Measurements and RRR Evaluation of ^{54}Fe

NCSP TPR

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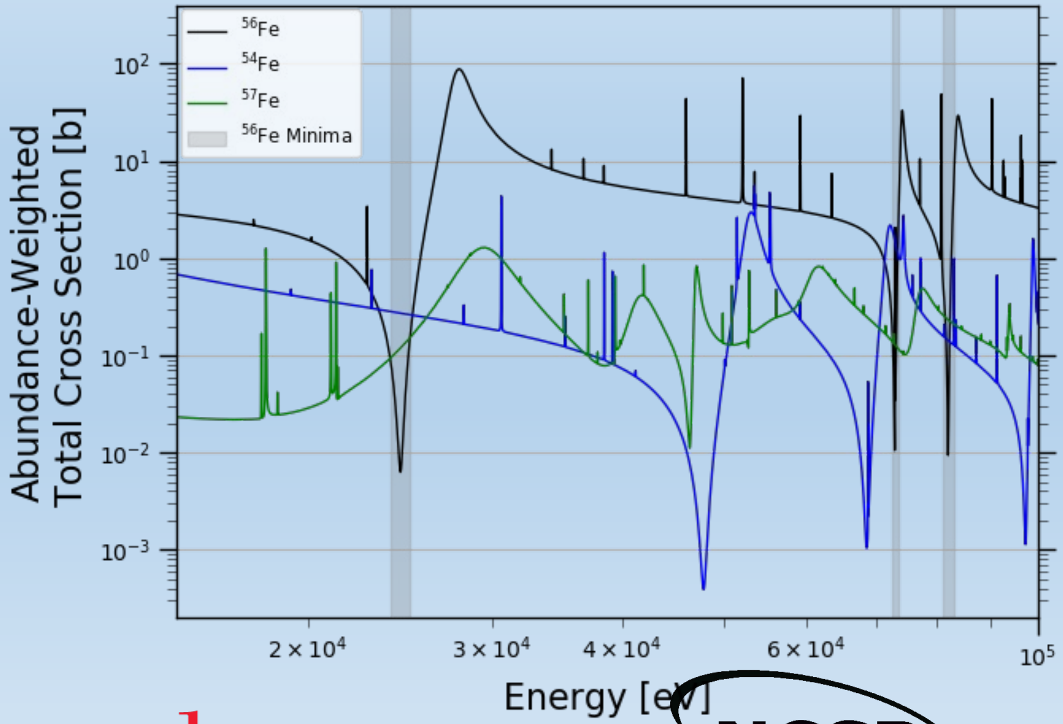
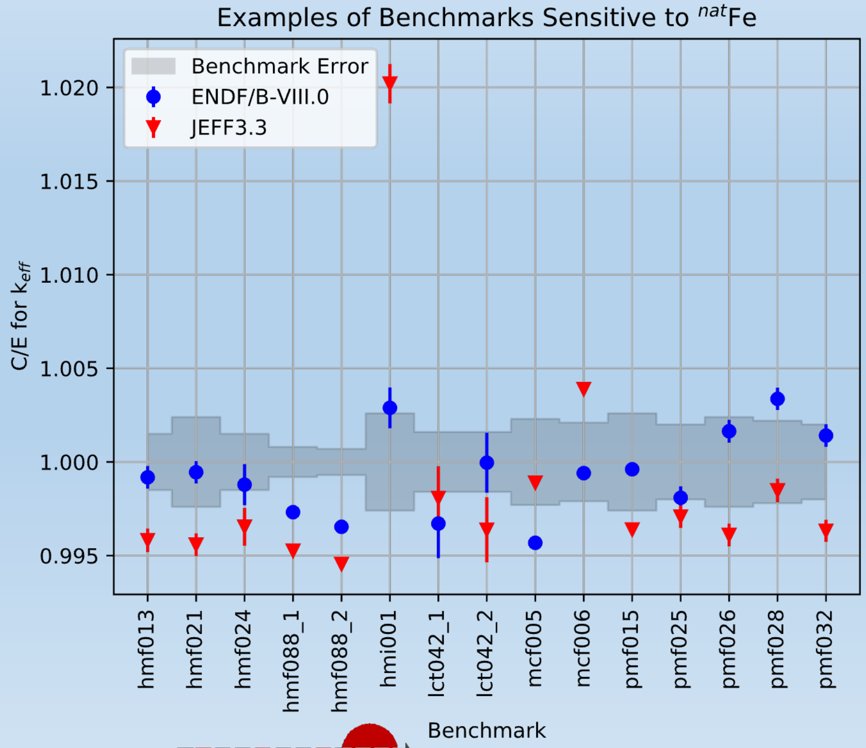
^{54}Fe Project Overview

- **Motivation:**
  - Criticality safety calculations require high accuracy nuclear data to reduce uncertainties
  - ^{54}Fe neutron cross sections have not been well-studied relative to ^{56}Fe.
- **Project Goals:**
  - Perform new RRR evaluation for ^{54}Fe cross section in the keV region using RPI and EXFOR nuclear data.
    - Evaluation will include covariances along w/ consideration of measurement covariances from RPI experiments.

