Validation and Evaluation Uses of Quasi-Differential High-Energy Scattering Data

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OUTLINE

- Motivation
- Quasi-Differential for Evaluation
- Quasi-Differential for Covariance
- Quasi-Differential for Validation
- Summary

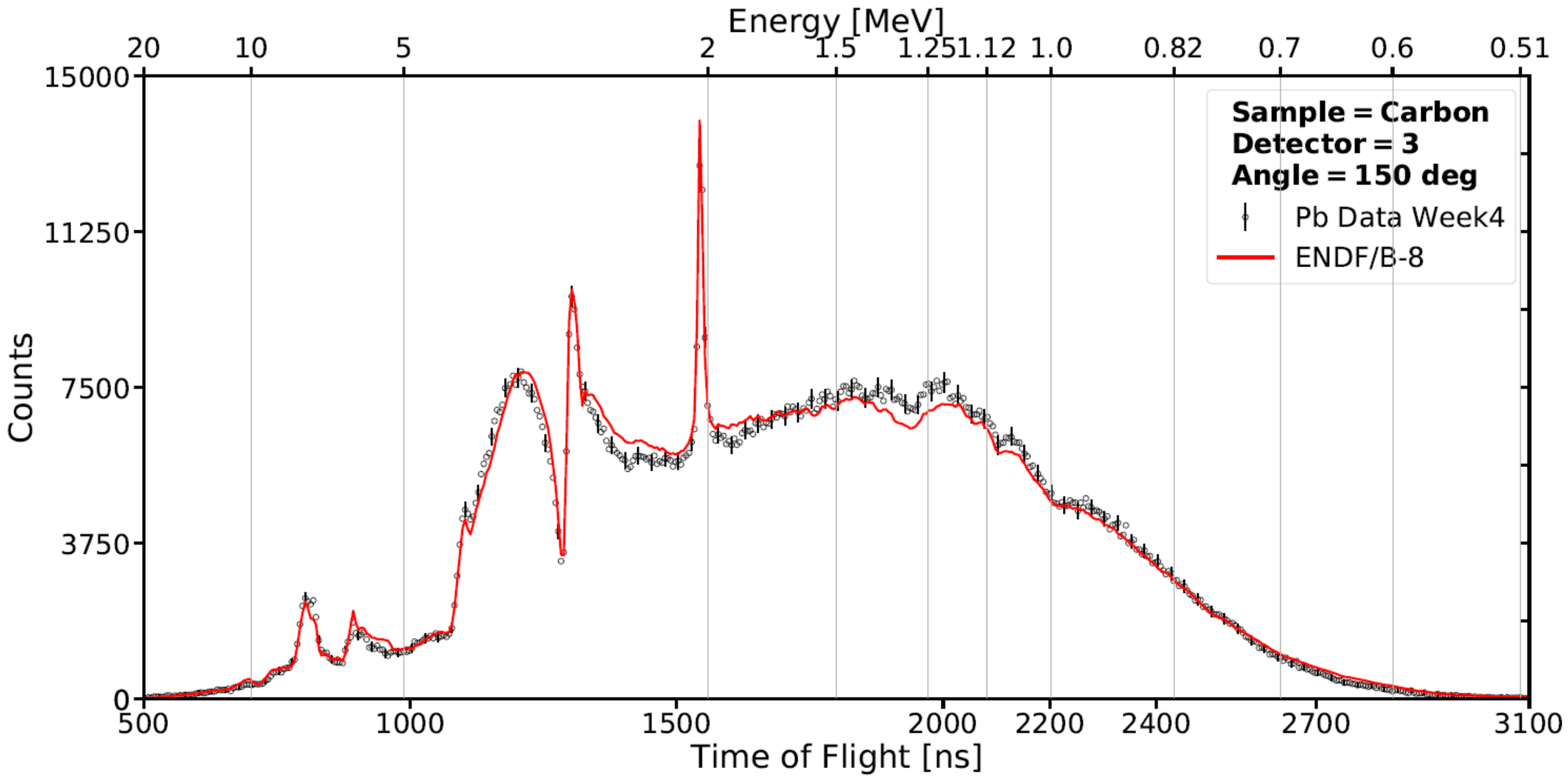
PROJECT OVERVIEW

- Motivation: Lead isotope evaluations for DOE-NEUP support of GEN-IV reactor technologies [1]
  - Lead Fast Reactors (LFRs), Molten Salt Reactors (MSRs), and Liquid Metal Fast Breeder Reactors (LMFBRs)
  - Accelerator driven systems (ADS)
  - Lead-cooled fast spectrum test beds

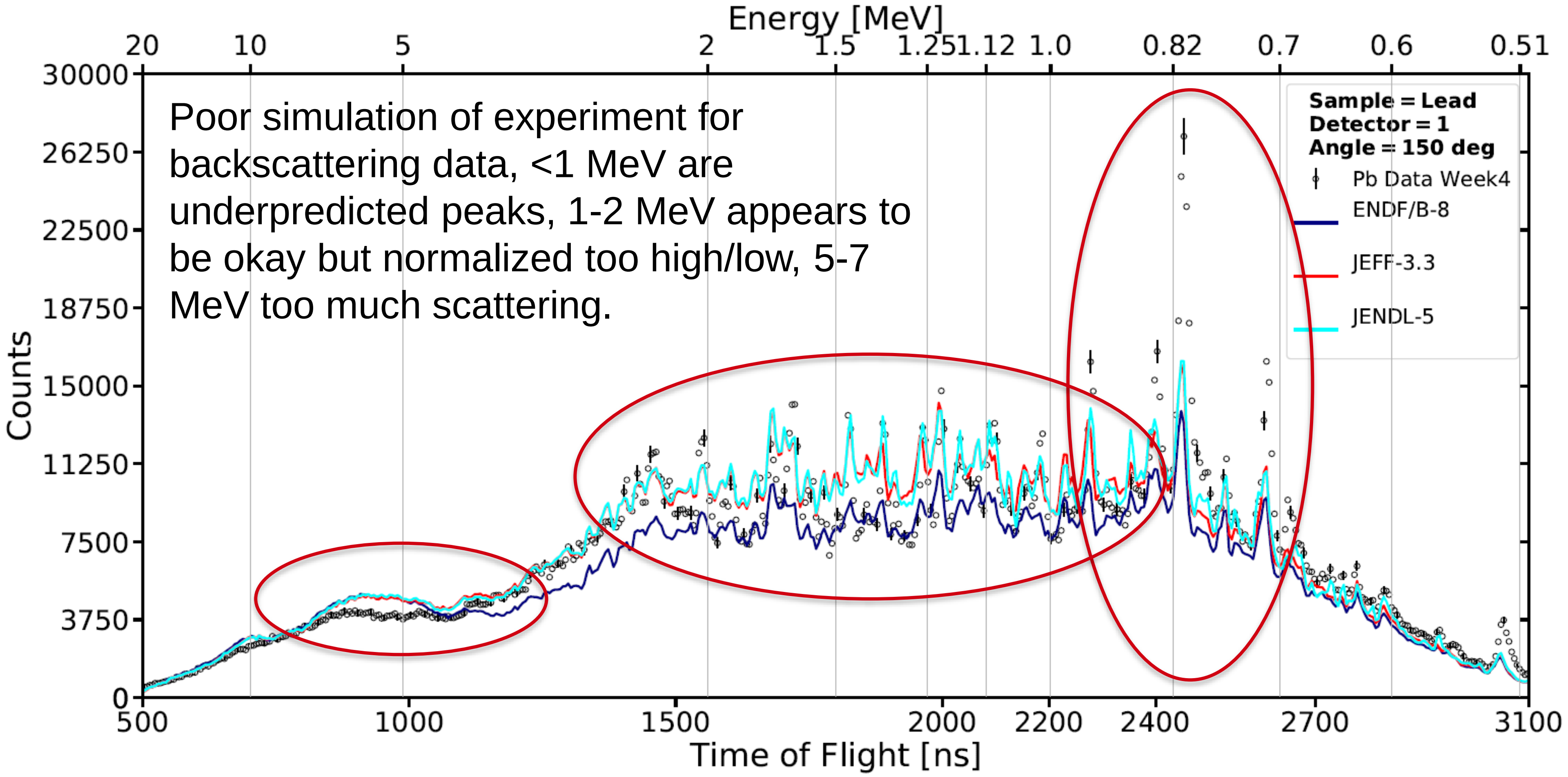
- Project Goals
  - Validate a suite of (quasi)integral experiments in order to test Pb libraries
  - Resolved Resonance and Fast Region Evaluations for Pb-206, Pb-207, Pb-208
  - Covariance development for all isotopes over the recently evaluated energy ranges

- For energies below 5 MeV, elastic scattering is primary reaction for lead isotopes
- The agreement between quasi-differential experimental data and simulation of the experiment should be directly proportional to how well the integral double-differential scattering cross section is known
- Work here will be using reduced data from Youmans, mimicking approach of someone who is outside RPI [2]

Carbon simulations perform relatively well for ENDF/B-VIII.0



Poor simulation of experiment for backscattering data, <1 MeV are underpredicted peaks, 1-2 MeV appears to be okay but normalized too high/low, 5-7 MeV too much scattering.



