

Measurements and evaluation of structural materials at RPI

Y. Danon¹, Devin Barry²
Greg Siemers¹, Alec Golas¹, Ian Parker¹, Katelyn Keparutis¹

¹Department of Mechanical, Aerospace and Nuclear Engineering
Rensselaer Polytechnic Institute
NES 1-9, 110 8th St., Troy, NY 12180-3590, USA

²*Naval Nuclear Laboratory, Schenectady, NY 12301, USA*

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Recent relevant work

- $^{90,91}\text{Zr}$ evaluation (Greg Siemers and Alec Golas)
 - New evaluation in progress for ^{90}Zr
 - Preliminary measurement of $^{\text{nat}}\text{Zr}$ thermal capture.
- Adding URR to Fe-56 ??
- Neutron capture gamma cascade spectra validation (Katelyn Keparutis, Ian Parker)

$^{90,91}\text{Zr}$ Overview

Motivation for Stable Zirconium Isotope Evaluation

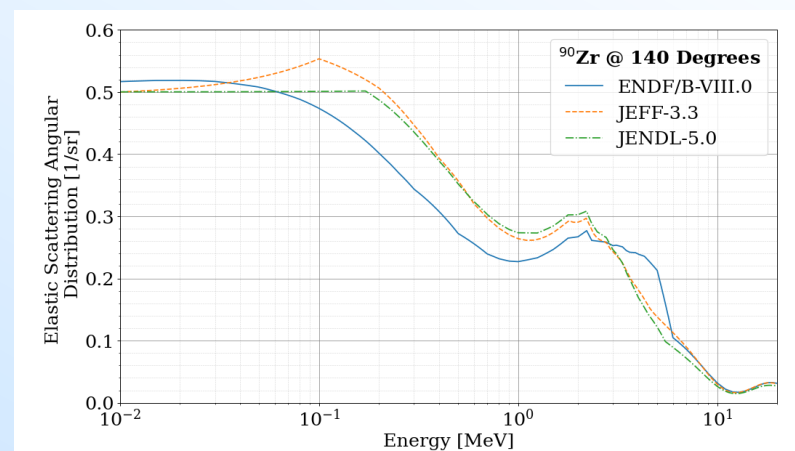
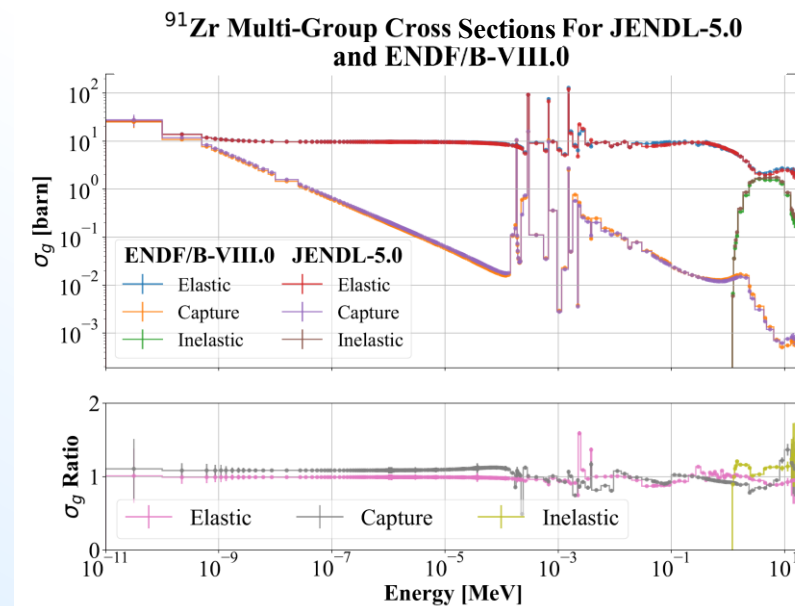
Zirconium is a ubiquitously used material in the nuclear industry, mainly as cladding for Uranium fuel rods. Zirconium hydride is also being developed as an advanced moderator. Evaluated zirconium nuclear data can be substantially improved.

Resolved Resonance Region

1. Resonances misassigned w.r.t transmission data
2. Large differences of thermal cross section between libraries
3. Previous evaluations do not use R-Matrix formalism
4. No/limited covariance

High Energy Region

1. Updated version of EMPIRE/OPTMAN which includes more modeling capabilities
2. Soft-rotor optical potential in RIPL 609 developed for Zr
3. Elastic scattering angular distributions of utmost importance



New Zirconium Evaluations for ENDF/B-IX

RRR: New evaluations will use R-Matrix resonance parameterization, replacing the current MLBW evaluations. Evaluations will incorporate new ORNL isotopic transmission and capture measurements.

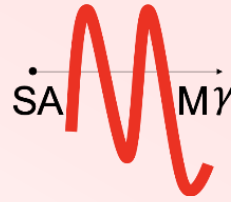
URR: New evaluations will leverage a new version of SAMMY which includes several new URR fitting capabilities.

Fast: New evaluations with modern version of EMPIRE using new soft-rotor OMP developed for Zr. Evaluations will leverage new ^{nat}Zr transmission from RPI, DT validation data from China, and others.

Isotope	New Measurement Status	Final Data Reduction	RRR Evaluation	Completion	URR Evaluation	Completion	Fast Evaluation	Completion
Zr-90	Complete	Completed (March 2024)	RPI –>NNL - ORNL	Q4 2025	RPI –>NNL - ORNL	Q4 2025	RPI –BNL	Q1 2026
Zr-91	Complete	Near Complete (May 2025)	RPI –>NNL - ORNL	Q4 2025	RPI –>NNL - ORNL	Q4 2025	RPI –BNL	Q1 2026
Zr-92	In Progress	2026	ORNL	TBD	NNL - ORNL	TBD	BNL - RPI	TBD
Zr-94	2025/2026	2026	ORNL	TBD	NNL - ORNL	TBD	BNL - RPI	TBD
Zr-96	N/A	N/A	ORNL	TBD	NNL - ORNL	TBD	BNL - RPI	TBD

$^{90,91}\text{Zr}$ Evaluation RRR

Resolved Resonance Region Evaluations



$^{90}\text{Zirconium}$

Datasets fit in the new evaluation:

- **Transmission:**

1. de L. Musgrove, et al. 1977^[1] - 0.08645 at/b metallic enriched ^{90}Zr @ 80m (^6Li)
 - Fit: 3 keV – 500 keV
2. de L. Musgrove, et al. 1977^[1] - 0.08645 at/b metallic enriched ^{90}Zr @ 200m (NE110)
 - Fit: 100 keV – 800 keV

- **Radiative Capture:**

1. ORNL/JRC-Geel 2021^[2] - 0.00558 at/b metallic enriched ^{90}Zr @ 58m (C_6D_6)
 - Fit: 3 keV – 94 keV
2. Tagliente, et al. 2008^[3] (nTOF) - 0.01308 at/b enriched $^{90}\text{ZrO}_2$ @ 185m (C_6D_6)
 - Fit: 94 keV – 500 keV

- Channel radius of 6.31 fm adopted from Fröhner recommendation^[4]
 - Large s-wave distant levels used to represent R_∞ contribution
 - New evaluation adopted the LRF-7 format

$^{91}\text{Zirconium}$

Datasets fit in the new evaluation:

- **Transmission:**

1. de L. Musgrove, et al. 1977^[5] - 0.06423 at/b metallic enriched ^{91}Zr @ 80m (^6Li)
 - Fit: 1 eV – 300 keV
2. de L. Musgrove, et al. 1977^[5] - 0.06423 at/b metallic enriched ^{91}Zr @ 200m (NE110)
 - Fit: 75 keV – 300 keV
3. ORNL/JRC-Geel^[6] 2022 – 0.00445 at/b metallic enriched ^{91}Zr @ 48m (^6Li)
 - Fit: 1 eV – 10 keV

- **Radiative Capture:**

1. ORNL/JRC-Geel 2022^[7] – 0.00445 at/b metallic enriched ^{91}Zr @ 58m (C_6D_6)
 - Fit: 150 eV – 94 keV

- Channel radius of 6.33 fm adopted from Fröhner recommendation^[4] and effective scattering radius of 7.20 fm used to match experimental data
 - Large s-wave distant levels used to represent R_∞ contribution
 - New evaluation adopted the LRF-7 format

Notable Improvements to Zr Evaluations

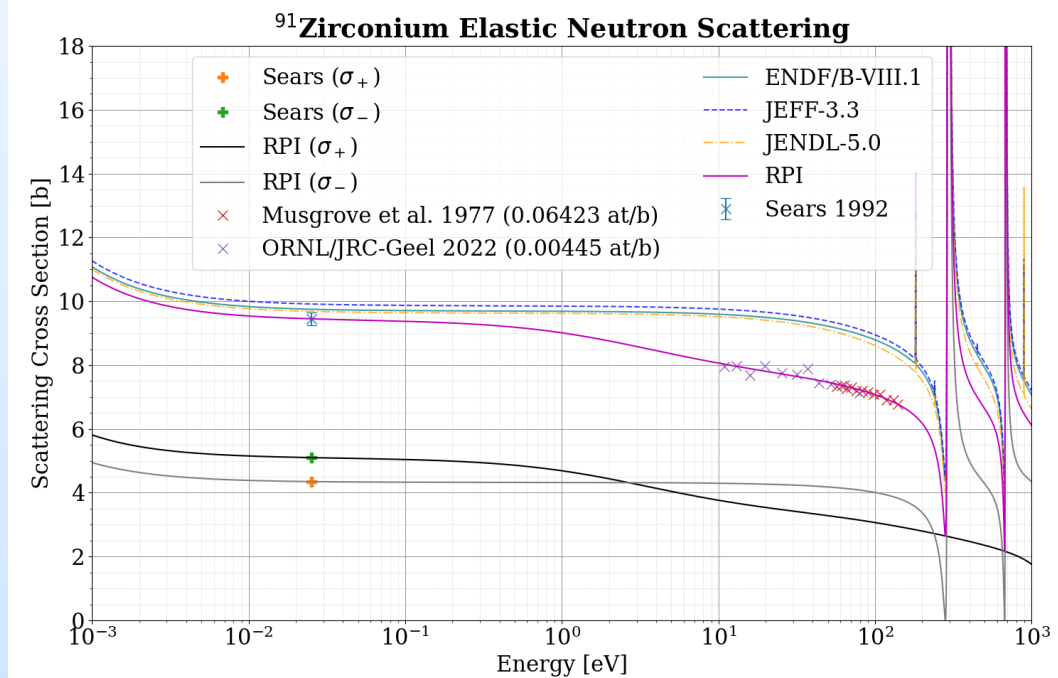
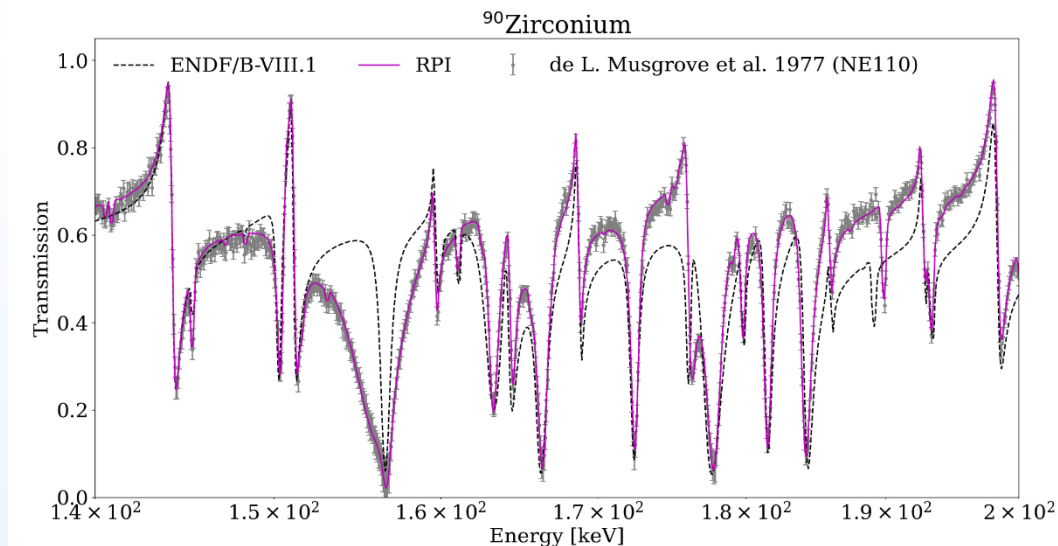
⁹⁰Zirconium