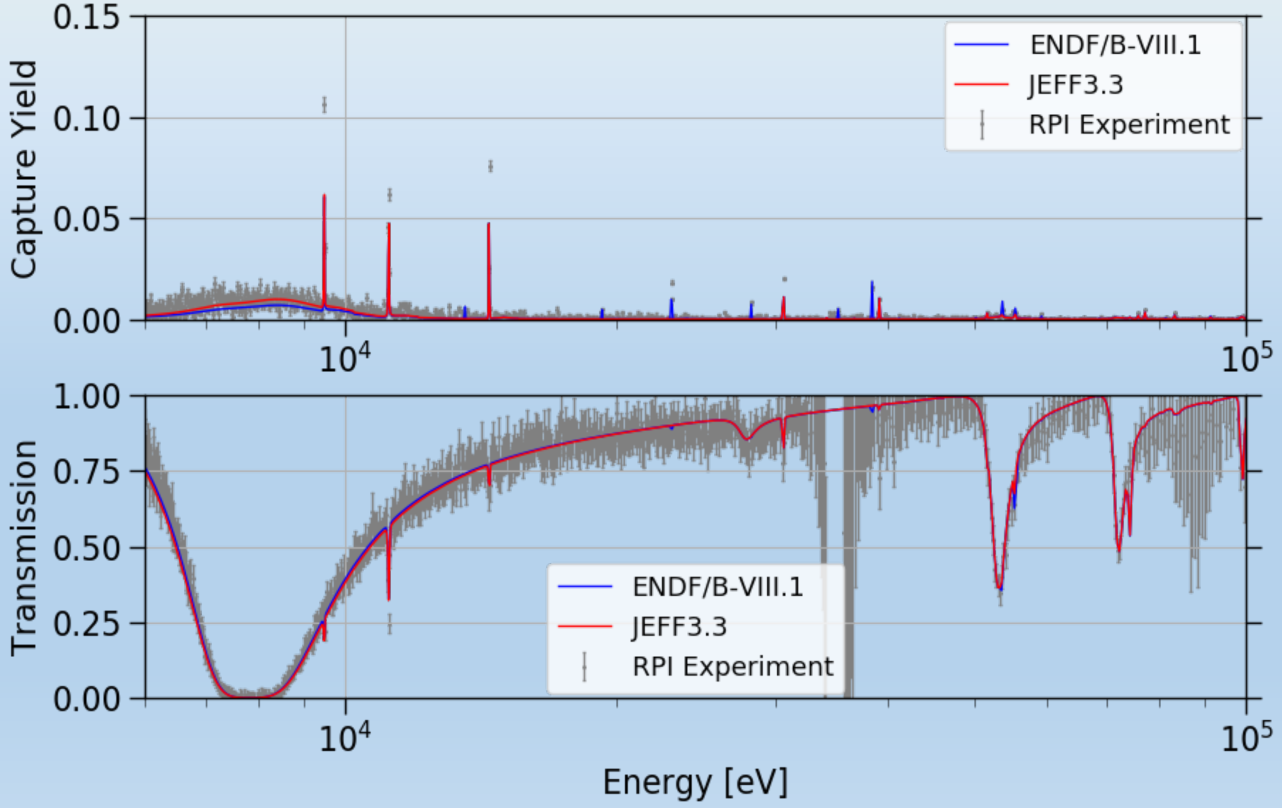




Overview of RPI Measurement Campaign

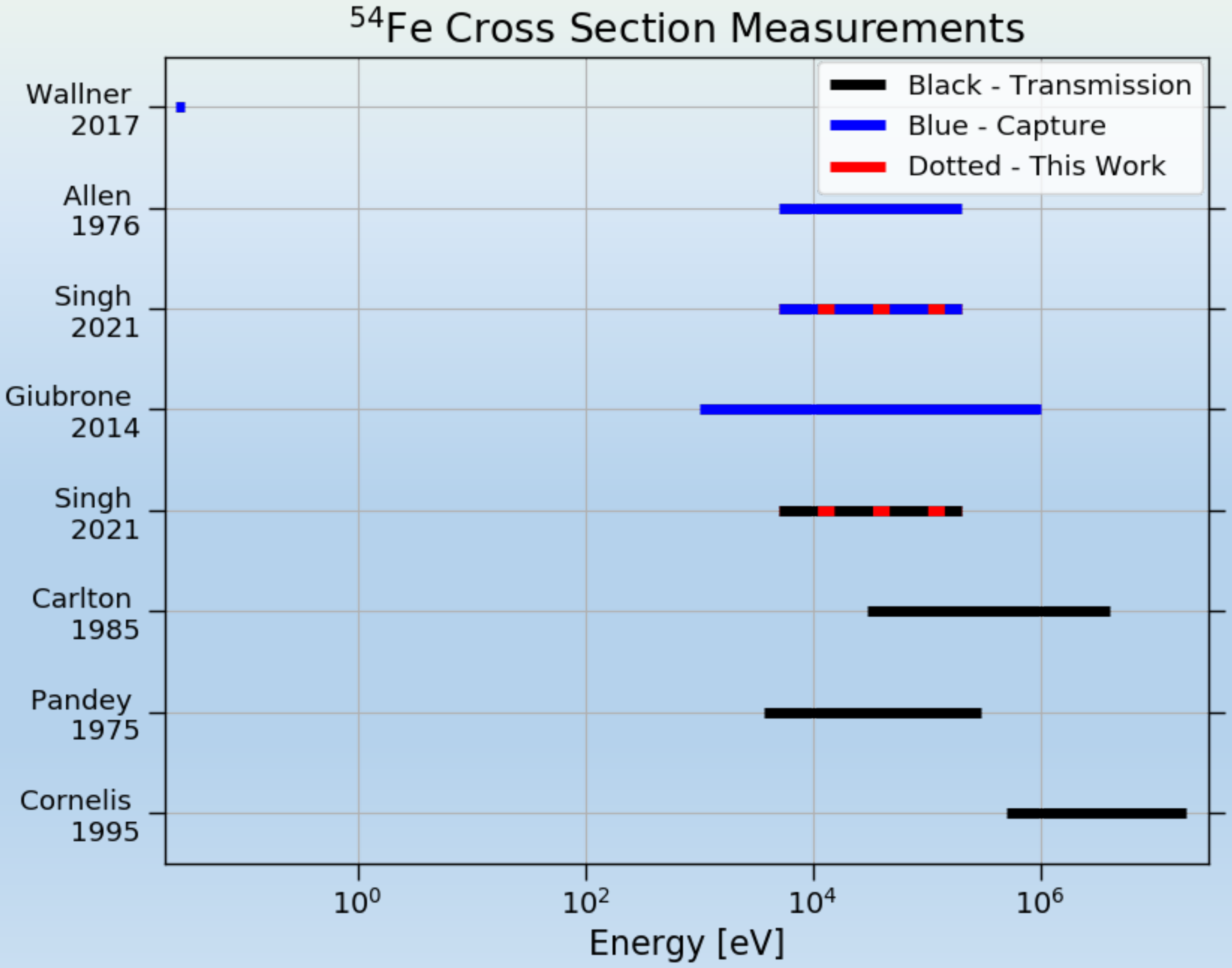
- RPI previously conducted transmission and radiative capture yield measurements as a part of this work
- 0.021 a/b enriched metallic ^{54}Fe sample was used for both experiments.
- Full energy-energy correlations were generated.
  - First time generating experimental covariances for radiative capture yield experiments at RPI.