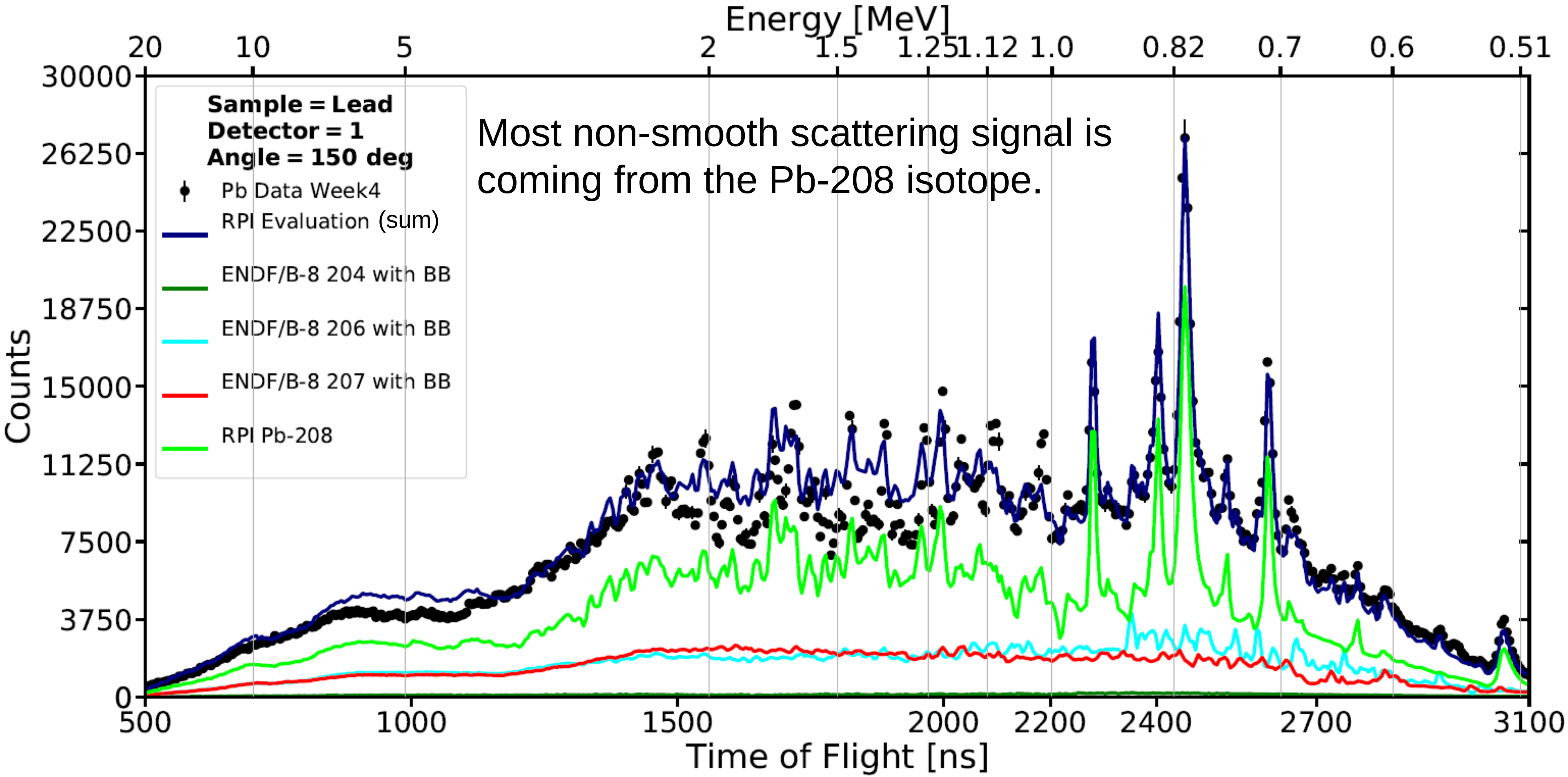
Evaluation uses of Quasi-Differential

- Large scattering peaks below 1 MeV are completely underpredicted from investigated evaluations
- Around1-2 MeV ENDF/B-VIII.0 agree with the valley of structure while JEFF/JENDL have the peaks
- Scattering at 5-8 MeV too high

Simulation using ENDF Pb isotopic data does not reproduce the natural lead scattering experiment as well as the carbon simulation matches experiment.