1. Removal of erroneous resonances and several width fixes between 100 keV and 200 keV
2. Extension of R-matrix resonance parameterization to 800 keV
3. Thermal scattering now consistent to experimental values (Sears 1992^[13])

⁹¹Zirconium

1. Total cross section below first resonance (~150 eV) now consistent with measurements^[11,12]
2. Extension of R-matrix resonance parameterization to ~300 keV (preliminary)
3. Scattering cross section distributed appropriately between s-wave spin groups^[14]
4. Thermal scattering and capture cross section now consistent with experimental data^[13,15,16]

End or RRR		
Isotope	ENDF-8.1	RPI
Zr-90	200 keV	800 keV
Zr-91	26 keV	195 keV



^{90}Zr Evaluation Parameters (293.6 K) (Preliminary)

Parameter	NIST	ATLAS-2018	ENDF/B-VIII.1	JENDL-5.0	JEFF-3.3	RPI ²
$*b_c$ [fm]	6.4 +/- 0.1	6.5 +/- 0.1	6.55	6.54	6.69	6.33
σ_s [b]	5.03 +/- 0.2**	5.3 +/- 0.16	5.30	5.29	5.53	5.21
S_0 (x 10^4)	-	0.61	0.57	0.64	0.71	0.57
S_1 (x 10^4)	-	4.79	2.81	2.97	2.90	5.17
S_2 (x 10^4)	-	-	1.20	0.25	-	2.06
σ_γ [mb]	11.0 +/- 5.0	14.0 +/- 6.0	10.25	10.93	9.98	10.67
I_γ [b]	-	0.13 +/- 0.03 ¹	0.16	0.16	0.17	0.16
Westcott (g)	-	1.004	1.000	0.999	1.000	0.999
MACS @ 30 keV [mb]	19.3 +/- 0.9 ³	19.3 +/- 0.9	18.69	19.25	20.10	17.70

¹Value reported at 0 K

²Preliminary

³Retrieved from KADoNiS/ASTRAL database

^{90}Zr ($I=0$) has no incoherent scattering component

**Converted to free scattering cross section

^{91}Zr Evaluation Parameters (293.6 K) (Preliminary)

Parameter	NIST	ATLAS-2018	ENDF/B-VIII.1	JENDL-5.0	JEFF-3.3	RPI ²
b_c [fm]	8.7 +/- 0.1	6.5 +/- 0.1	8.82	8.79	8.89	8.68
b_i [fm]	-1.08 +/- 0.15	-	-1.03	-1.04	-1.06	-1.08
σ_s [b]	9.45* +/- 0.2	9.82 +/- 0.23	9.75	9.69	9.92	9.45
S_0 (x 10 ⁴)	-	0.55 +/- 0.15	0.42	0.45	0.52	0.40
S_1 (x 10 ⁴)	-	7.04 +/- 1.00	4.88	0.27	4.98	4.79
σ_γ [b]	1.17 +/- 0.1	1.30 +/- 0.15	1.21	1.31	1.22	1.30
I_γ [b]	-	8.30 +/- 0.83 ¹	5.83	5.75	6.05	6.21
Westcott (g)	-	1.004	1.000	1.000	0.999	0.999
MACS @ 30 keV [mb]	62.0 +/- 3.4 ³	63.0 +/- 4.0	66.1	63.4	76.1	72.4

¹Value reported at 0 K

²Preliminary (v1.3.2)

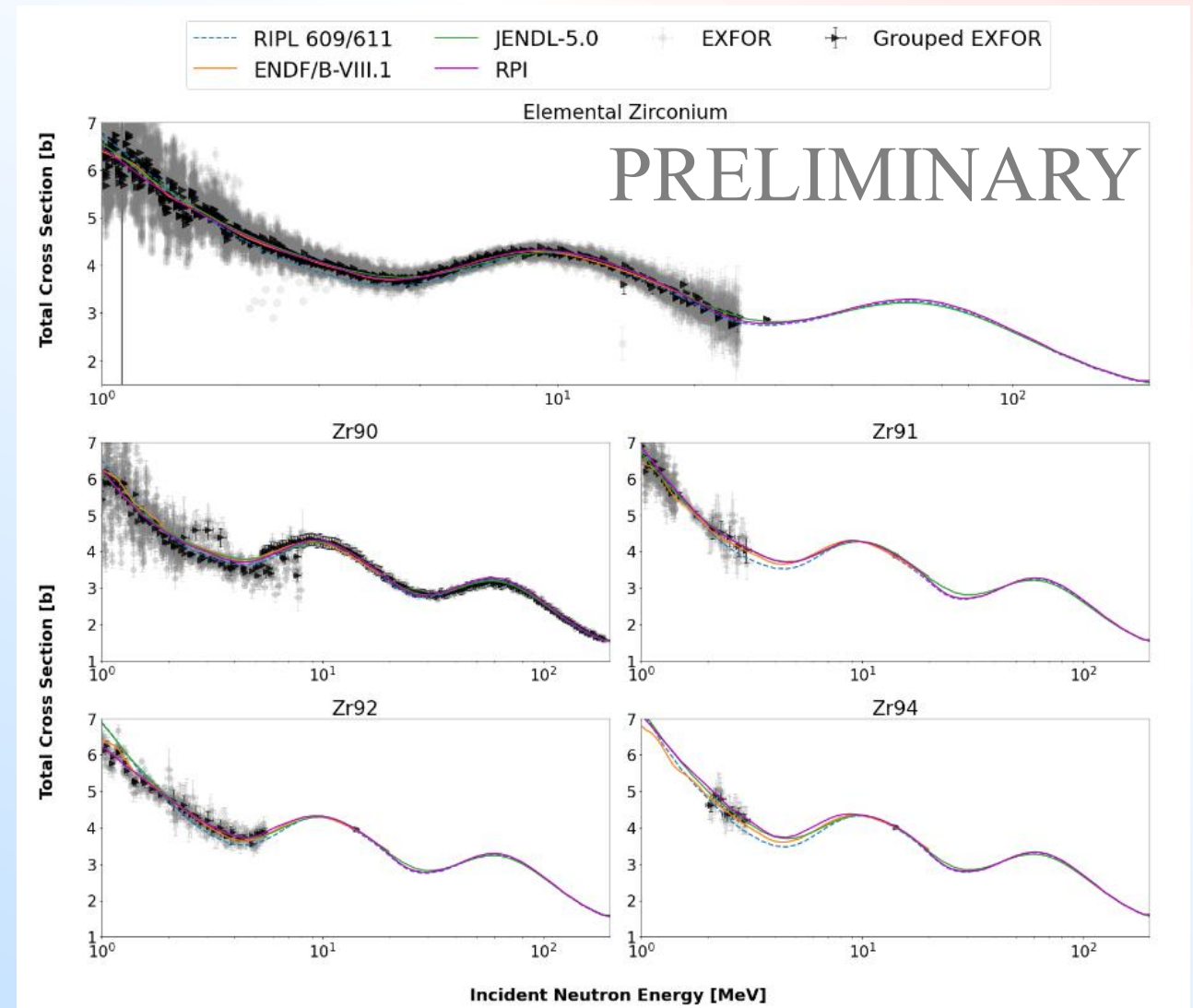
³Retrieved from ASTRAL/KADoNiS database

*Converted from bound to free scattering cross section

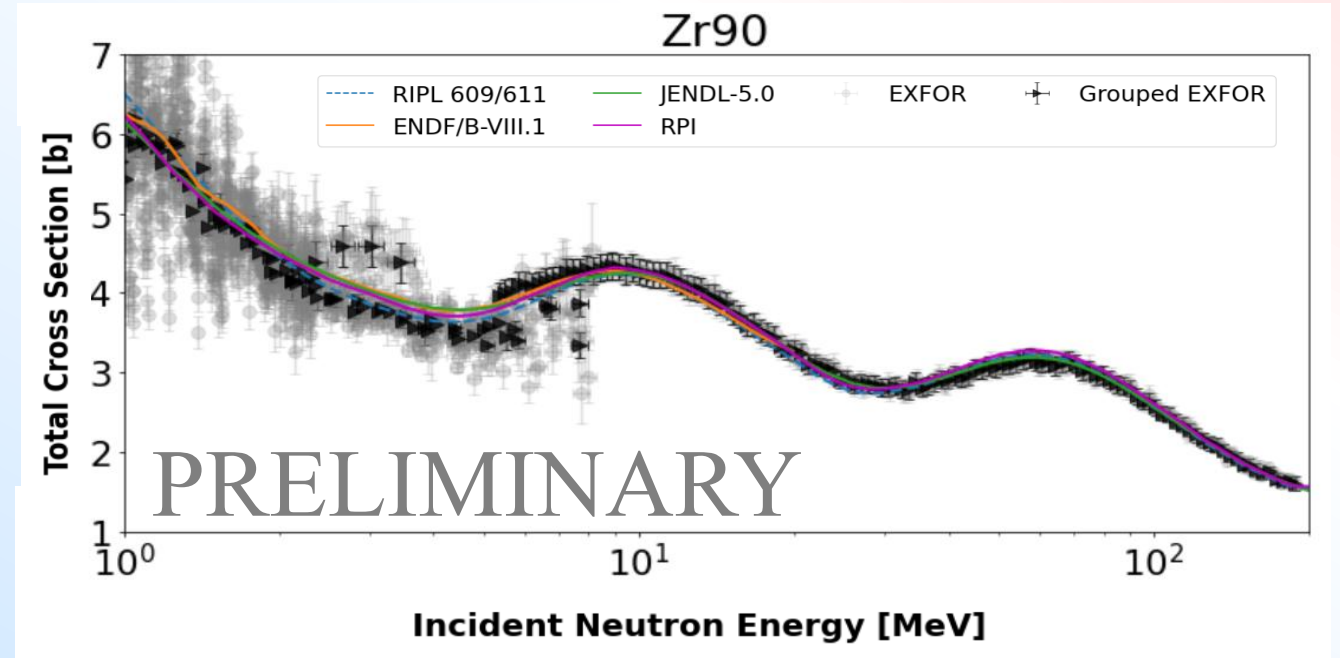
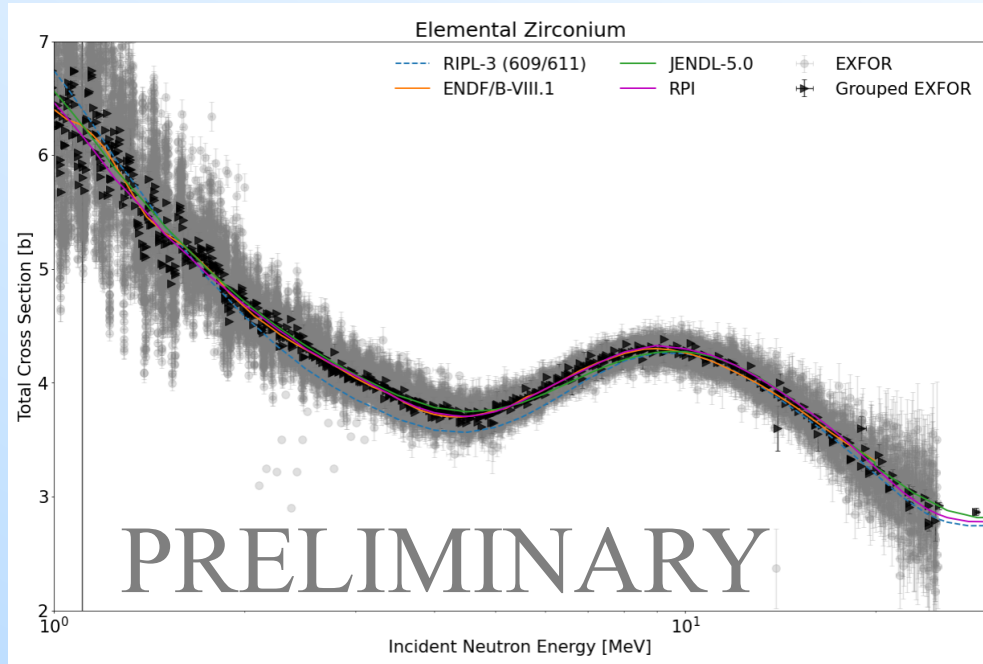
$^{90,91}\text{Zr}$ Evaluation Fast