Parameter	Capture	Transmission
Flight Path [m]	45	35
Energy Region [keV]	1-150	0.01 - 150
Detector	C_6D_6	^{6}Li Glass



Fitted Experimental Data

- In addition to RPI ^{54}Fe measurements, other energy-differential TOF data from EXFOR was identified and included in the RRR evaluation.
- Very limited data exists for the thermal point of ^{54}Fe
- Giubrone n_TOF data was made available following RPI capture experiments
- Pandey transmission data requires additional background correction below 30 keV



RPI Evaluation Results

Experiment or Evaluation	Value [mb] @ 30 keV
ENDF/B-VIII.0	27.13
RPI Eval	29.8 ± 0.9
KADoNiS-0.3	29.6 ± 1.3
n_TOF Exp	30.8 ± 1.6
Allen Exp	33.6 ± 2.7

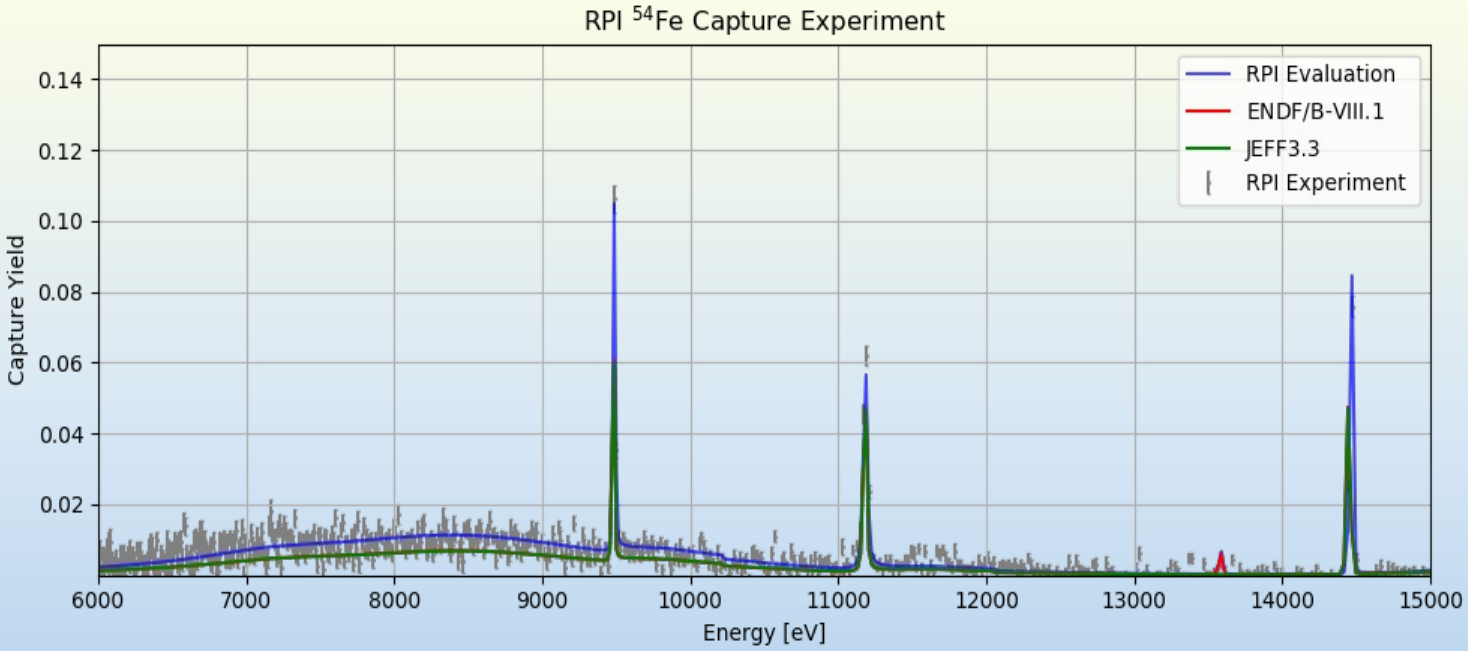
Source	σ_γ [barns] at 0.0253 eV
RPI Evaluation	2.27 ± 0.02
ENDF/B-VIII.0	2.25
JEFF-3.3	2.25
Litvinskij Capture	2.28
Wallner Capture	2.26 ± 0.15
NIST	2.25
Atlas (2018)	2.30 ± 0.07