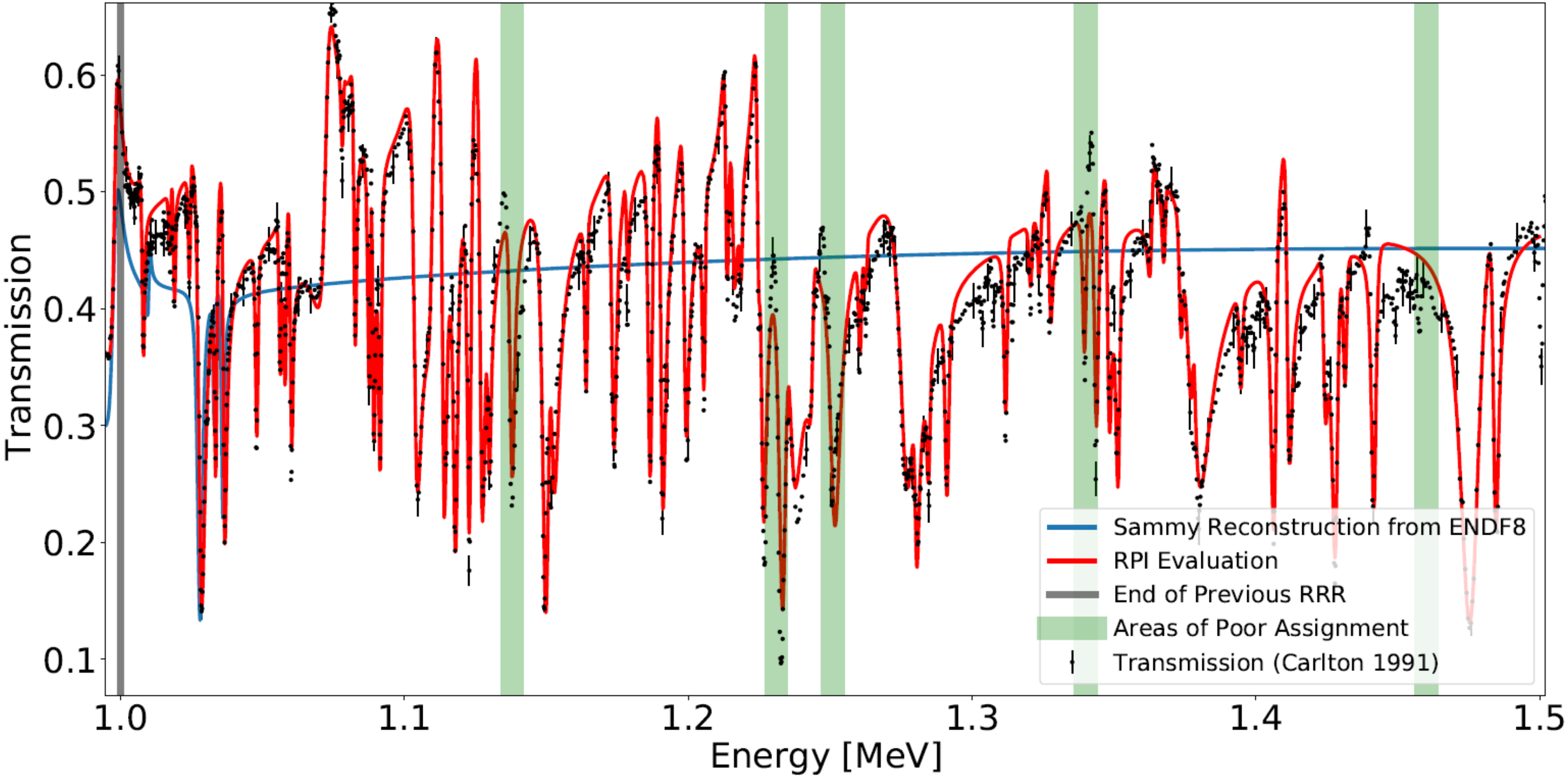
Evaluation uses of Quasi-Differential

- The upper limit of resolved resonance regions for Pb isotopes (Pb-206: 0.9 MeV, Pb-207: 0.475 MeV, Pb-208: 1 MeV)
- The total and capture cross sections are well known for isotopes in this region, so elastic (and inelastic) scattering distributions (ESAD) may be the issue
- Use Blatt-Biedenharn (BB) in NJOY[3] to recalculate ESAD (MF-4, MT-2) and then simulate pure isotopic samples in MCNP [4]

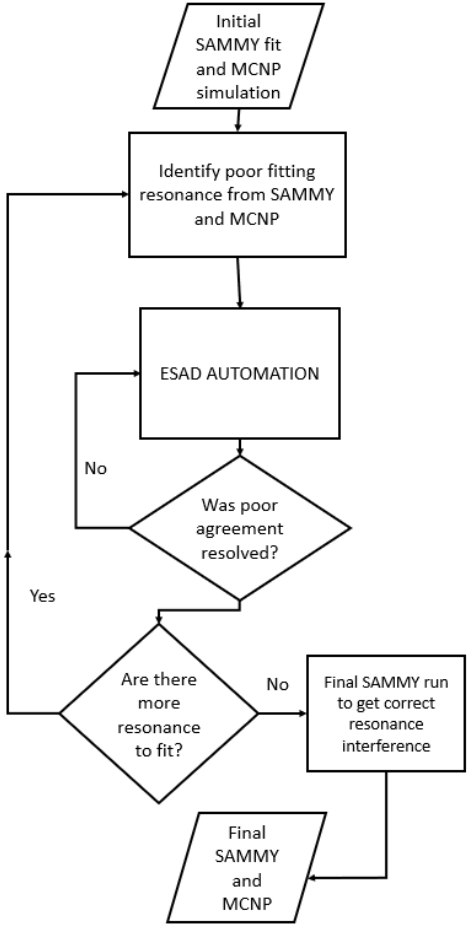

Energy [MeV]
20
10
5
2
1.5
1.25
1.12
1.0
0.82
0.7
0.6
0.51
Sample = Lead
Detector = 1
Angle = 150 deg
Pb Data Week4
RPI Evaluation (sum)
ENDF/B-8 204 with BB
ENDF/B-8 206 with BB
ENDF/B-8 207 with BB
RPI Pb-208
Most non-smooth scattering signal is coming from the Pb-208 isotope.
Counts
30000
26250
22500
18750
15000
11250
7500
3750
0
500
1000
1500
2000
2200
2400
2700
3100
Time of Flight [ns]

- The current upper limit of the RRR for Pb-208 is 1 MeV, based on a ORELA transmission by Carlton [5]
- The RRR was extended out to 1.5 MeV, but there are several areas in transmission that are spin insensitive

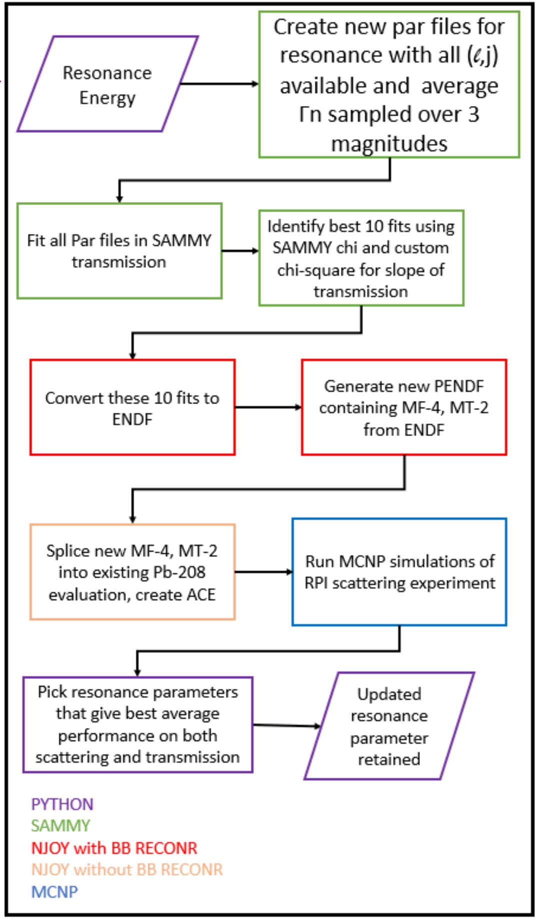
Pb-208 Transmission



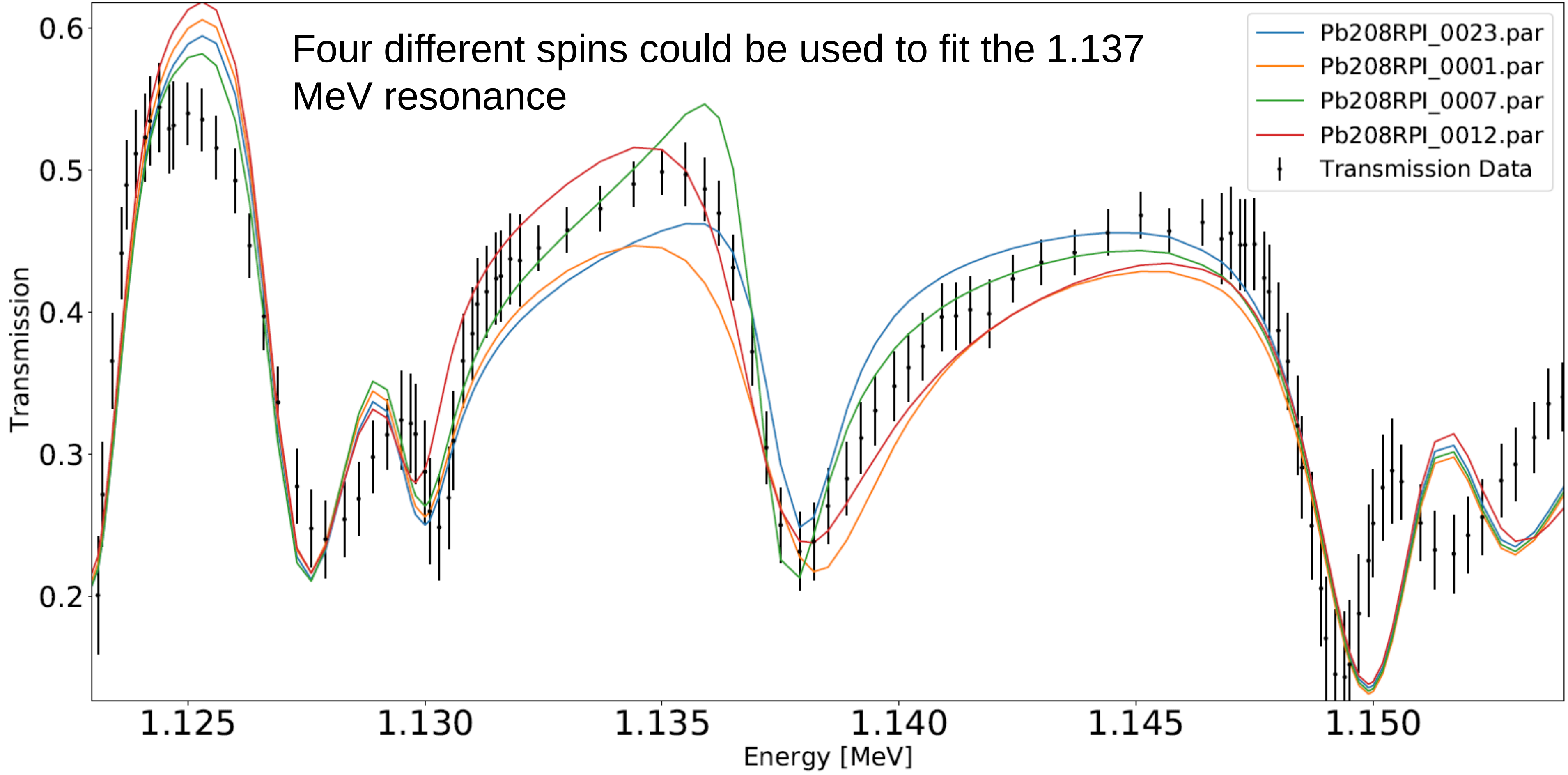
- Even though transmission is spin insensitive, the scattering data will be spin sensitive
- ESAD Methodology developed to sample the most probable spin assignments based on empirical fits (transmission)