Fitting Zr Optical Model Parameters

- EMPIRE – KALMAN utilized to tweak RIPL initial OMPs <1% for $^{90,91,92,94}\text{Zr}$ isotopes
- Model brought within uncertainty to 14.1 MeV total cross section measurements from Dyumin, et al. (1977)
- At lower energies (< 5 MeV) manual total cross section tweaks performed using TOTRED (energy-dependent scaling) to best match experimental data



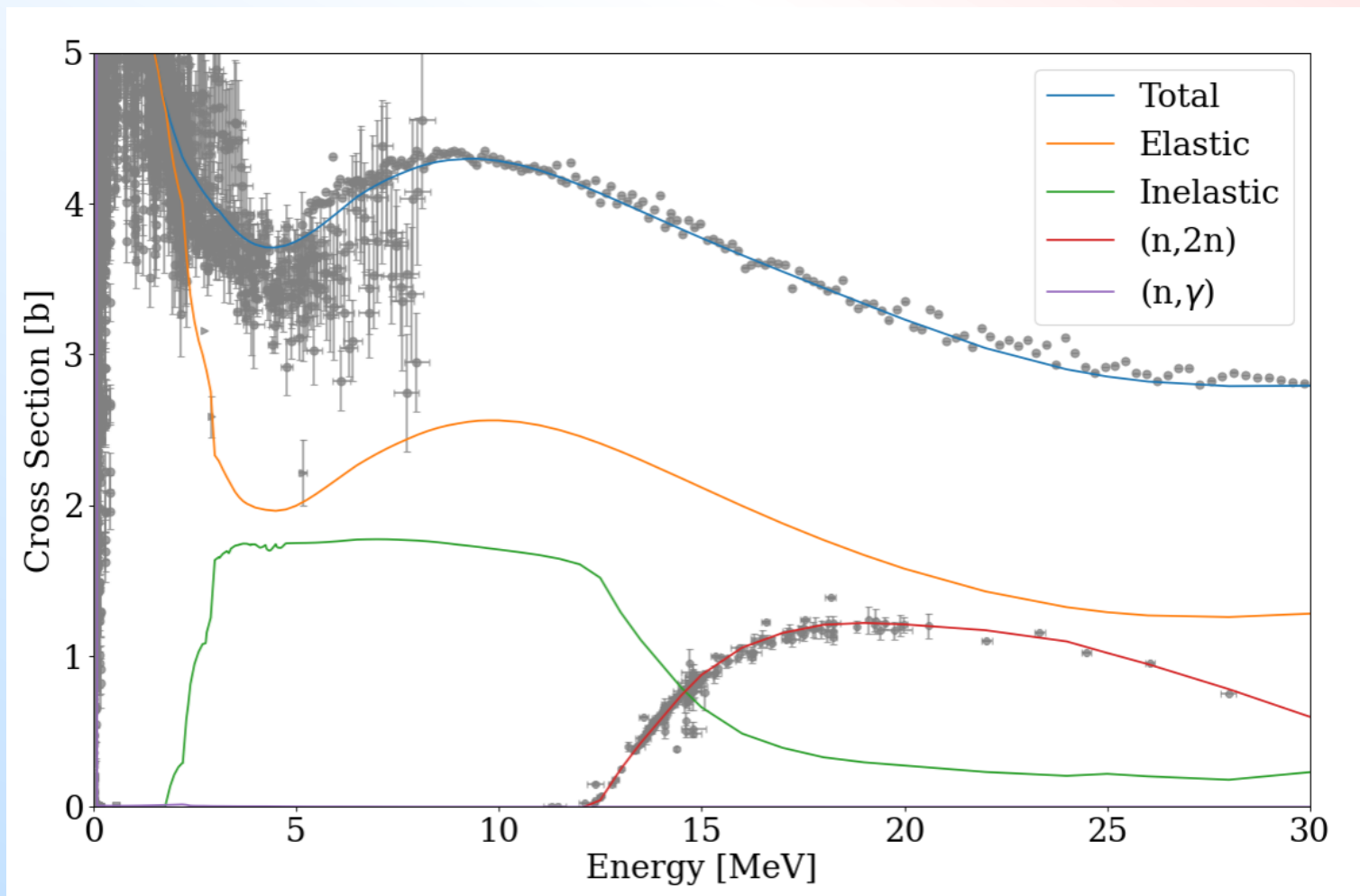
Total cross section



- ^{90}Zr total cross section was increased between 2 MeV and 5 MeV to ensure agreement to elemental Zr data.
- A discontinuity in the isotopic ^{90}Zr total cross section data is also apparent around 6 MeV between the Guenther and Green experiments and the Finlay measurement.
- A new transmission measurement of enriched ^{90}Zr from 1 MeV to at least 10 MeV is needed resolve these discrepancies.

^{90}Zr Fast Evaluation Overview

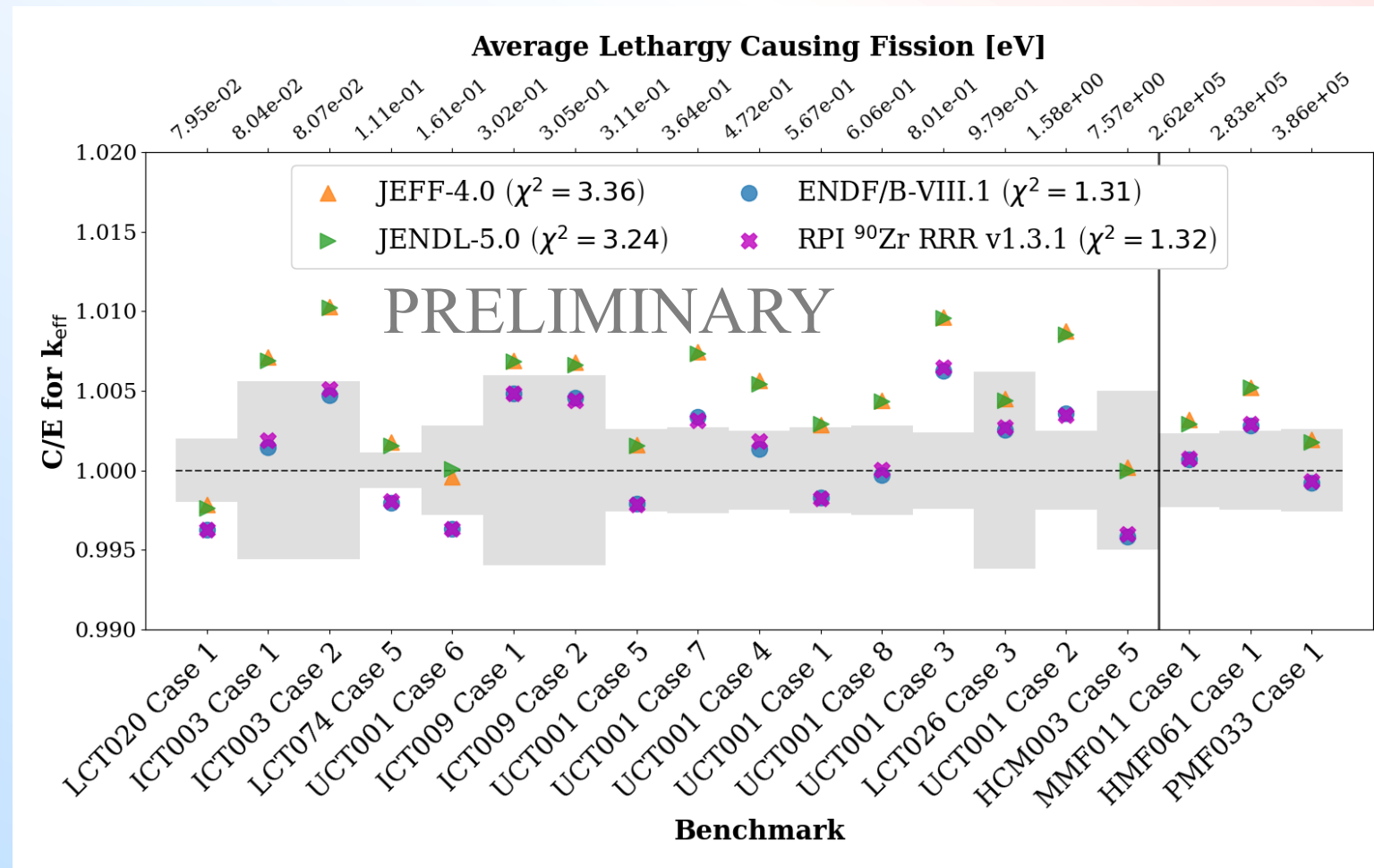
- EMPIRE^[11] – 3.2 (Malta) to be used for the $^{90,91}\text{Zr}$ fast neutron evaluations
- Good amount of experimental data available for ^{90}Zr
 - Disagreement found between ^{90}Zr and $^{\text{nat}}\text{Zr}$ total cross section data which is unresolvable with the minor isotopes alone
 - Lots of (n,2n) data since $^{90}\text{Zr}(\text{n},2\text{n})$ is heavily used in dosimetry (IRDFF)
 - Inelastic data only available for individual levels



$^{90,91}\text{Zr}$ Some integral testing of RRR only

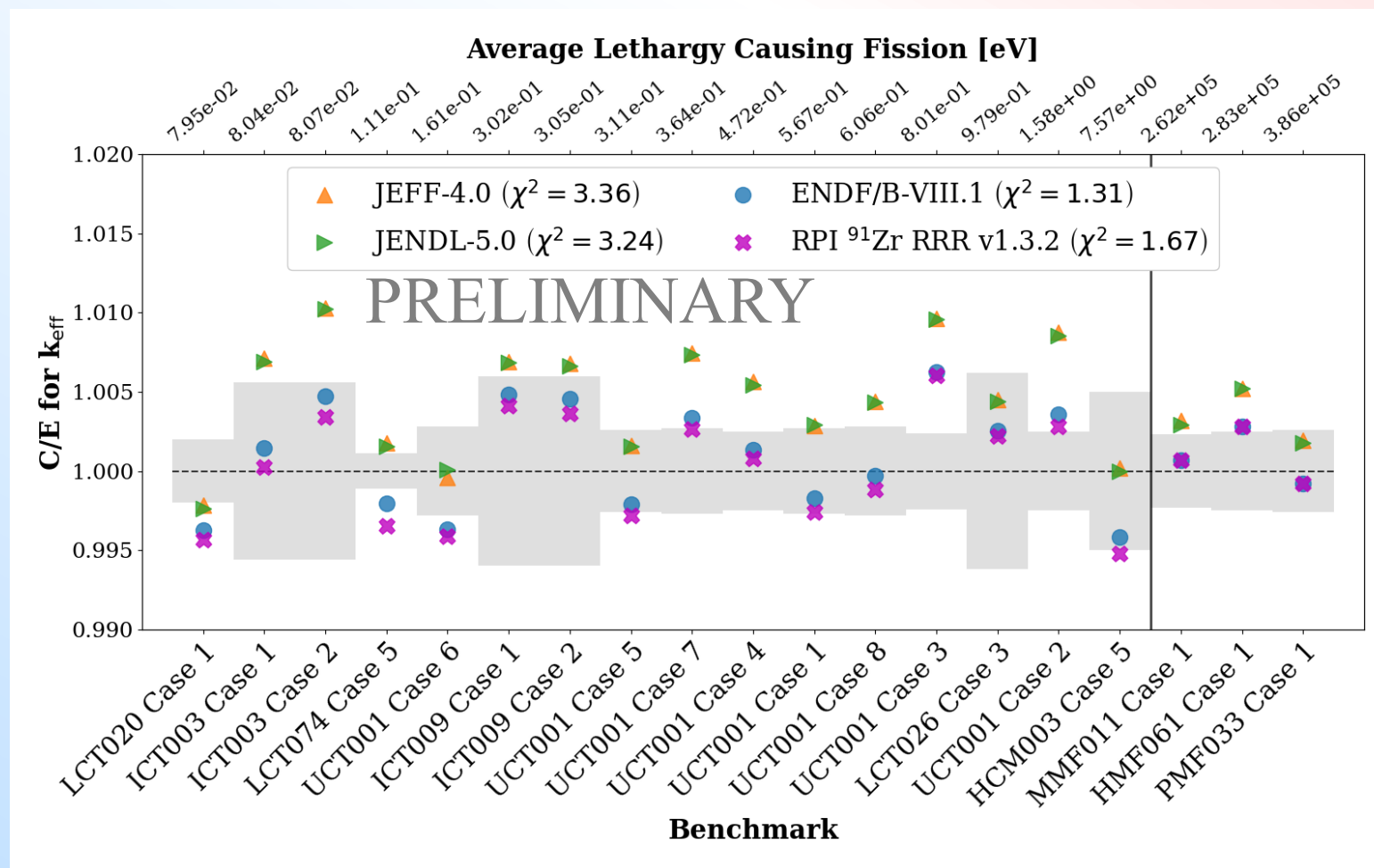
Preliminary Validation of New ^{90}Zr RRR Evaluation