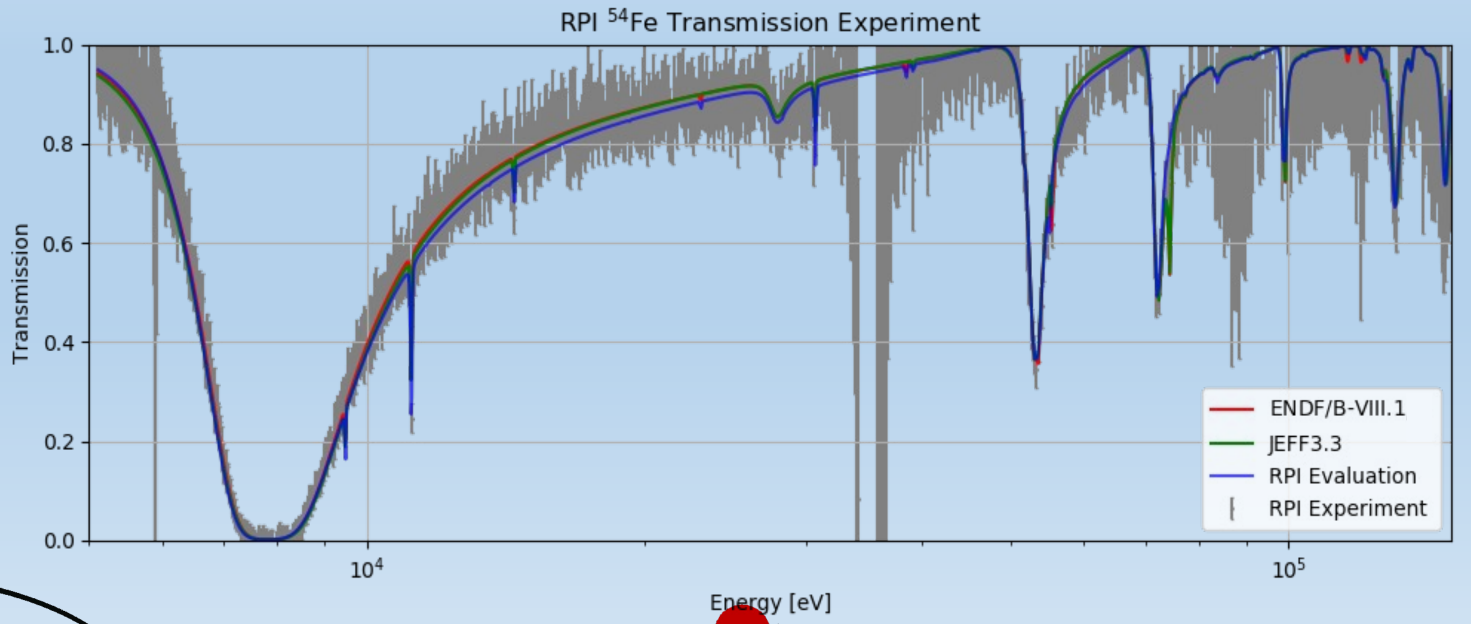
Source	σ_t [barns] at 0.0253 eV
RPI Evaluation	4.46 ± 0.05
ENDF/B-VIII.0	4.43
JEFF-3.3	4.45
NIST	4.45
Atlas	4.47 ± 0.12

Experiment	Value @ 481 keV
Wallner	6.01 ± 0.28 [mb]
n_TOF Exp	6.04 [mb]
RPI Eval	6.10 ± 0.14 [mb]