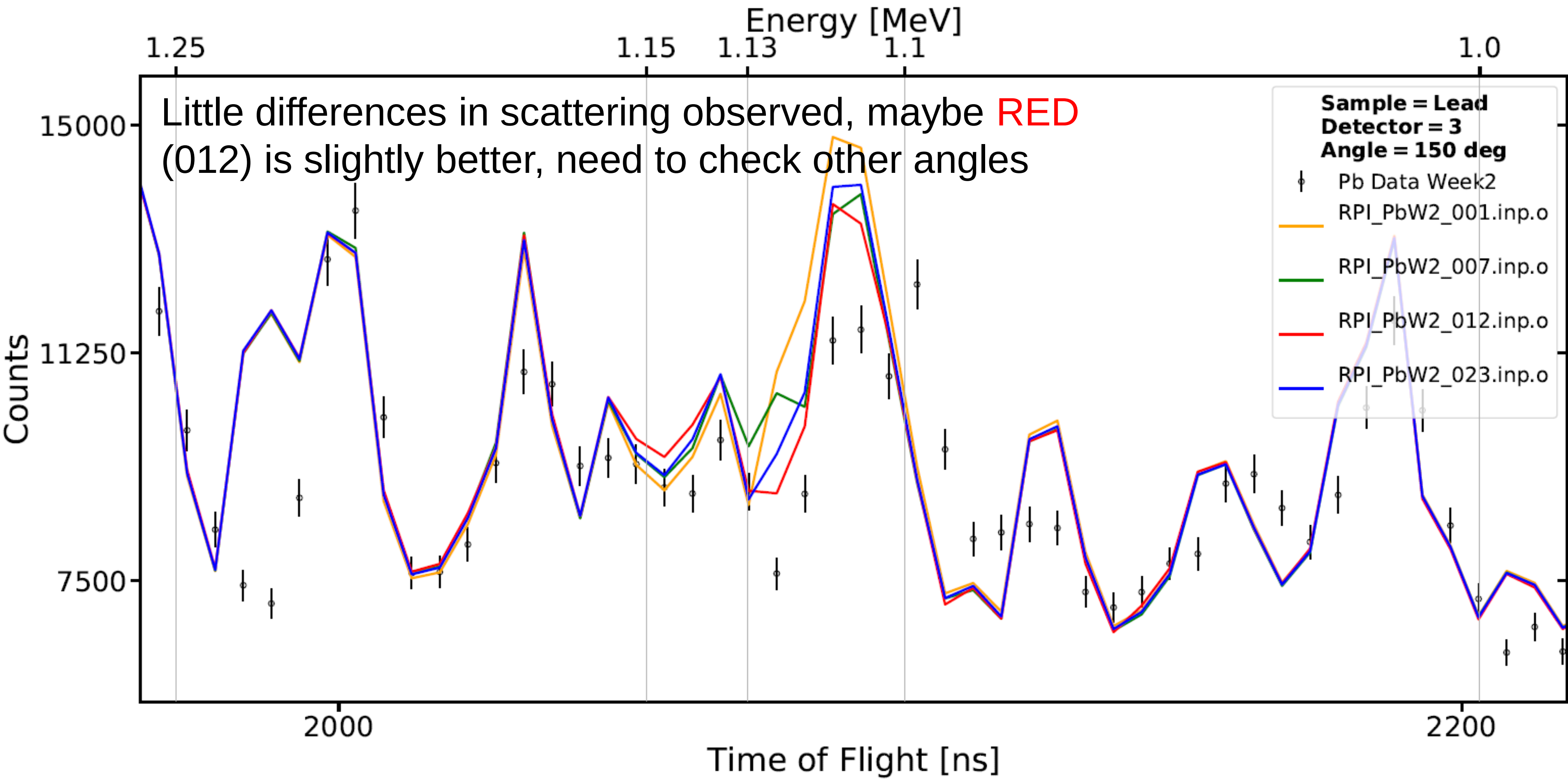


ESAD AUTOMATION

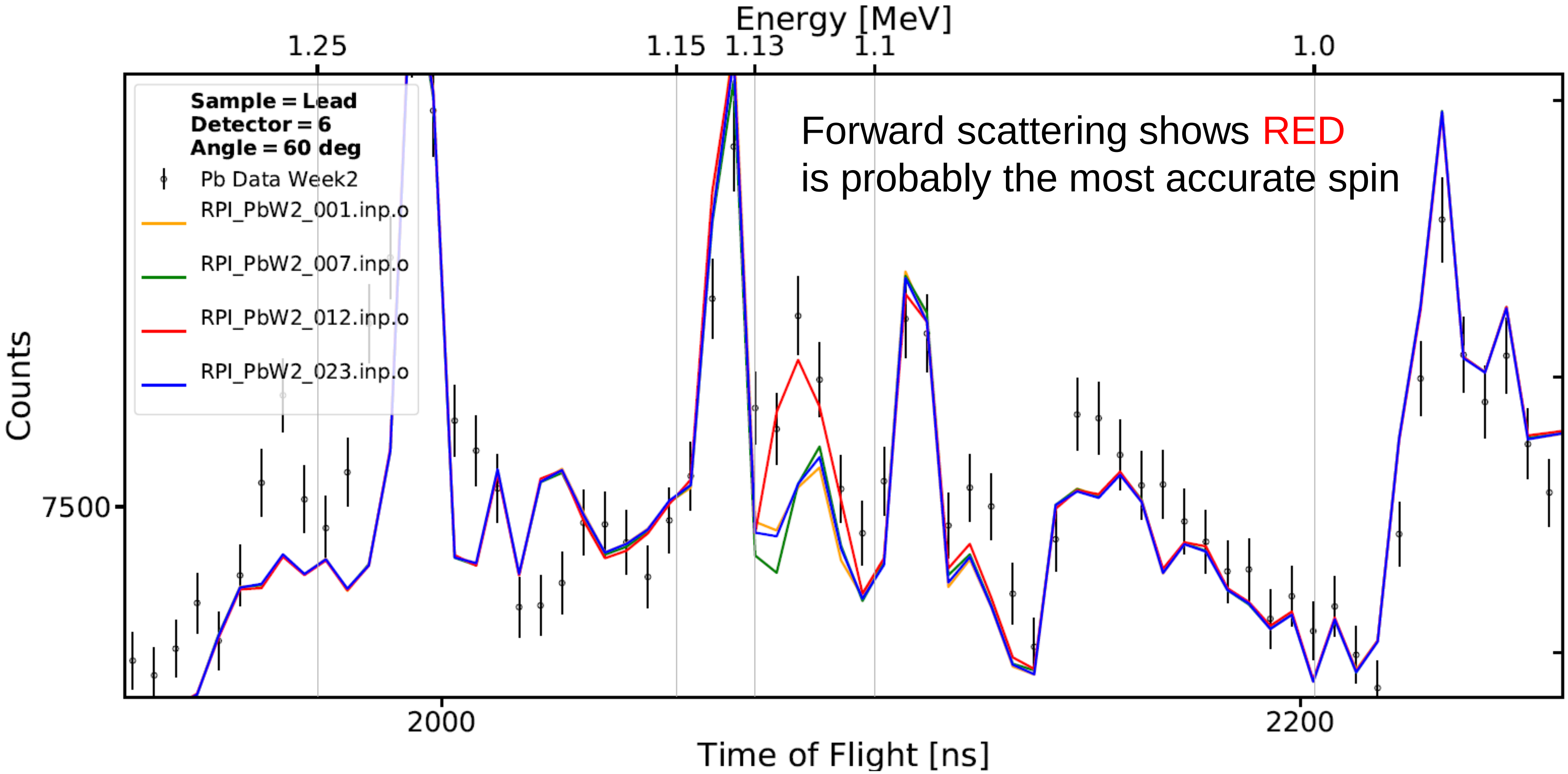


Four different spins could be used to fit the 1.137 MeV resonance

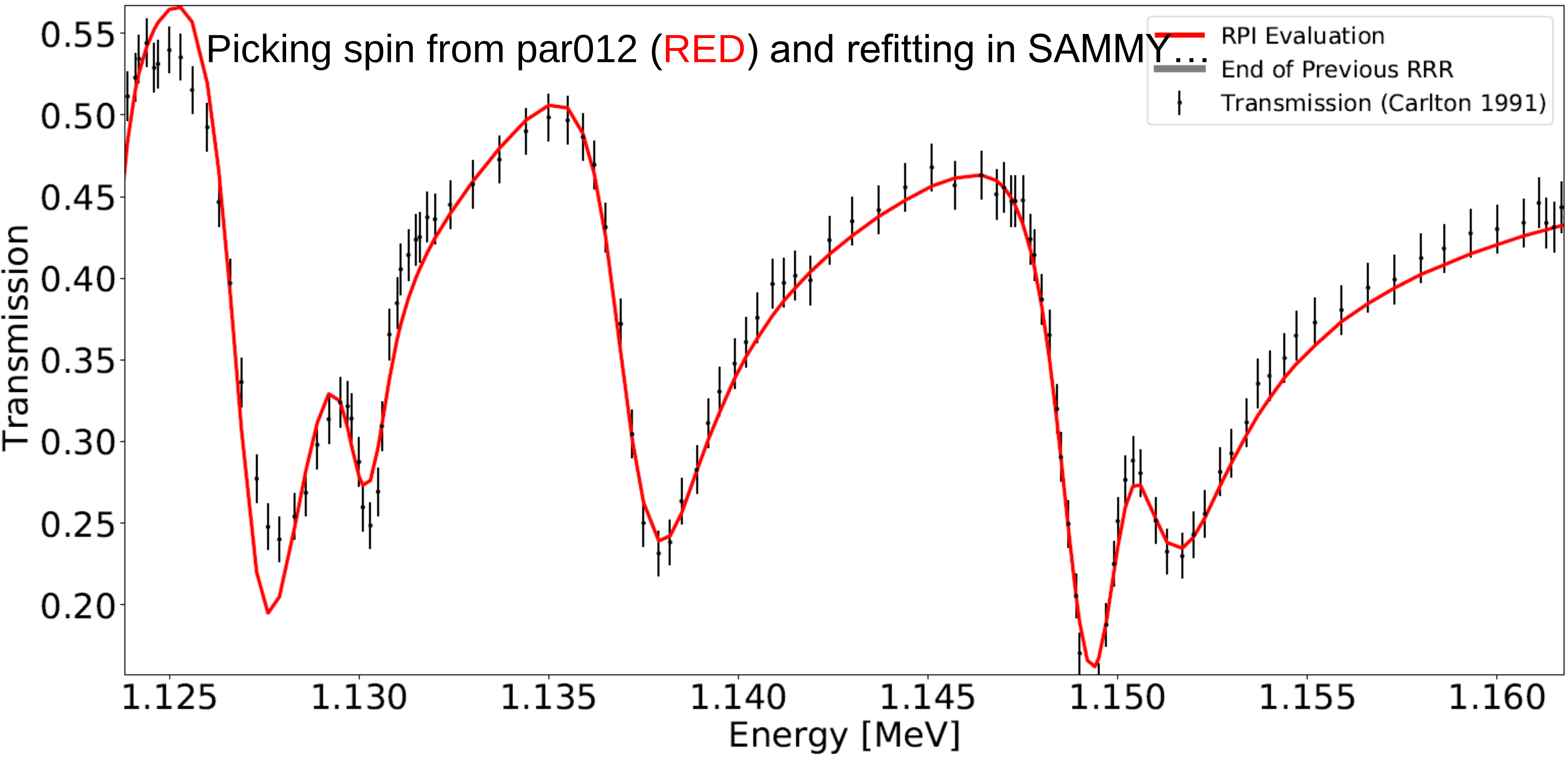




Little differences in scattering observed, maybe RED (012) is slightly better, need to check other angles



Forward scattering shows RED
is probably the most accurate spin


Picking spin from par012 (RED) and refitting in SAMMY…
RPI Evaluation
End of Previous RRR
Transmission (Carlton 1991)
Transmission
0.55
0.50
0.45
0.40
0.35
0.30
0.25
0.20
1.125
1.130
1.135
1.140
1.145
1.150
1.155
1.160
Energy [MeV]

- Useful in determining individual isotopic contributions to natural Pb scattering, determining problematic isotopes for evaluation
- Quasi-differential scattering can be used to assign resonance spins
  - Transmission data, elastic dominance, isotope separation