- RPI ^{90}Zr evaluation tested with ENDF/B-VIII.1 for other Zr isotopes
- All simulations performed using ENDF/B-VIII.1 as the base evaluation
 - Uncertainty: 6-8 pcm
- JEFF-4.0 and JENDL-5.0 indicate substitution of Zr evaluations only, other materials are ENDF/B-VIII.1



Preliminary Validation of New ^{91}Zr RRR Evaluation

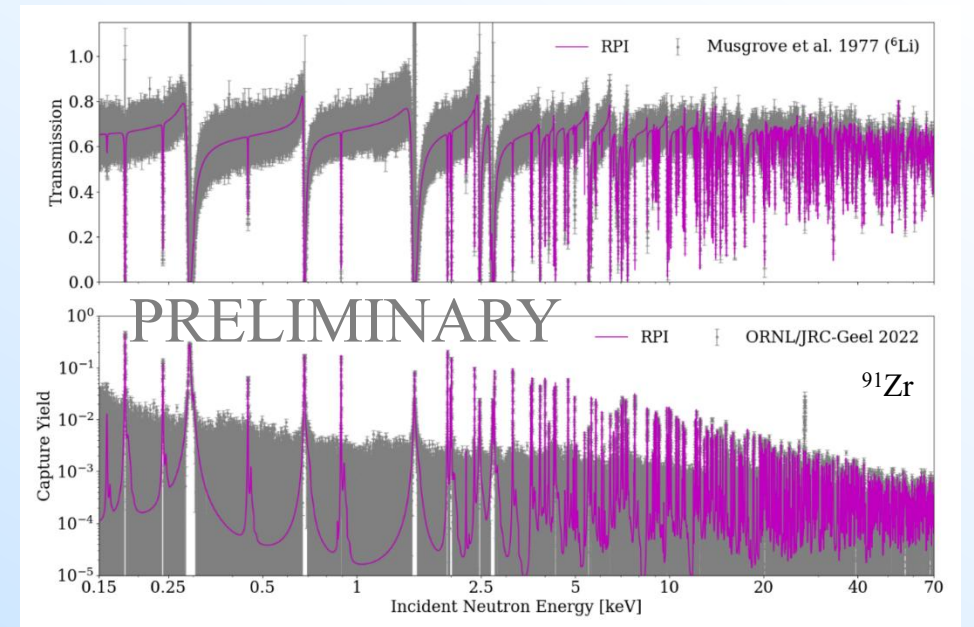
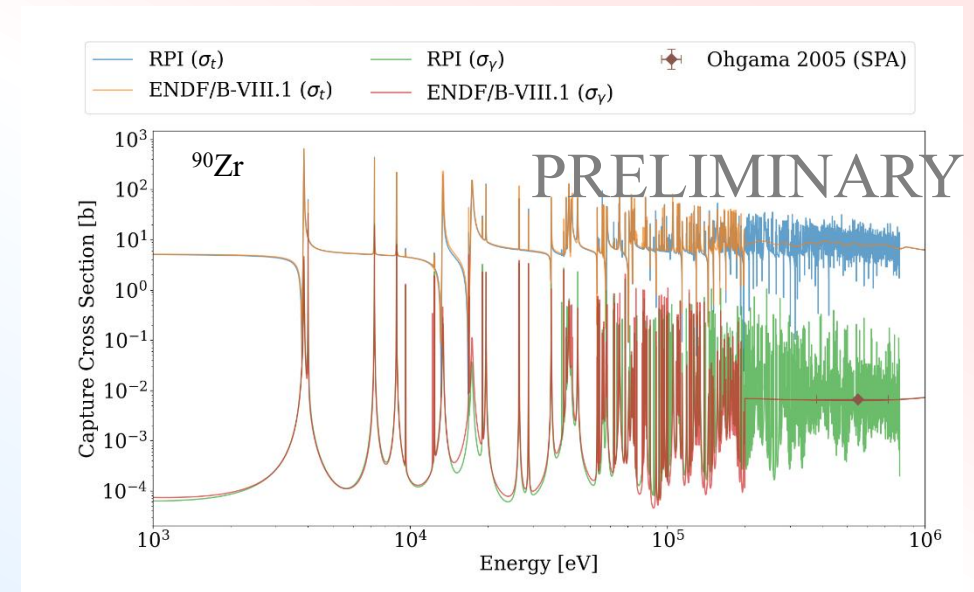
- ^{91}Zr evaluation tested with ENDF/B-VIII.1 for other Zr isotopes (RPI on legend)
- Decrease in reactivity due to increase in resonance ^{91}Zr resonance integral – which is expected to be compensated by ^{90}Zr elastic scattering angular distributions in fast evaluation



$^{90,91}\text{Zr}$ RRR and Fast Evaluation Outlook

Going Forward

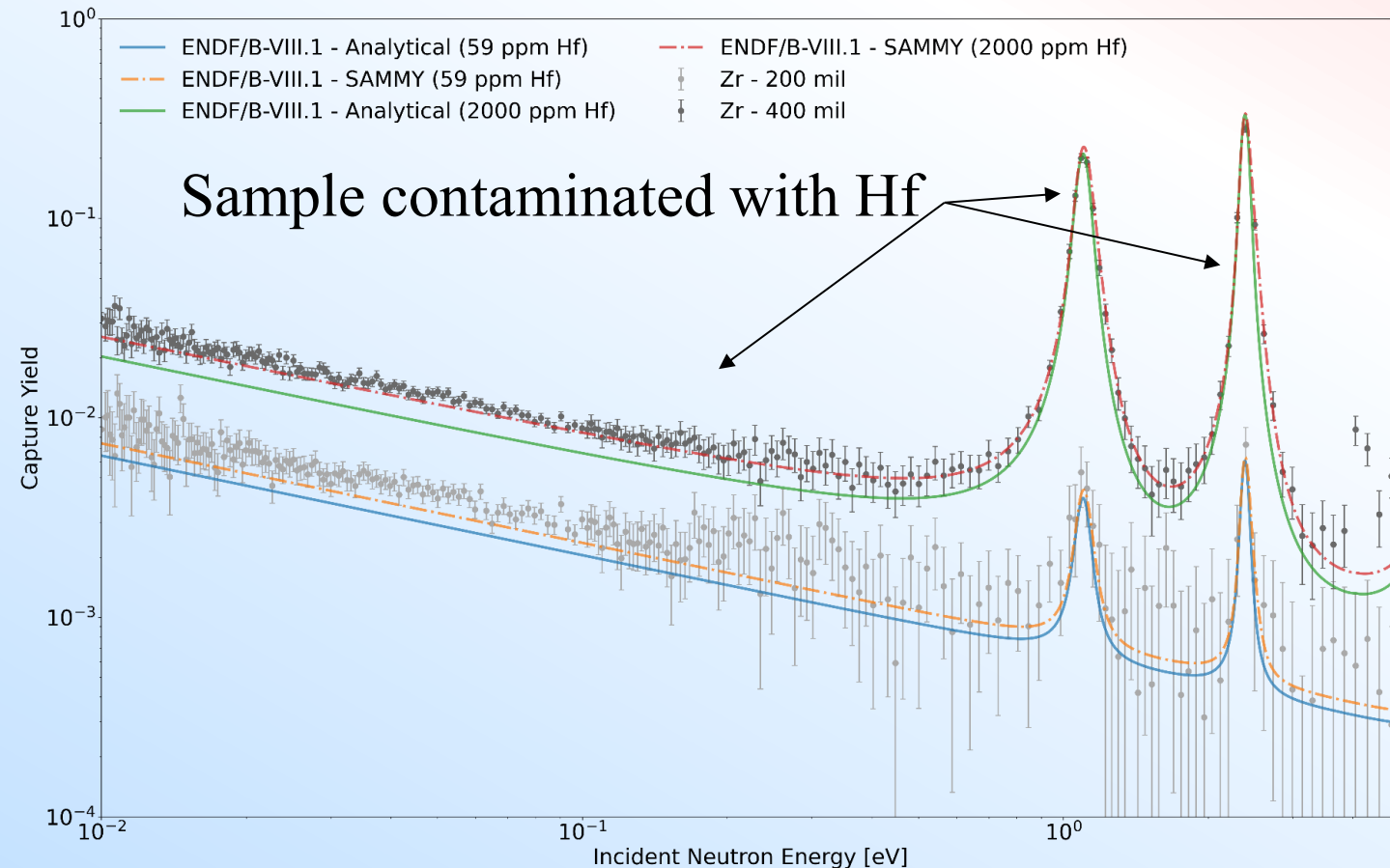
- Uncertainty quantification and covariance determination of $^{90,91}\text{Zr}$ resolved resonance region evaluations
- Finalize OMPs fitted for each Zr isotope with shape elastic and ESAD data
- Finalize level densities for $^{90,91}\text{Zr}$ fast evaluations
- Test and adjust preequilibrium models of $^{90,91}\text{Zr}$ to improve agreement to differential data for the other reaction channels: n,n' , $n,2n$, etc. and emission spectra
- Assemble final ENDF-6/GNDS $^{90,91}\text{Zr}$ files for submission to the NNDC