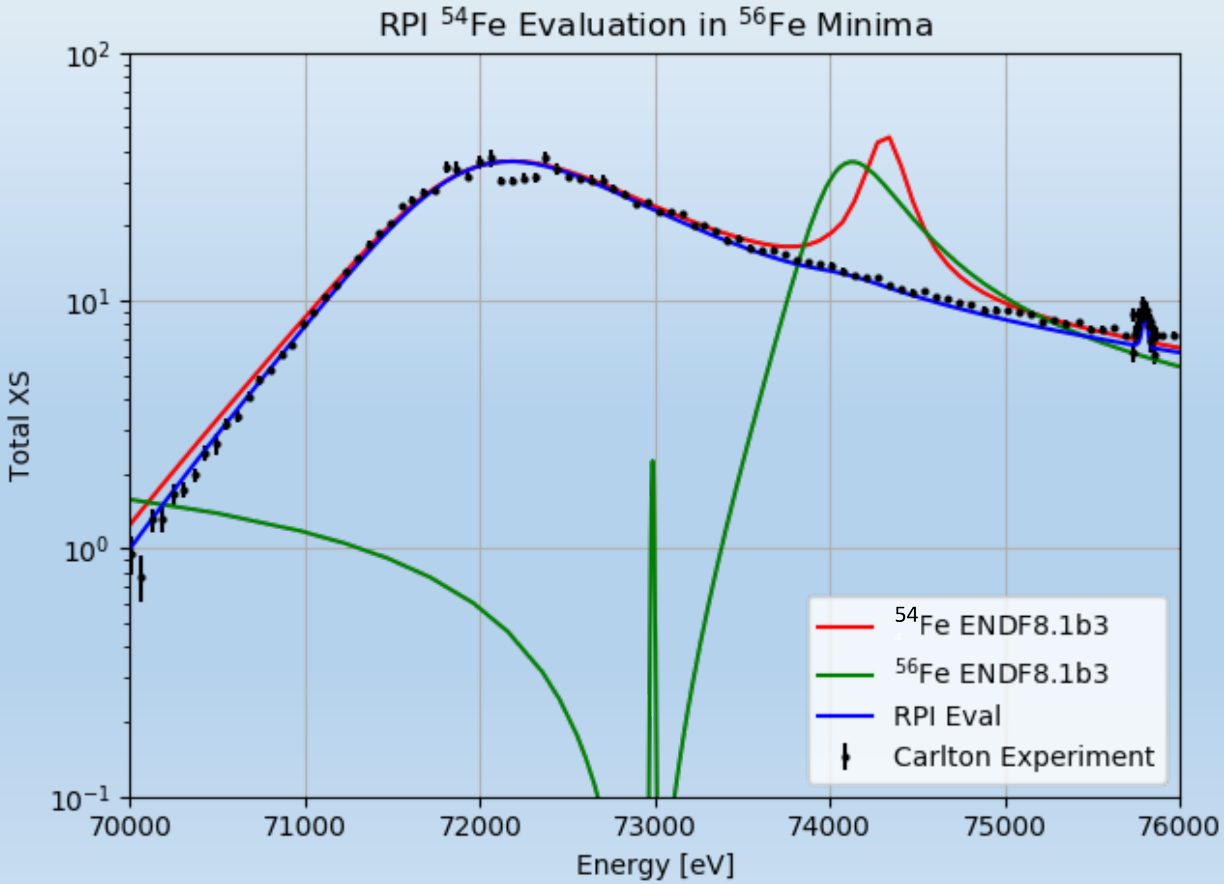
RPI Evaluation

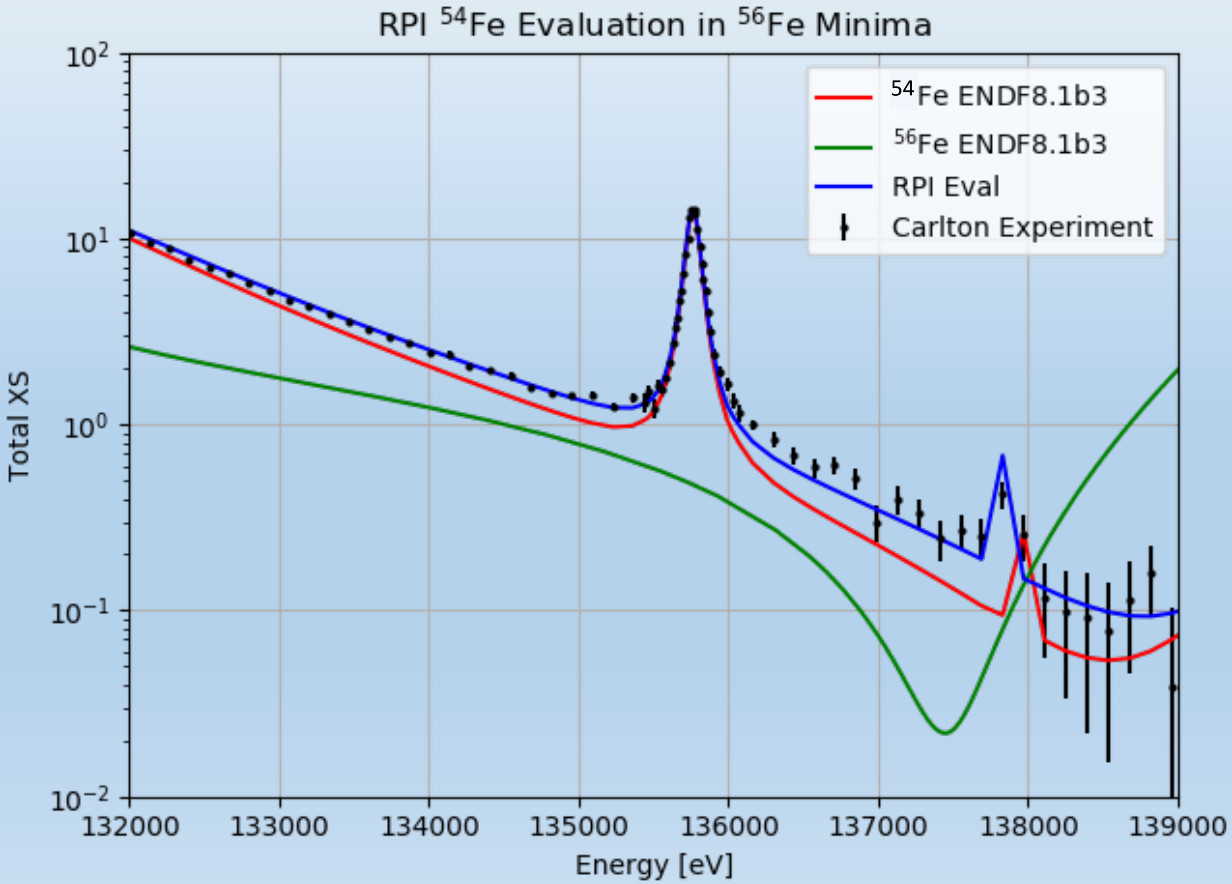
- Capture widths were increased for prominent capture resonances
  - Both experiments suggested an increase was needed in the capture cross section for these d-wave resonances
- The direct capture process was considered in the evaluation, a direct capture background was discarded in favor of bound levels.
  - Collaboration w/ Luiz Leal (ORNL) and Goran Arbanas (ORNL) to determine magnitude of direct capture cross section.
- **Resonance parameter fitting considered experimental data covariances.**
  - This has not been done in the past.