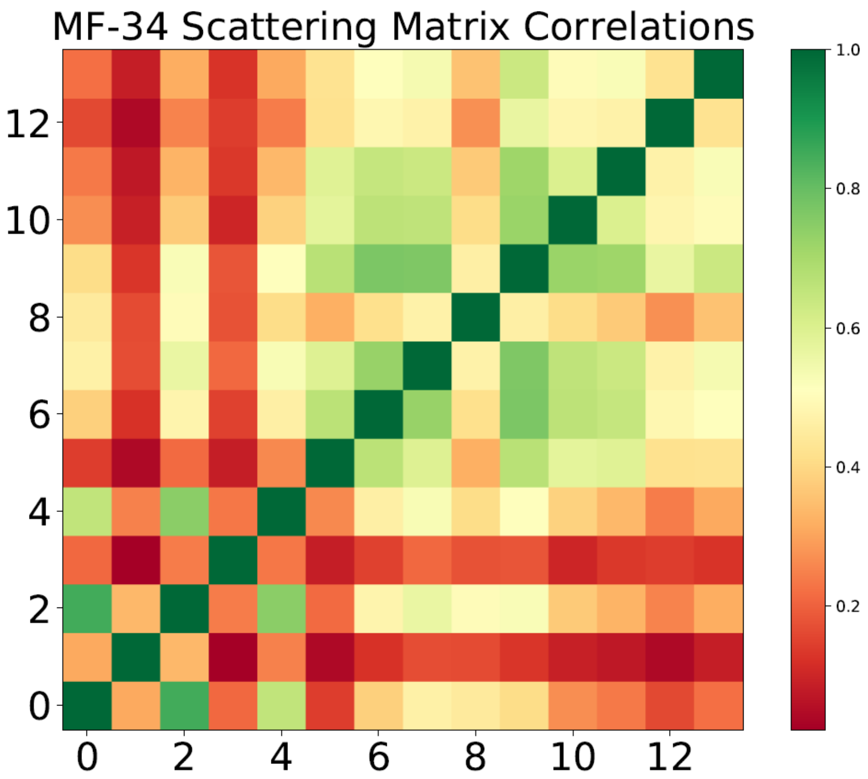
Covariance uses of Quasi-Differential

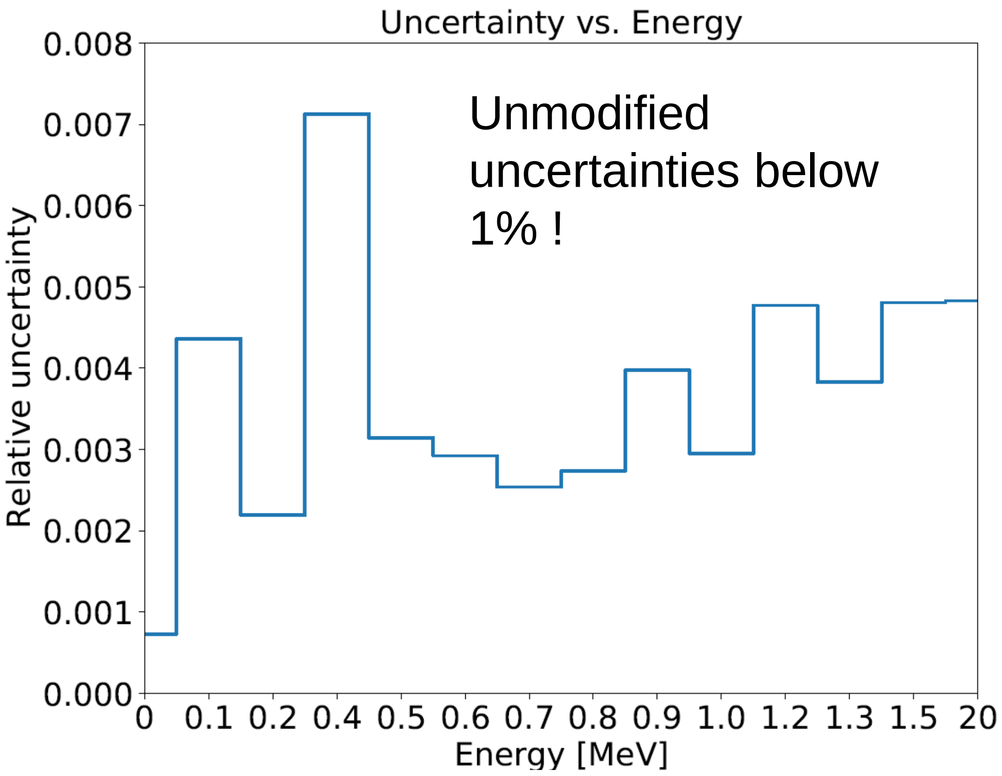
- V. Sobes on ENDF/B-8 covariance: "… [covariance] in the ENDF/B libraries is not an estimation of a physical quantity. It is rather a statement of the belief or a confidence in the estimated mean value." [6]
- The final use of quasi-differential scattering data is determining the magnitude of the covariance for scattering distributions MF-34

Covariance uses of Quasi-Differential

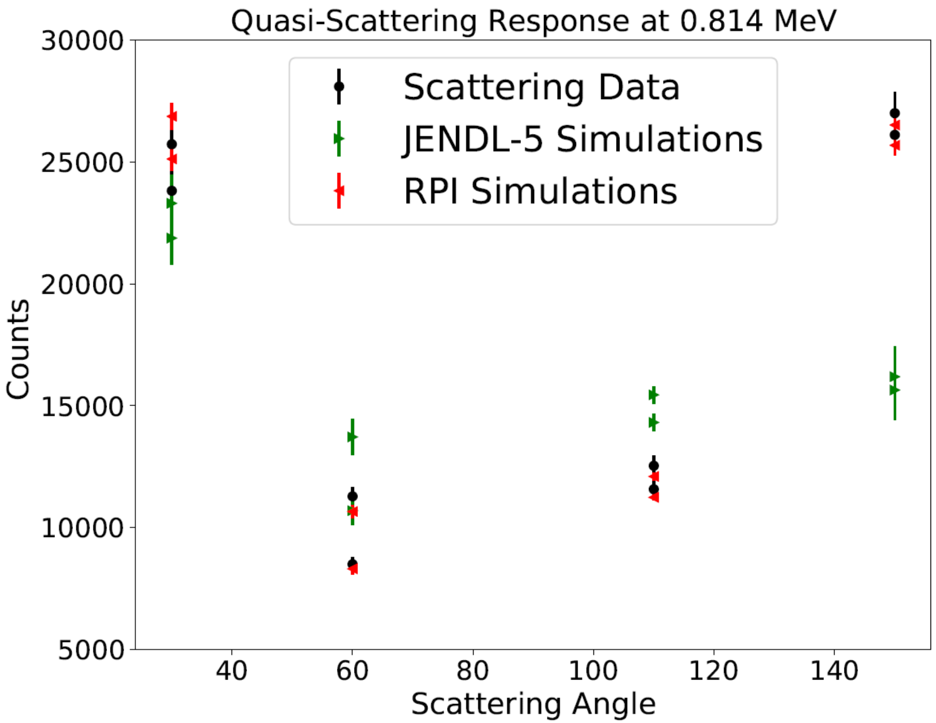
- Use Monte Carlo (MC) approach to generate new MF-2 resonance parameters using MF-32 uncertainties and generating new MF-4 using SAMMY [7]
- Run 100s of synthetic MF-2 through Blatt-Biedenharn to get a spread of $a_1(E)$ coefficients (can track others but not supported in NJOY)
- Calculate and format covariance matrix in Python code
- Any energy higher than the RRR limit gets the uncertainty from the last bin within the RRR, this means a constant uncertainty on a_1 past 1.5 MeV