$^{\text{nat}}\text{Zr}$ Thermal capture experiment

Elemental Zirconium (n, γ) Measurement

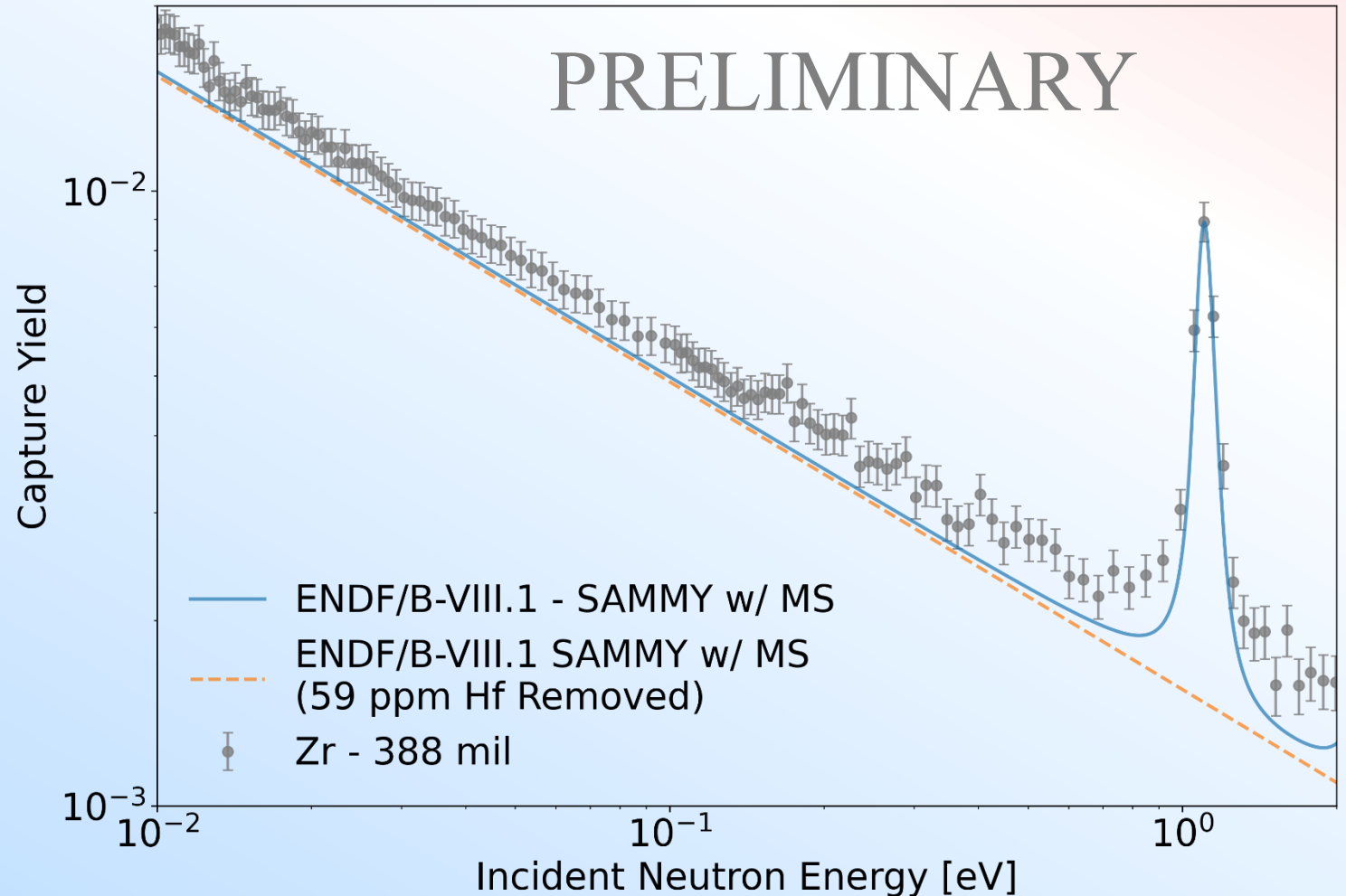
- Measurement performed in late August 2025 using the RPI multiplicity detector
- Several available Zr samples of varying thickness (and two procurement batches) stacked to obtain measurable yield
- Hf content in measured yield did not match the anticipated result from vendor provided mass spec
- 200 mil (batch #1) and 400 mil (batch #2) samples were split and measured independently



Preliminary Zirconium Capture Yield

$$Y_{Zr} = \frac{\dot{C}_{Zr} - \dot{C}_{Open} \cdot \left(\frac{M_{Zr}}{M_{Open}} \right)}{\phi} \cdot f_n \cdot \left(\frac{\eta_{Cd}^{\gamma}}{\eta_{Zr}^{\gamma}} \right)$$

- Final measured sample was six stacked batch #1 elemental Zr samples totaling 388 mil
 - Difficulties limited total Zr data acquisition time to a few hours
 - Preliminary results find the ENDF/B-VIII.1 evaluation low
 - Longer measurement needed to verify initial findings
- Both In and Cd measured to assess the merit of each material as neutron flux normalizer
- Pb measured to determine false capture signal due to neutron scattering into detector Al
 - Effects of which were shown to be small ($\sim 1e-4$ yield)



$^{90,91}\text{Zr}$ URR evaluation

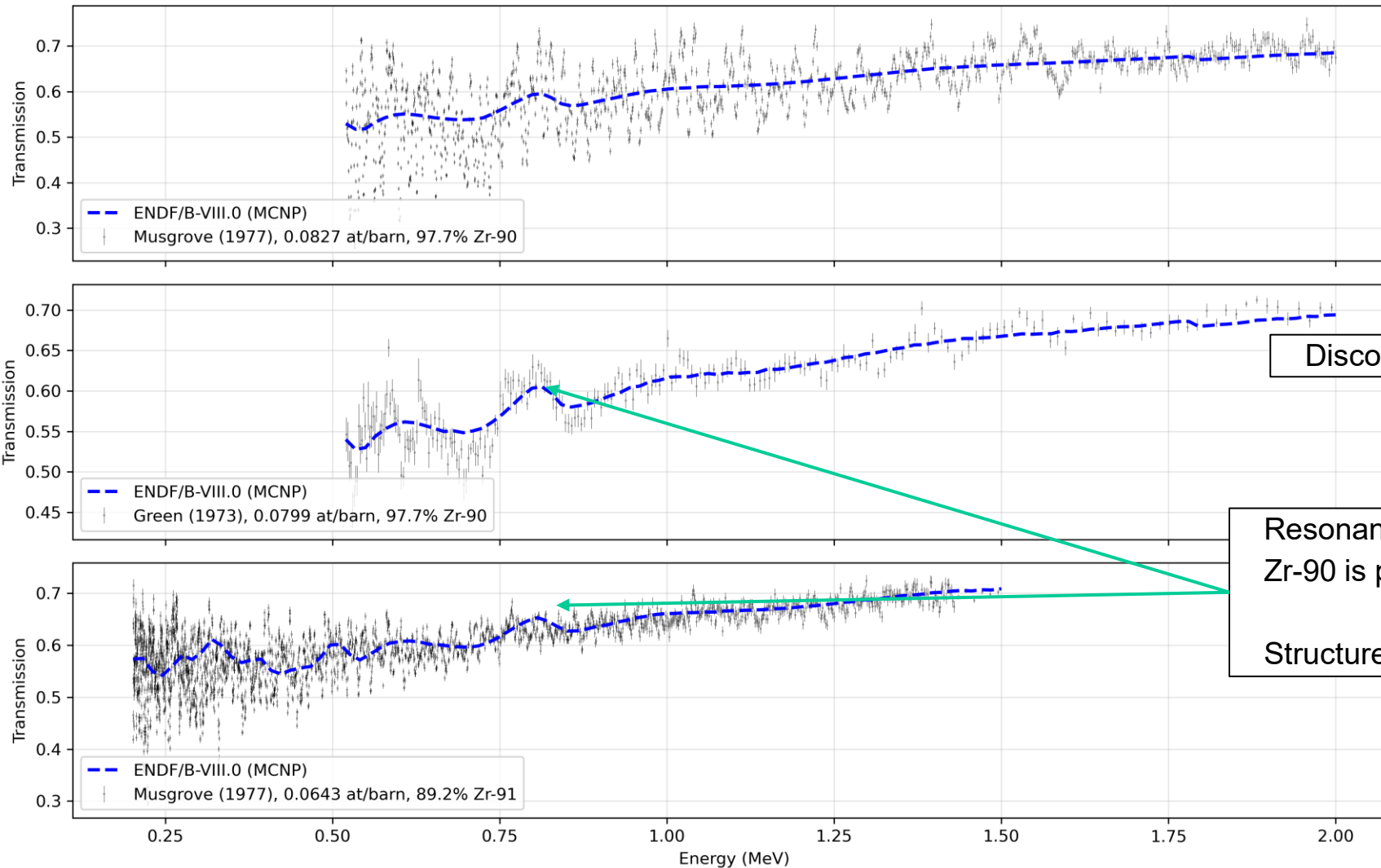
Current Deficiencies

File 3 background cross-sections are currently sourced from natural Zirconium - not isotopic data

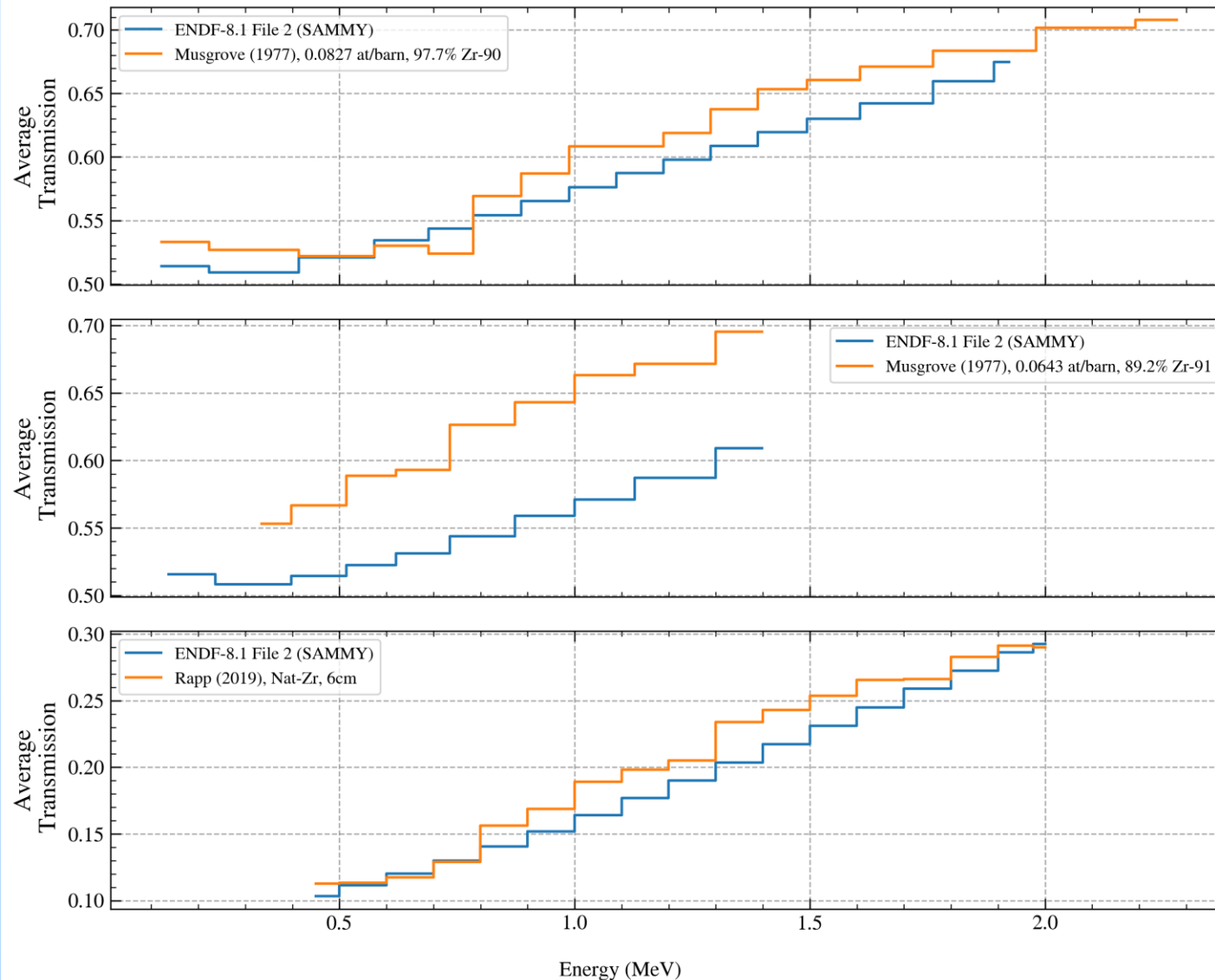
Discontinuity at 1st inelastic state

Resonant structure that is observable in Zr-90 is propagated to Zr-91

Structure not observable in Zr-91 data



Current Deficiencies



File 2 parameters don't accurately represent isotopic behavior by themselves

Significant deviation between theoretical cross-section calculated from Zr-91 URR parameters and experiment

Natural Zr is arguably *better* represented – compensating errors between isotopes

Objectives

- Perform URR evaluation concurrently with a new Resolved Resonance (RR) evaluation.
- **Utilize new RPI developed SAMMY functionality** to fit parameters to multi-isotope self-shielded URR measurements, (discussed in SG-51).
- Implement a physical model to capture the non-resonant intermediate structure (doorway states).
- Improve UQ on parameters (add File 32 to evaluation)