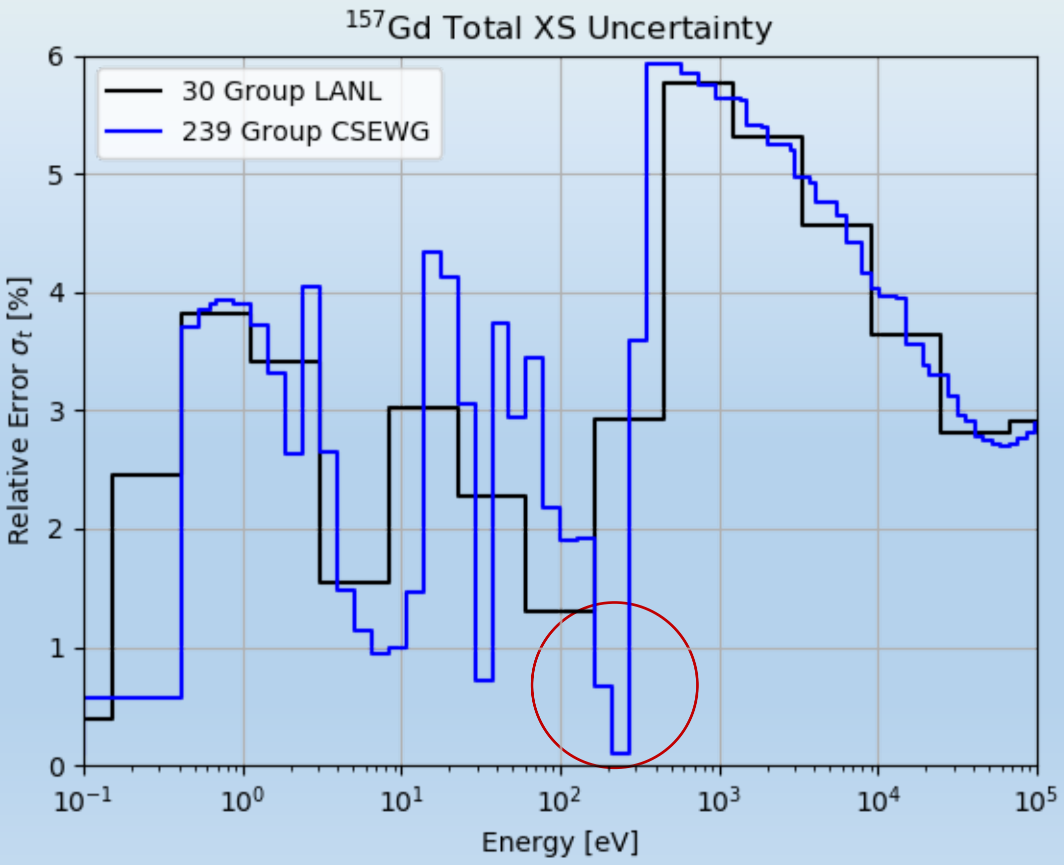
^{54}Fe Changes Near ^{56}Fe XS Minima





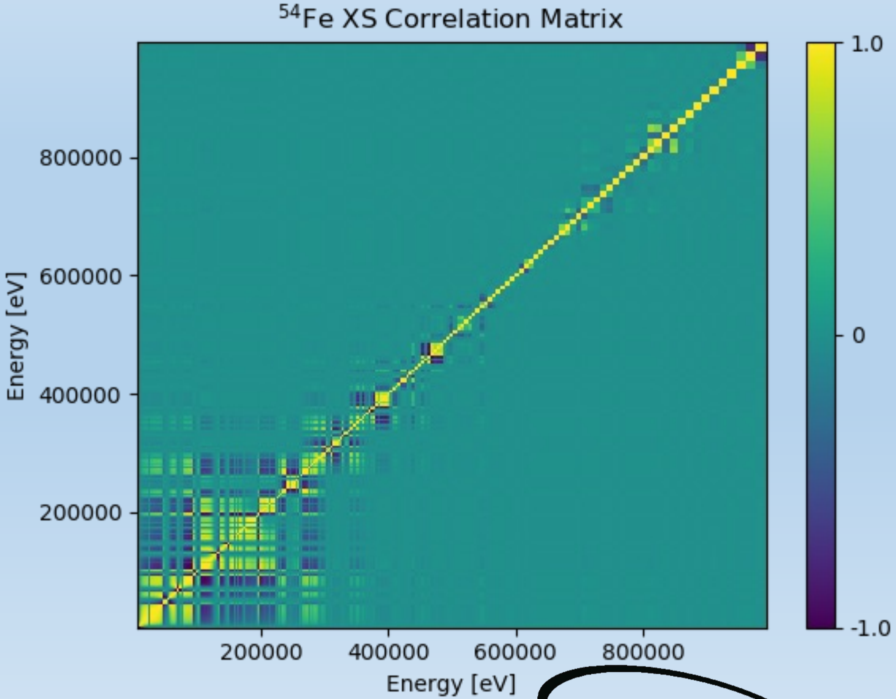
The Issue with Nuclear Data Covariances

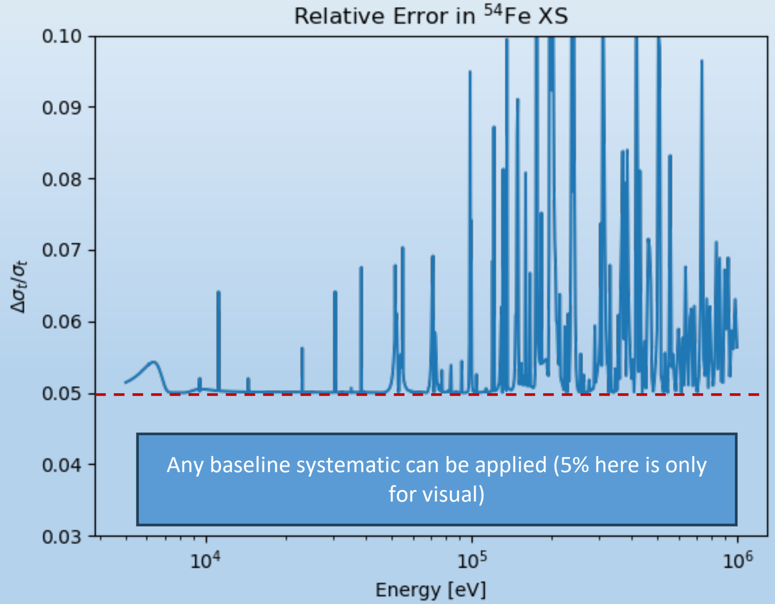
- Covariance information is <u>required</u> when submitting a new evaluation to ENDF
- Grouped cross section uncertainties are often tuned to the standards set by the nuclear data community
- Two issues arise with this approach:
  - **Resonance parameter covariances when converted to cross section covariances lose systematic uncertainties**
  - Grouped cross section uncertainties are sensitive to the grouping structure chosen.
- Several examples of <u>accepted</u> evaluations in ENDF/B-VIII.1 show issues when inspecting covariance data



A Proposed Solution for Future Evaluations

- A different approach for including uncertainties into the ENDF format is currently being investigated.
  - Compatible with ENDF format, preserves correlations and constrains total XS.