Covariance uses of Quasi-Differential



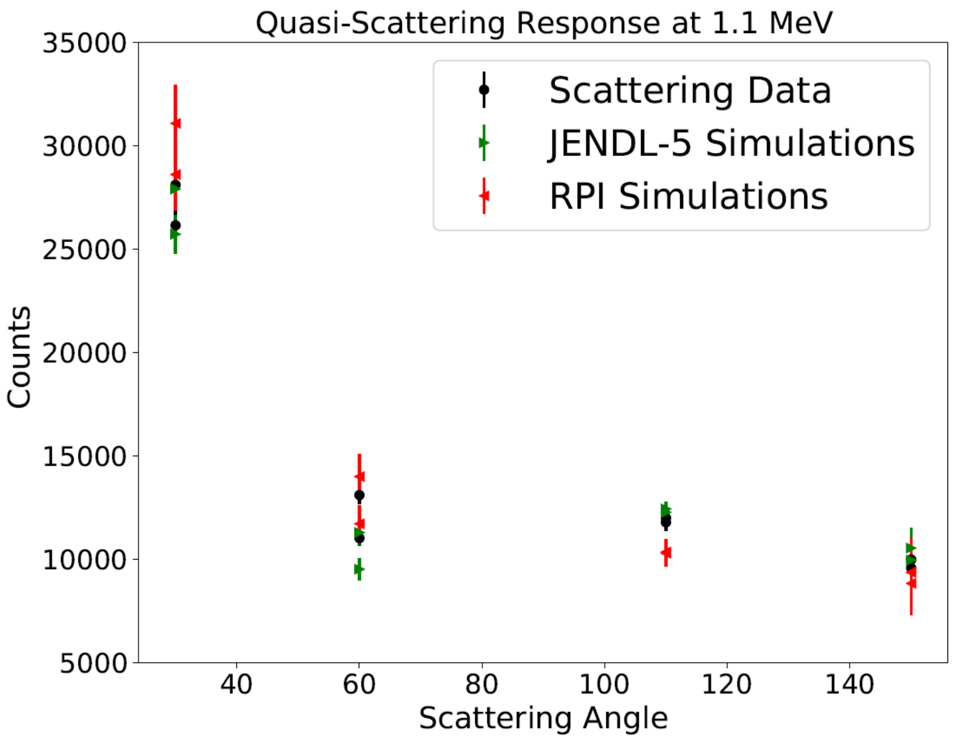


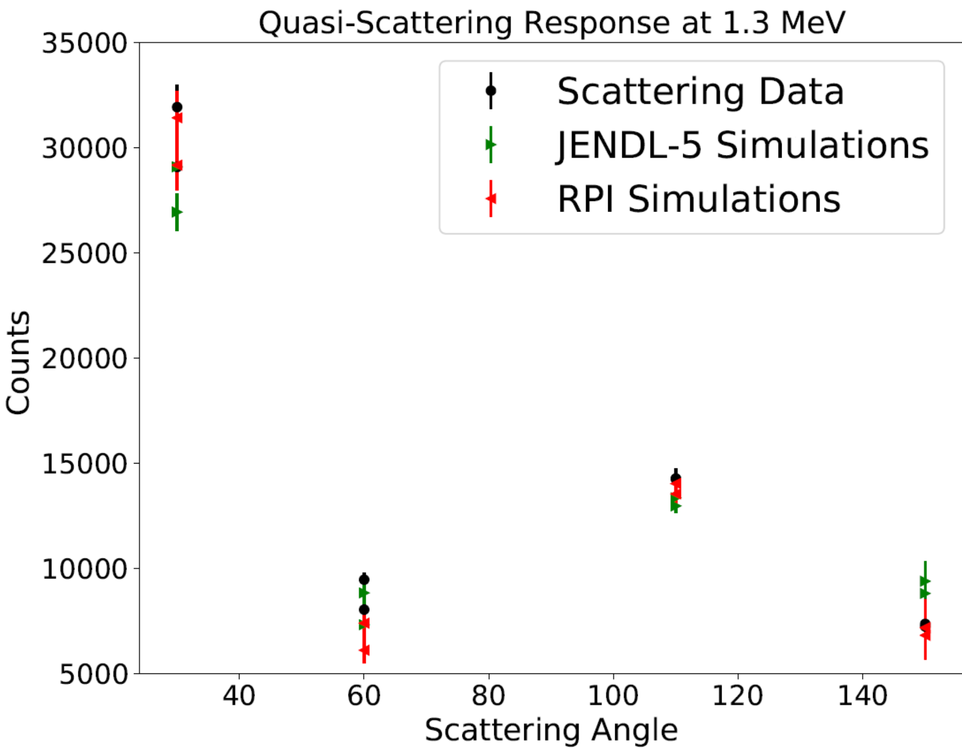
- Want to find the uncertainty on P1 which give us 5% uncertainty on experimental counts
- Manually perturbed P1 by 20-30% for RPI and JENDL-5
- 24% P1 uncertainty on Pb-208 gives back 5% experimental uncertainty at 814 keV



Covariance uses of Quasi-Differential

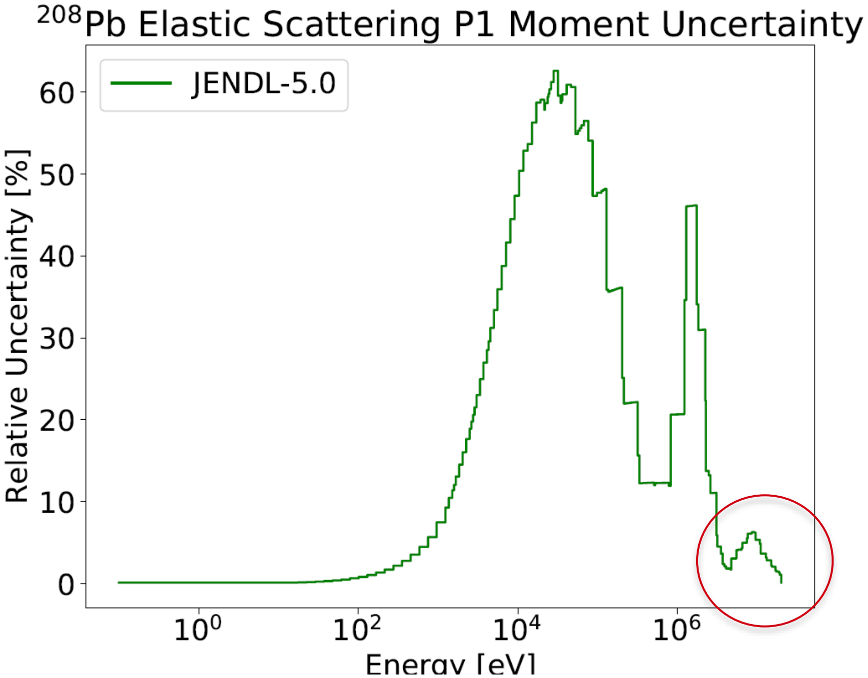
Different angles/energies are more/less sensitive to this type of analysis



