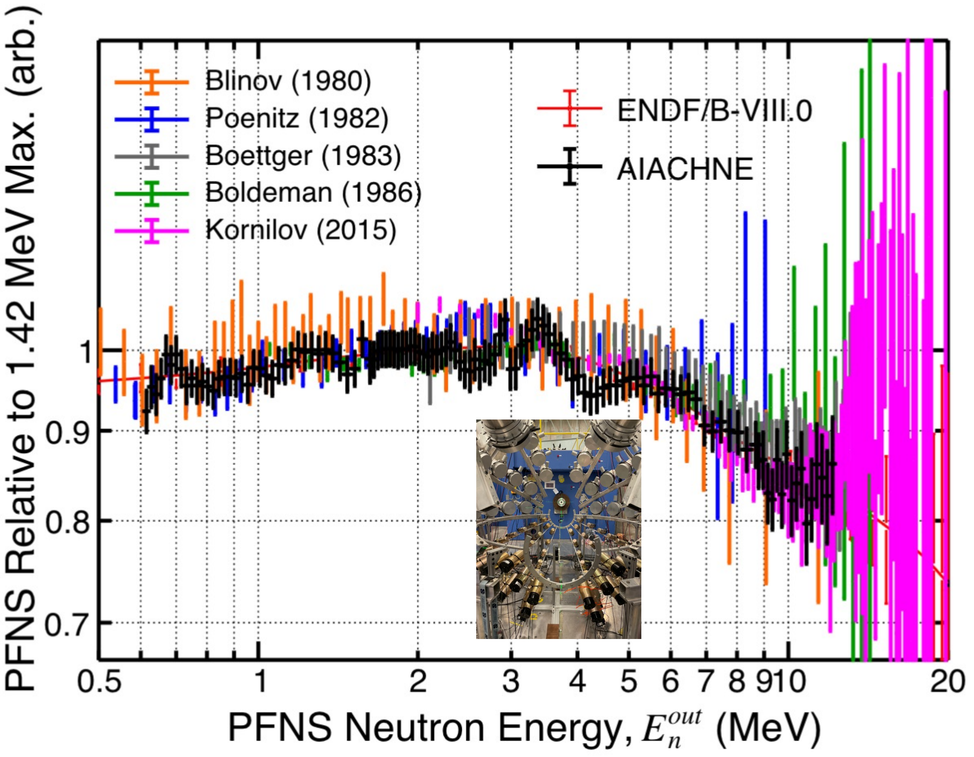




ML provided the clues to what is wrong with Knitter data substantiating decision for rejection.

Adoption after correction.

ML clues indicated what was the major open issues in ^{252}Cf PFNS exp. and guided the design of a new measurement.

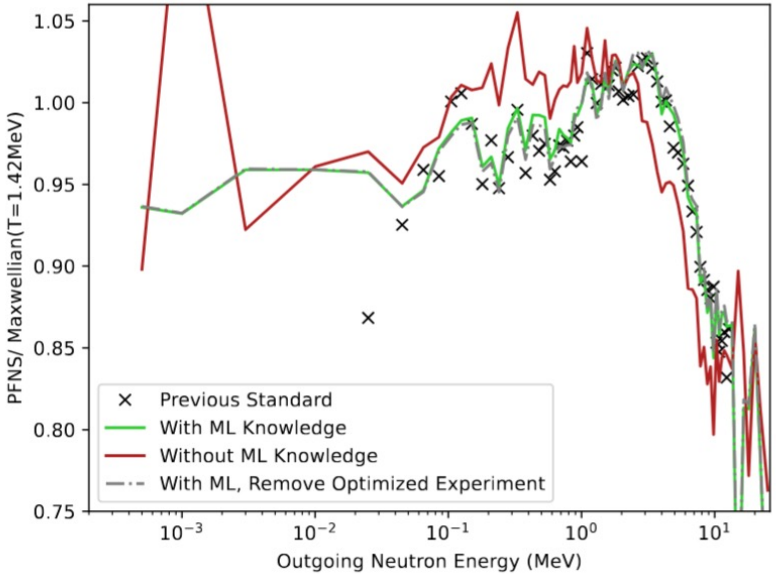


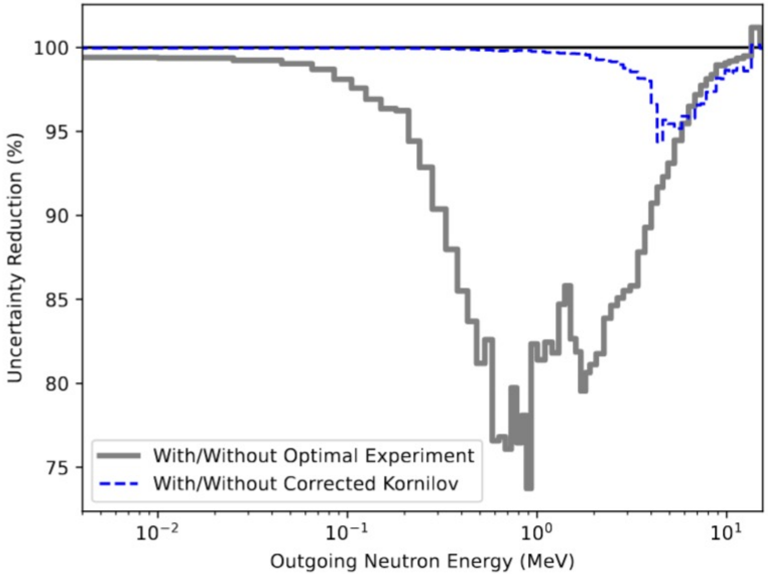
<u>AIACHNE experiment:</u>

- The key remaining issue is neutron detector response; often relies on knowing ^{1}H, ^{6}Li, ^{235}U.
- Here, we validate that by using ^{9}Be & ^{12}C(n,n) elastic neutron scattering.
- Uses CoGNAC array (K. Kelly).
- Structures highlight issues in ^{9}Be nuclear data!

K.J. Kelly, submitted (2025).

Impact assessment: Without ML clues we get strongly biased evaluation but with ML-guided exp. we reduce unc. by 25%!





Benefit of using this ML-supported process is that it highlights potential physics biases in data that can be followed up by simulations of historical data and gives clues what new experiment can unravel discrepancies.

D. Neudecker, in preparation (2025).

Thank you for your attention!

Summary:

- After nearly 40 years, a new $^{252}Cf(sf)$ PFNS Standard will be released.
- AIACHNE developed a tool that allows you to study via ML what is the physics root cause of discrepancies (USU). **This tool can be applied to nuclear data evaluations with good experimental**

Acknowledgements

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