  - ENDF file contains MF=32 and systematics are propagated separately into MF=33.





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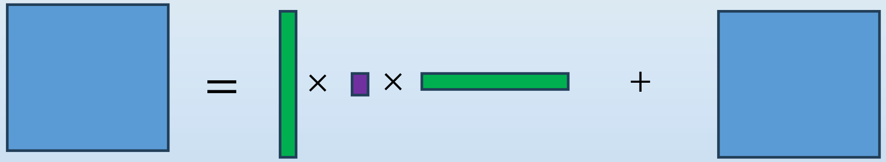
A Proposed Solution for Future Evaluations

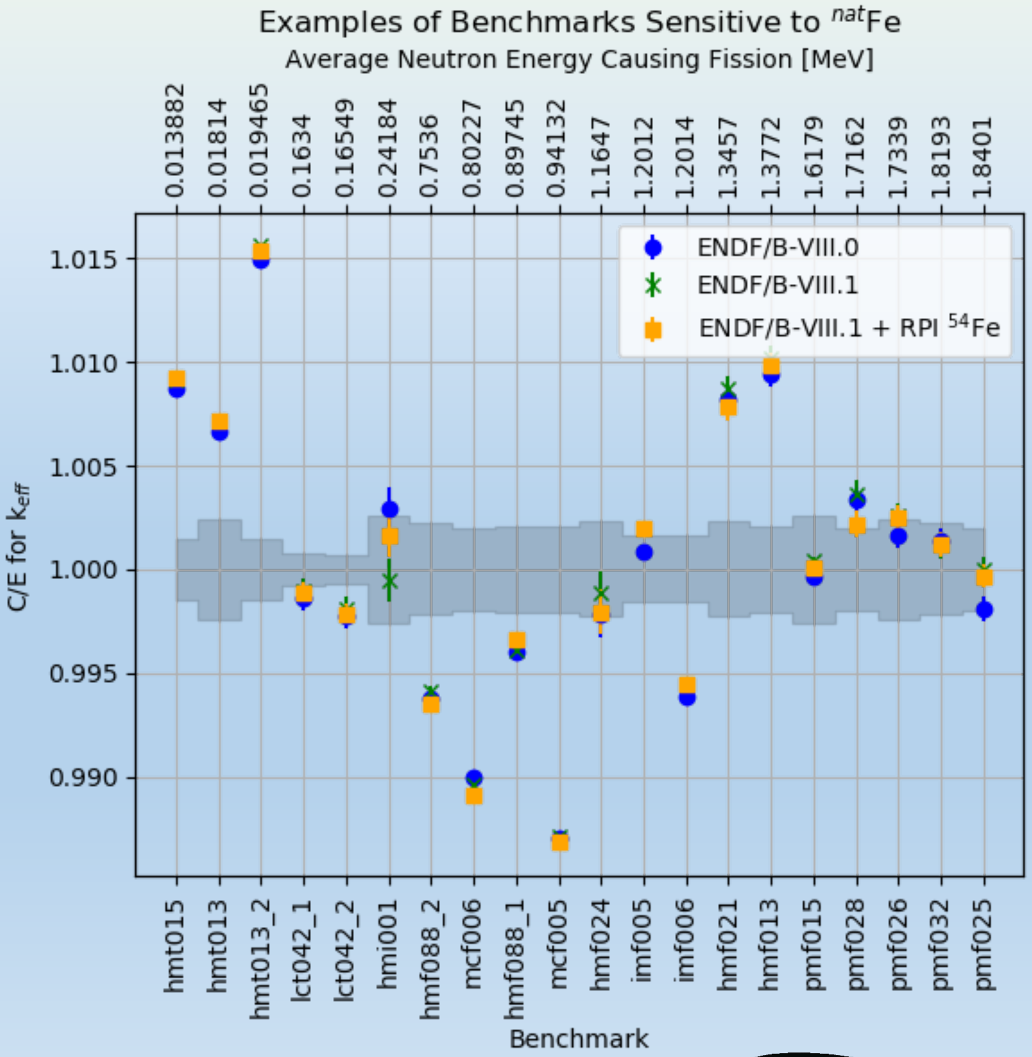
- MF=32 contains resonance parameter covariance matrix, determined a priori via normal evaluation procedure
- MF=33 contains cross section covariance that reflects a baseline systematic uncertainty desired
  - Can be determined by evaluator to be constrained by a desired value
  - Energy-dependent systematic uncertainty can be chosen as well
  - Energy grid of cross section covariance matrix must be sufficiency dense to properly reflect the systematic uncertainty, which is again, up to the evaluator
- SAMMY can produce cross section covariance, resonance parameter covariance, and file containing partial derivatives w.r.t all varied parameters.