Original Ranges

Isotope	Start Energy (MeV)	End Energy (MeV)
^{90}Zr	0.2	1.78
^{91}Zr	0.0261	1.0

Updated Ranges

Isotope	Start Energy (MeV)	End Energy (MeV)
^{90}Zr	0.8	1.78
^{91}Zr	0.220	1.24

Prior Parameter Calculation

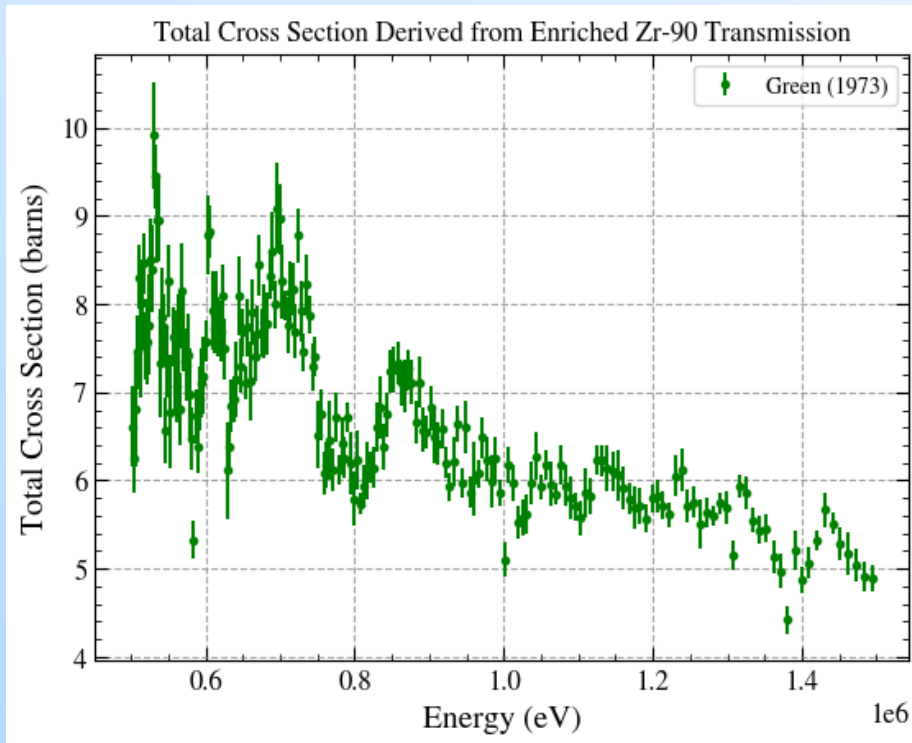
Isotope	ℓ	$S_\ell (\times 10^{-4})$	R^∞	$\langle \Gamma_\gamma \rangle$ (eV)	D (eV)
^{90}Zr	0	0.617 ± 0.064	-0.1658 ± 0.0630	0.224 ± 0.0162	8337.57
	1	5.387 ± 0.274	-0.1949 ± 0.086	0.662 ± 0.0268	-
	2	2.099 ± 0.208	-0.2308 ± 0.1170	0.224 ± 0.0162	-
^{91}Zr	0	0.399 ± 0.021	-0.1886 ± 0.0440	0.1649 ± 0.0049	540.96
	1	5.006 ± 0.277	-0.22640 ± 0.0630	0.2370 ± 0.007	
	2	0.325 ± 0.0921	-0.27440 ± 0.089	0.1649 ± 0.0049	

Available Data

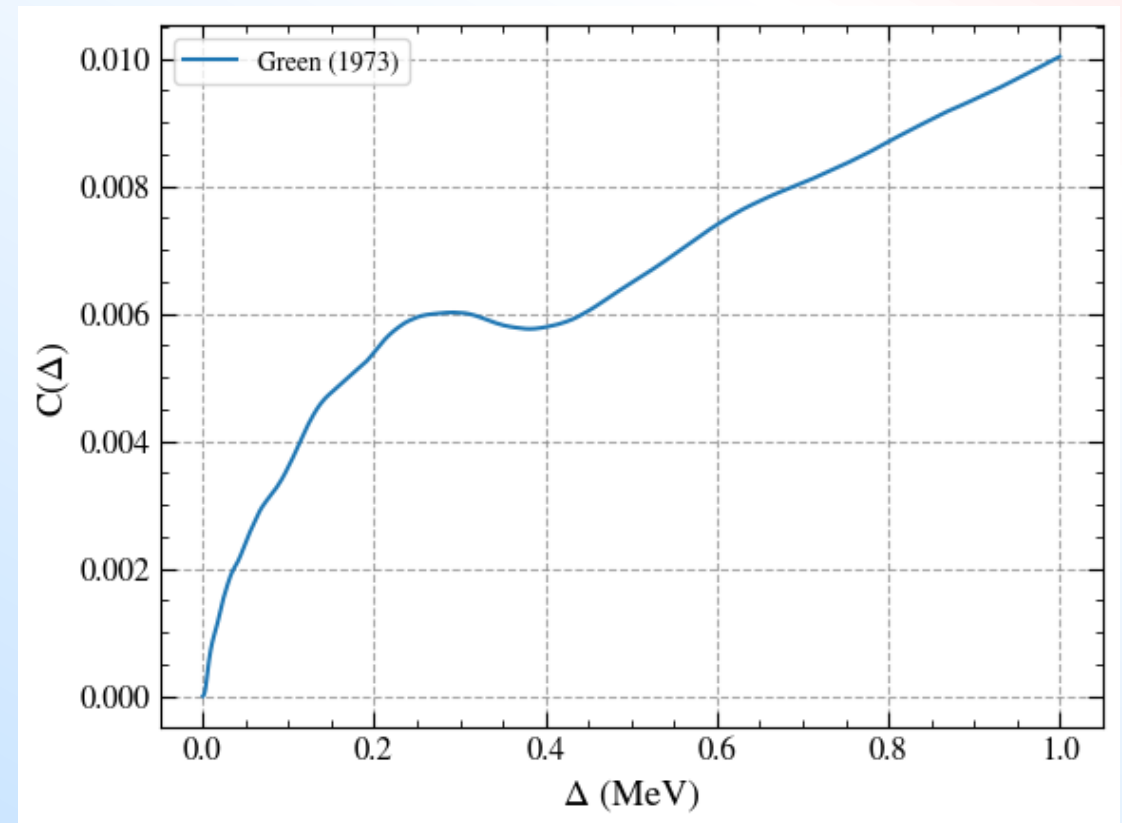
Isotope	Author	Reaction Type	Energy Range Utilized (MeV)	Notes
⁹⁰ Zr	Musgrove (1977)	Transmission	[0.12, 1.86]	Zr090 Enriched (97.7%) Thickness: 0.0827 at/barn
	Green (1973)	Transmission	[0.52, 1.94]	Zr-90 Enriched (97.7%) Thickness: 0.0799 at/b
	Ohgama (2005)	Capture XS	0.550	
	Macklin (1963)	Capture XS	0.030	
	Tagliente (2011)	Capture Yield	[0.150, 0.500]	ZrO ₂ sample, processing still in progress
⁹¹ Zr	Musgrove (1977)	Transmission	[0.324, 1.858]	Zr-91 Enriched (89.2%)
	Ohgama (2005)	Capture XS	[0.02, 0.550]	
	Gan (2024)	Capture XS	[0.026, 0.177]	

^{90}Zr Intermediate Structure

- Long-range non-resonant structure in Zr-90 cross-section
- Musgrove suggests presence of intermediate structure in Zr-90 P-wave at ~1 MeV
- Autocorrelation function used to confirm presence of intermediate structure



$$C(\Delta) = \frac{1}{N} \sum_{i=1}^N \left[\sigma(E_i) - \frac{1}{\Delta} \int_{E_i - \frac{\Delta}{2}}^{E_i + \frac{\Delta}{2}} \sigma(E) dE \right]^2$$



^{90}Zr Intermediate Structure (not used for now)

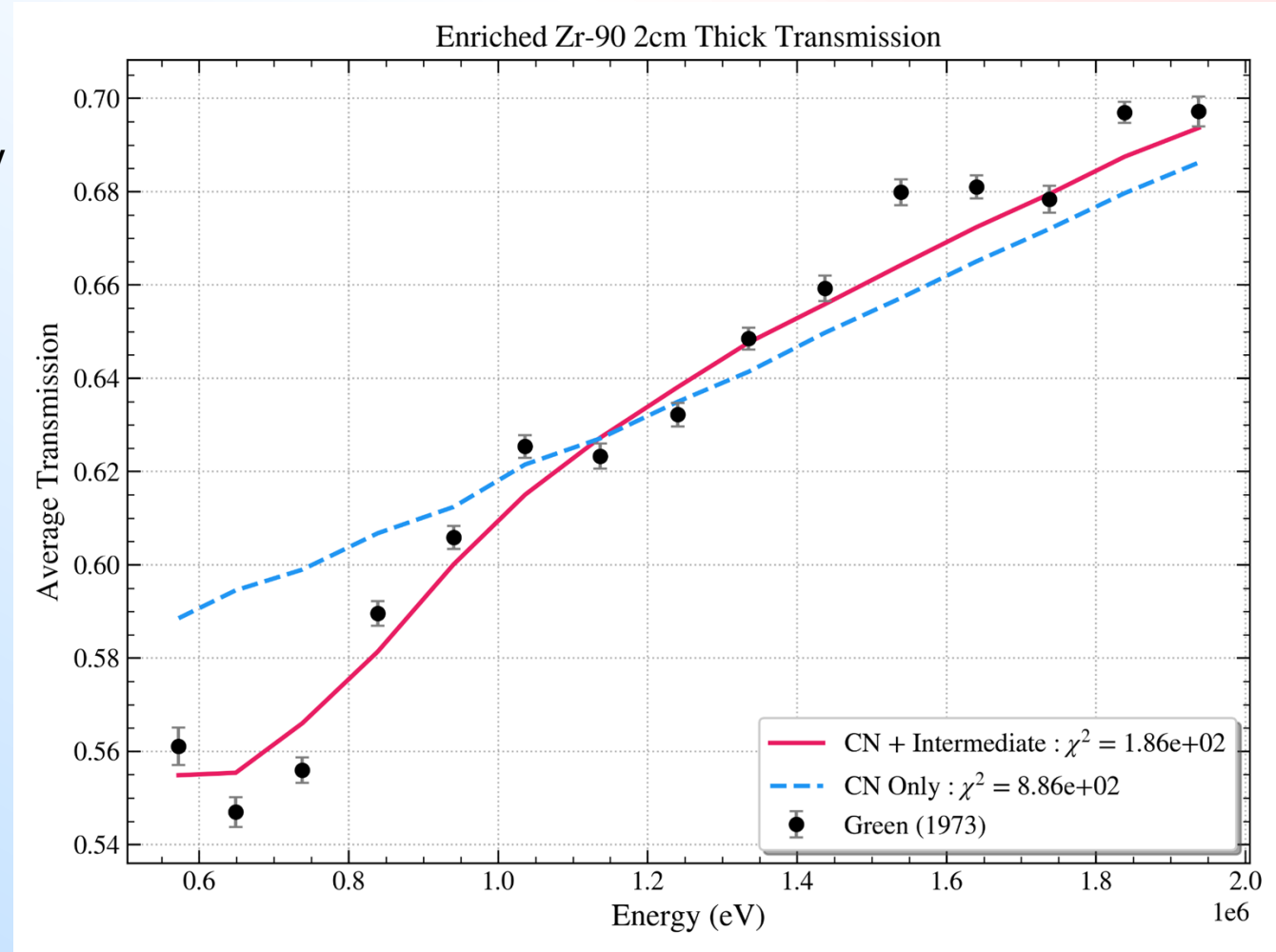
- Added functionality to SAMMY to support modeling intermediate structure
- Parameters to model intermediate structure roughly derived from RR parameters and autocorrelation result

$$S_{ds} = \frac{1}{\pi} \sum \frac{W\gamma_p^2}{(E_p - E)^2 + W^2}$$

$$S_1 = S_{CN} + S_{ds}$$

$$E_p = 750 \text{ keV} \quad W = 275 \text{ keV} \quad \gamma_p^2 = 403 \text{ keV}$$

- Significantly stronger agreement with data than from fitting with compound nucleus parameters alone