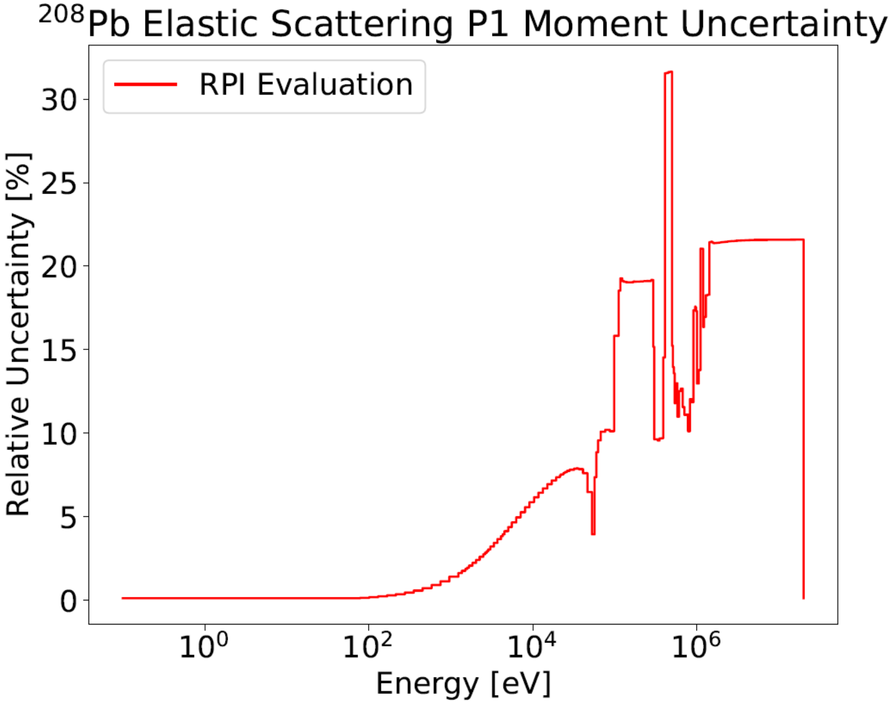


Covariance uses of Quasi-Differential

JENDL-5.0



RPI Evaluation

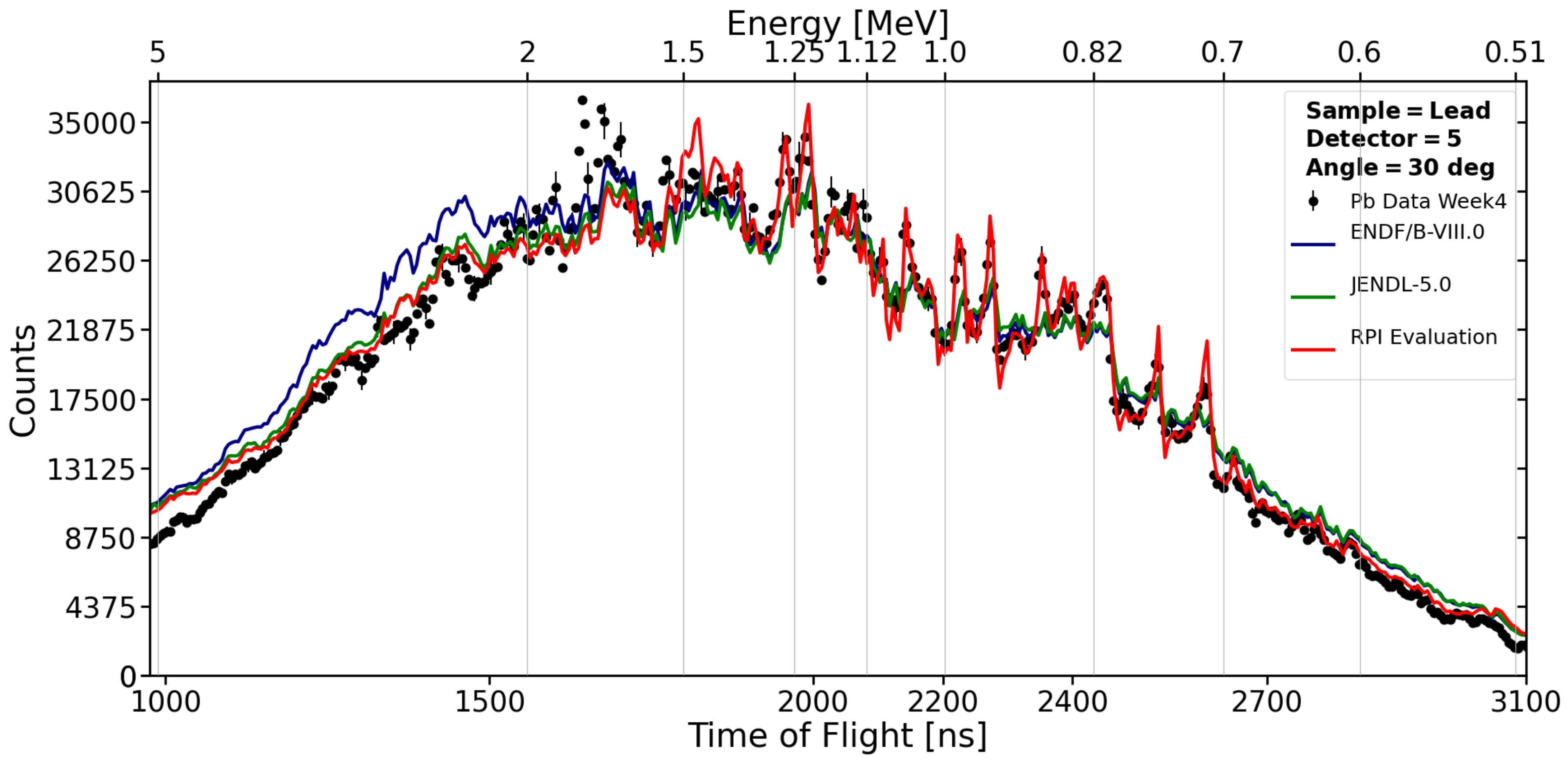


JENDL-5.0 reporting scattering distribution uncertainties with similar magnitude to total cross sections after 2 MeV

Covariance uses of Quasi-Differential

- Uncertainties between 10-30% on Pb-208 ESAD result in 5+% scattering uncertainties → upper bounds for unc.
- The choice to keep the last bin uncertainty (>1.5 MeV) equal to the previous bin (1.3 – 1.5 MeV) is deliberate as there is no basis for saying the scattering kernel is better known at higher energies
- The low uncertainties in JENDL library are a result of the KALMAN filtering from both cross sections and distributions
- However, the applicability of the OMP in Pb-208 below 2 MeV is poor and uncertainties above 2 MeV are small, covariances are then suspect

- After all the evaluation work of changing the elastic and inelastic channels can any difference be observed?


Energy [MeV]
5
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0.7
0.6
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Sample = Lead
Detector = 5
Angle = 30 deg
Pb Data Week4
ENDF/B-VIII.0
JENDL-5.0
RPI Evaluation
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17500
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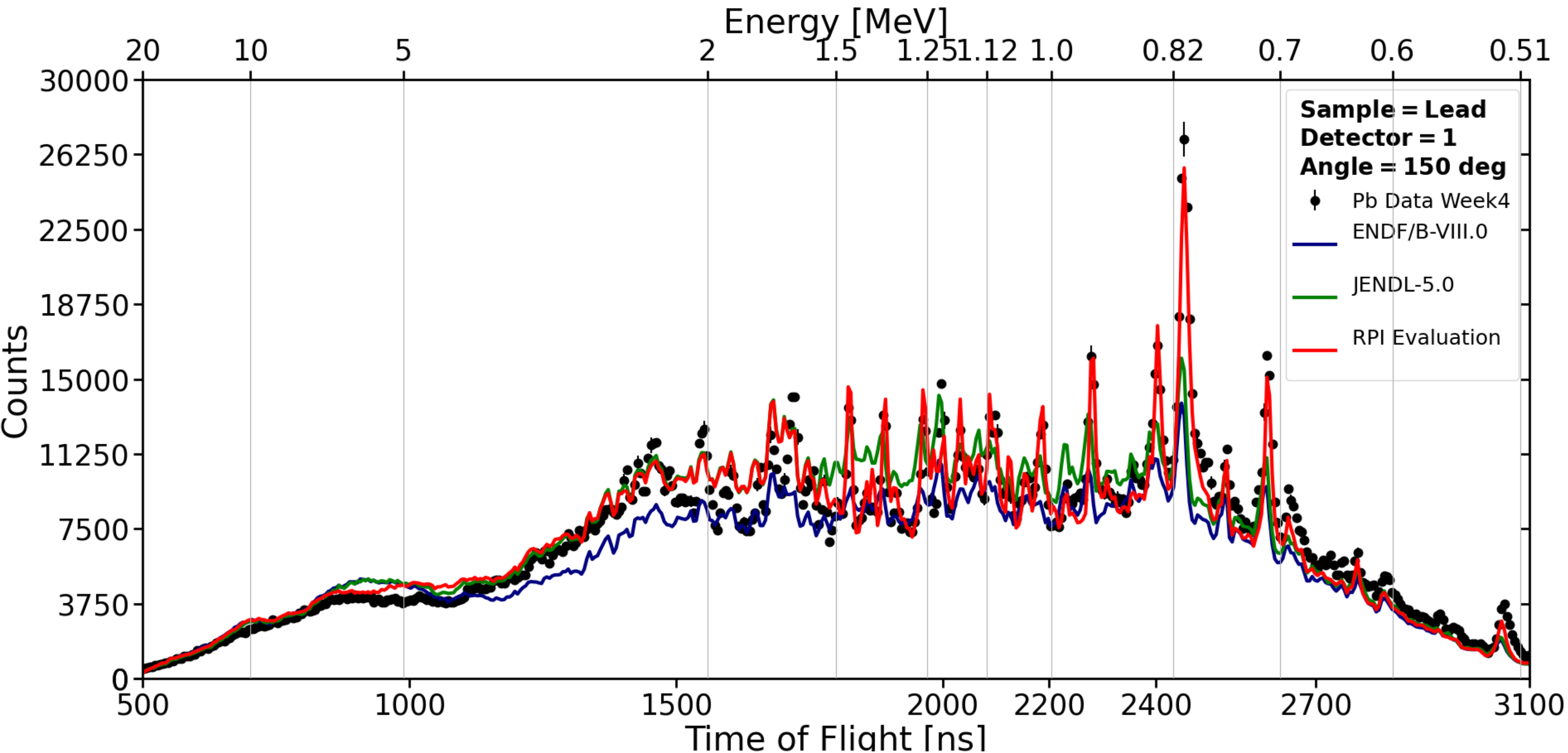
2700
3100
Time of Flight [ns]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22500
18750
15000
11250
7500
3750
0
Counts
500
1000
1500
2000
2200
2400
2700
3100
Time of Flight [ns]
Sample = Lead
Detector = 1
Angle = 150 deg
Pb Data Week4
ENDF/B-VIII.0
JENDL-5.0
RPI Evaluation

Summary of Uses for Quasi-Differential Scattering Data

- Many evaluation strategies can utilize the quasi-differential data
  - Identifying deficient isotopes, picking and reinforcing spin assignments, ad-hoc adjustments to cross sections (see talk later)
- Quasi-differential scattering data can be used to scale and understand the covariances derived for secondary neutron distributions (MF-34)
- MCNP simulations of quasi-differential measurements are ideal candidates for validation, even preferable over critical experiments for reflector materials with low number of integral experiments

References

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7. N. M. Larson, “Updated User’s Guide for SAMMY: Multilevel R-Matrix Fits to Neutron Data Using Bayes Equations”, Oak Ridge National Laboratory, Oak Ridge, TN, 2008, ORNL/TM-9179/R8 ENDF-364/R2.

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