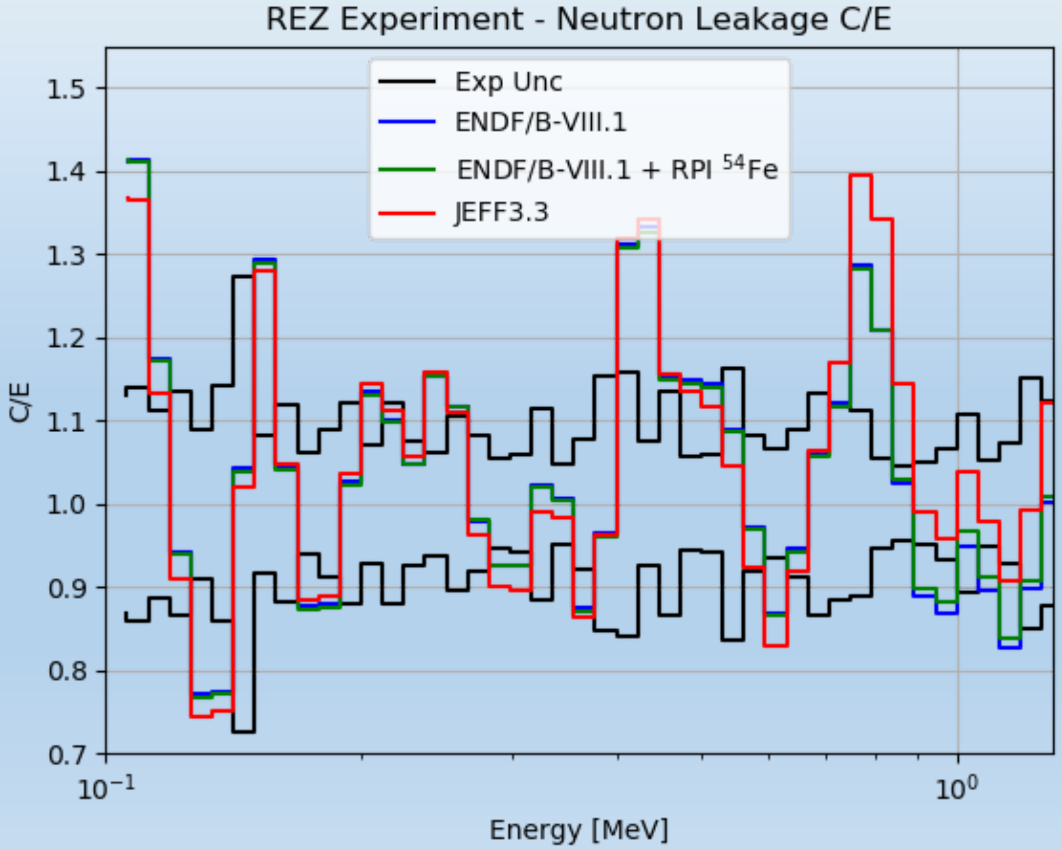
$$V = g \times m \times g' + X$$



$\boldsymbol{V}$ = Full xs covariance matrix
$\boldsymbol{g}$ = Partial derivatives of resonance parameters w.r.t. cross section
$\boldsymbol{m}$ = Covariance matrix of resonance parameters + nuisance variables
$\boldsymbol{X}$ = Systematic cross section covariance matrix

Validation Testing





Conclusions and Future Work

- The ^{54}Fe measurement campaign was completed, and the resulting data and experimental covariances were used for the RPI RRR evaluation.
  - Results will be published in Annals of Nuclear Energy – currently under review internally.
  - Paper regarding evaluation and covariances will be published separately
- Re-evaluation of Fe isotopes is currently on the NCSP 5-year plan.
- The current approach to producing evaluated covariances in the RRR has some flaws that need to be addressed by the nuclear data community.
  - MF=33 provides a way to include missing systematics from conversion of RP covariance to XS covariance.