Self-Shielding Uncertainty Quantification

^{90}Zr

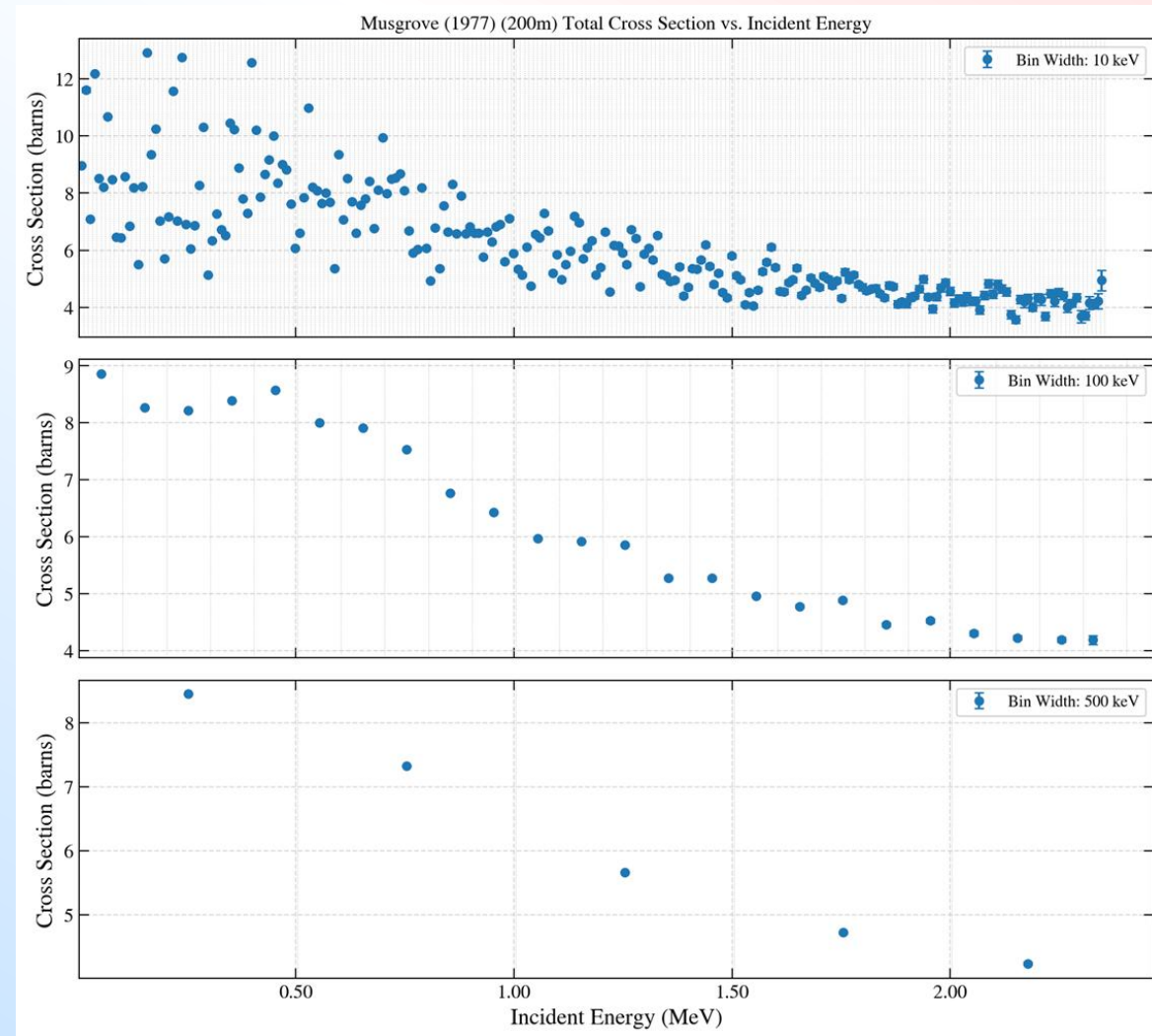
Two assumptions are used for correcting self-shielded measurements:

1. There are a statistical number of resonances in an energy bin
2. Energy bin is narrow enough to ignore energy dependent effects

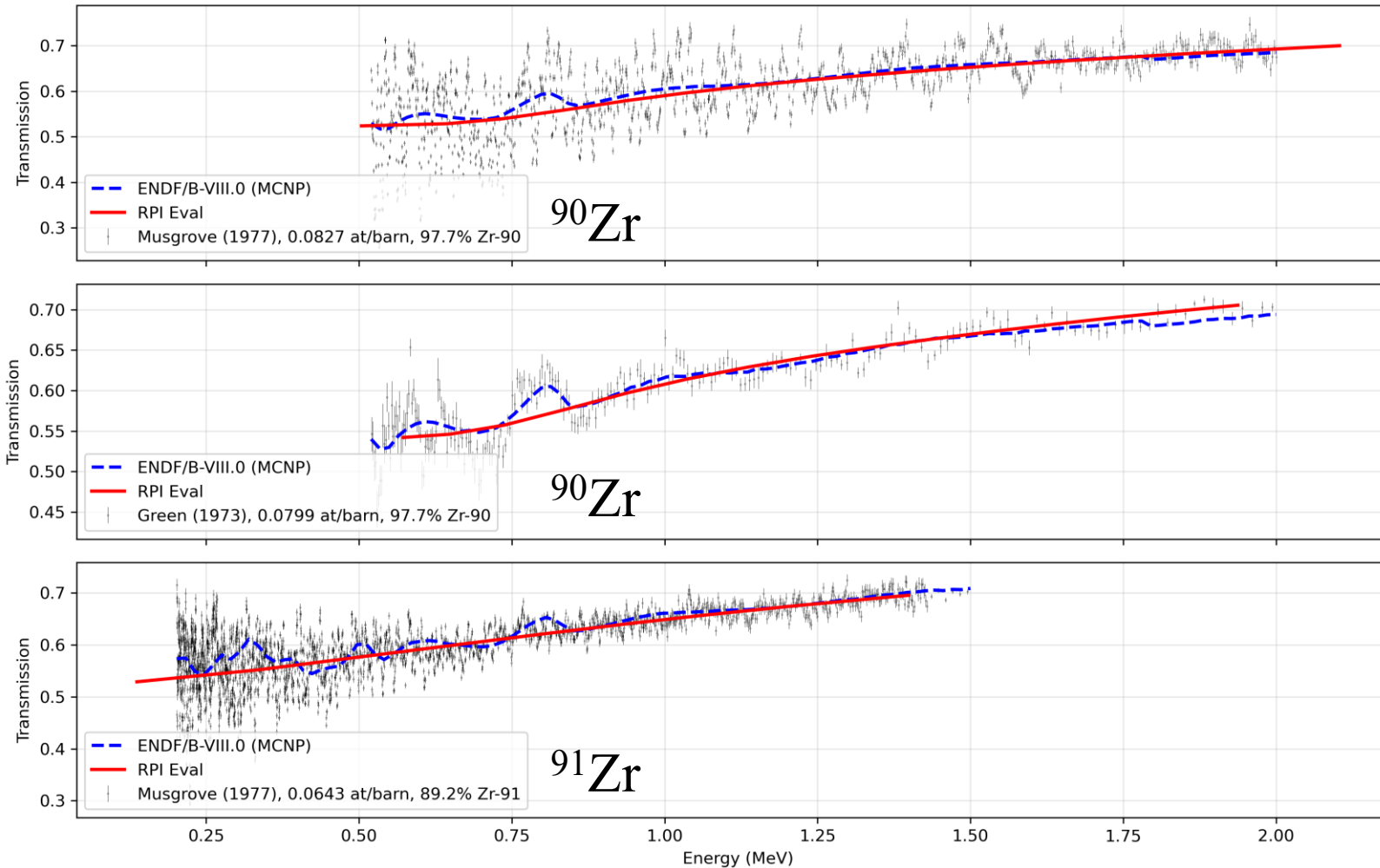
Zr-90 cannot meet both assumptions

- 8.3 keV average level spacing
- 200 resonances would require a 1.6 MeV energy bin (!!)
- Intermediate structure present requires “finer” energy grid for fitting

Issue: Finite number of resonances per energy bin can inaccurately represent average parameters – introduces uncertainty on correction factor

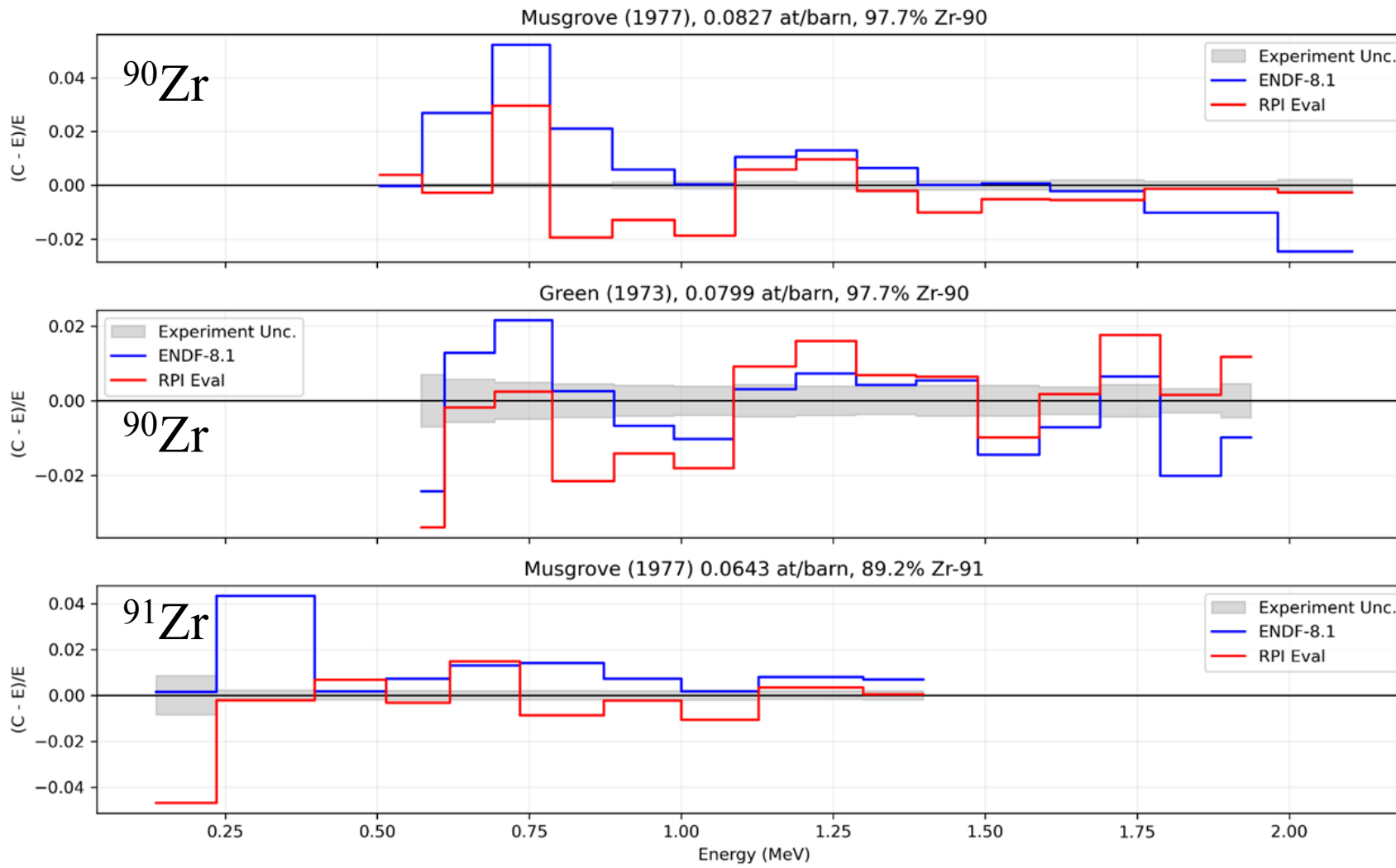


Fitting Results



- Intermediate structure model improves fit, but needs more work
- Reminder
 - New eval ^{90}Zr URR starts at 800 keV
 - New eval ^{91}Zr URR starts at 220 keV

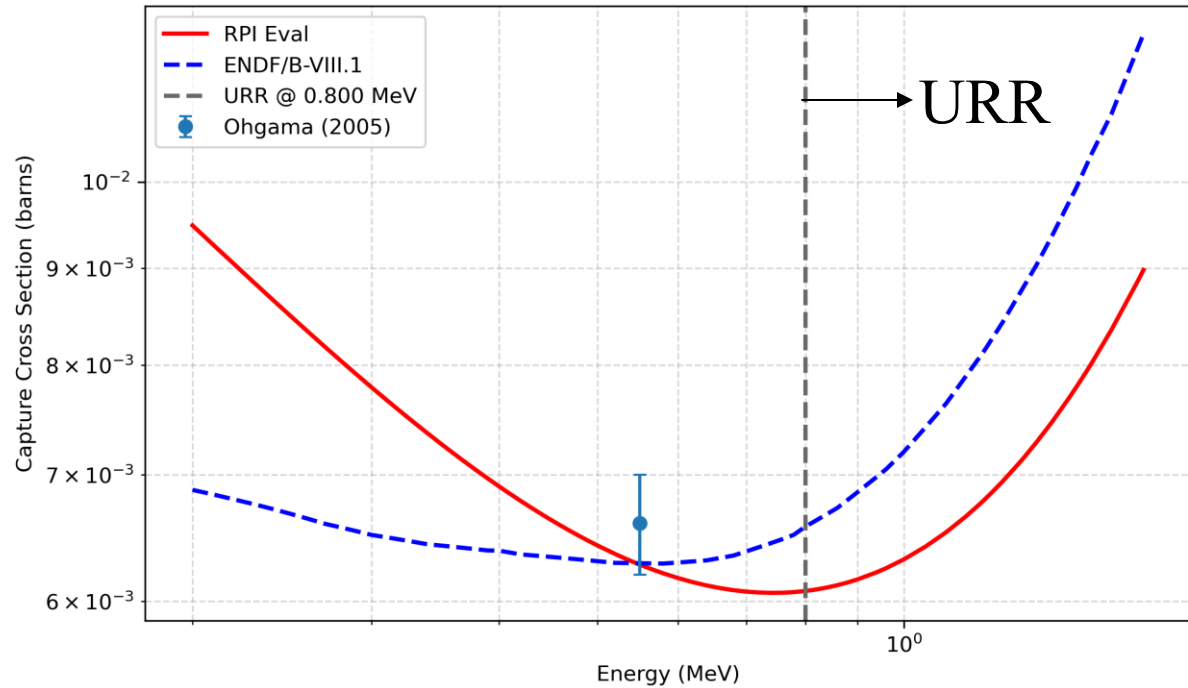
Fitting Results: Transmission Zr-90



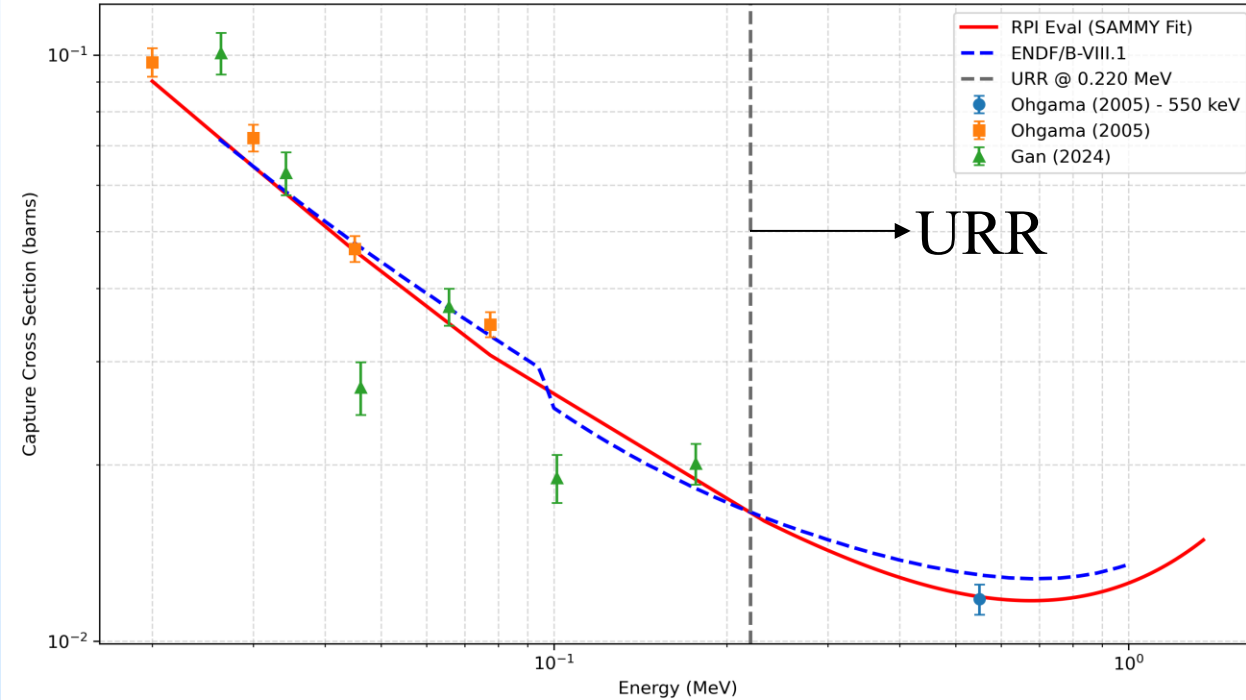
- Larger errors in new evaluation occur at intermediate structure peak
- A better model is required for more accurate representation

Fitting Results: Capture Cross-section

Zr-90 Capture Cross Section Comparison



Zr-91 Capture Cross Section Comparison

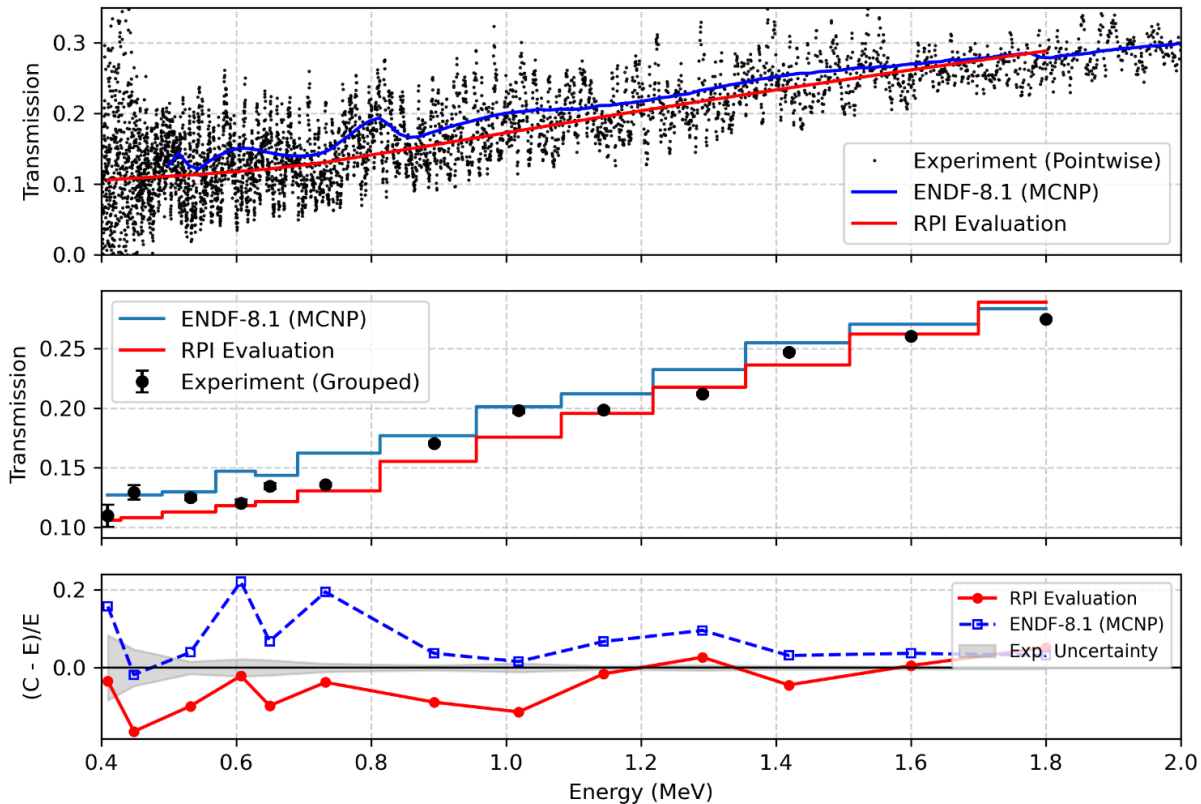


- Zr-90 capture data is very restricted in this new URR - not a single capture cross-section point lies in its range.
- Excessively unconstrained – poses a challenge for ensuring continuous URR energy boundaries

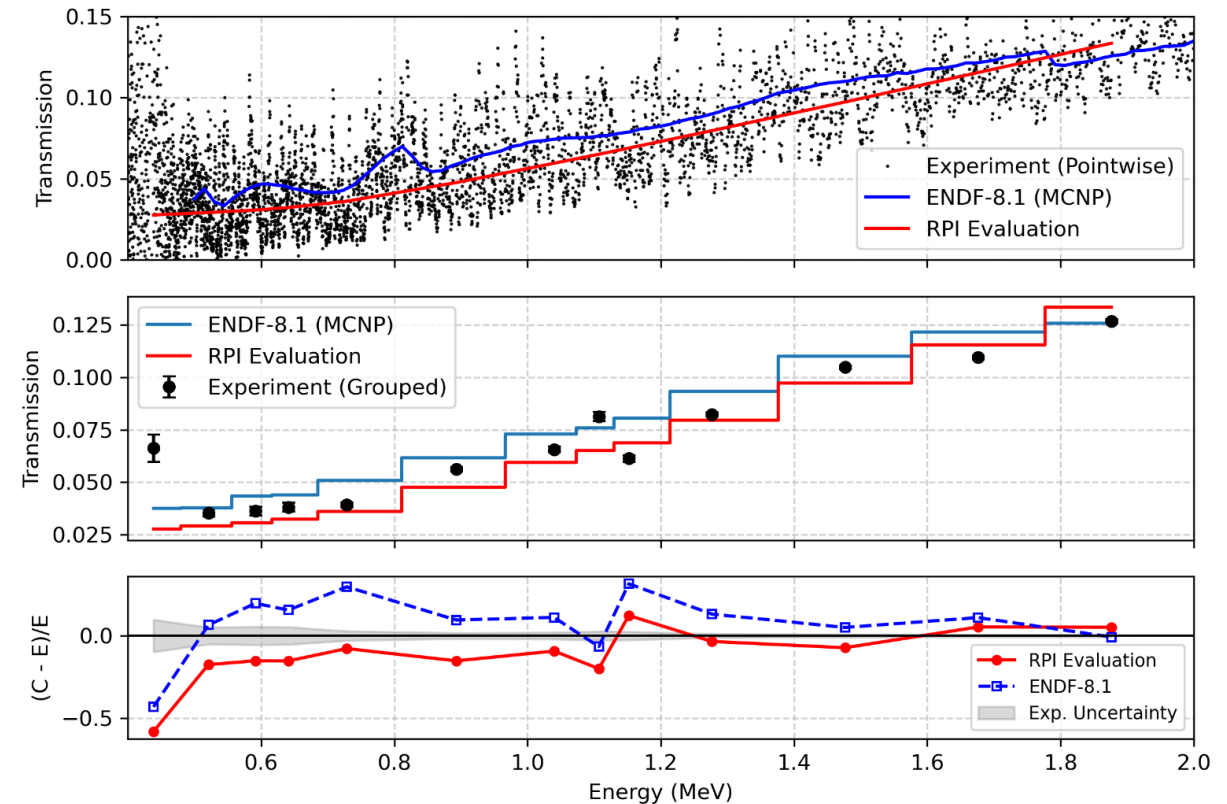
Fitting Results: Validating with ^{nat}Zr

- New evaluation is in slightly better agreement for the thick sample
 - Depends on other isotopes.

Nat-Zr Transmission for 6cm Sample (Rapp 2019)

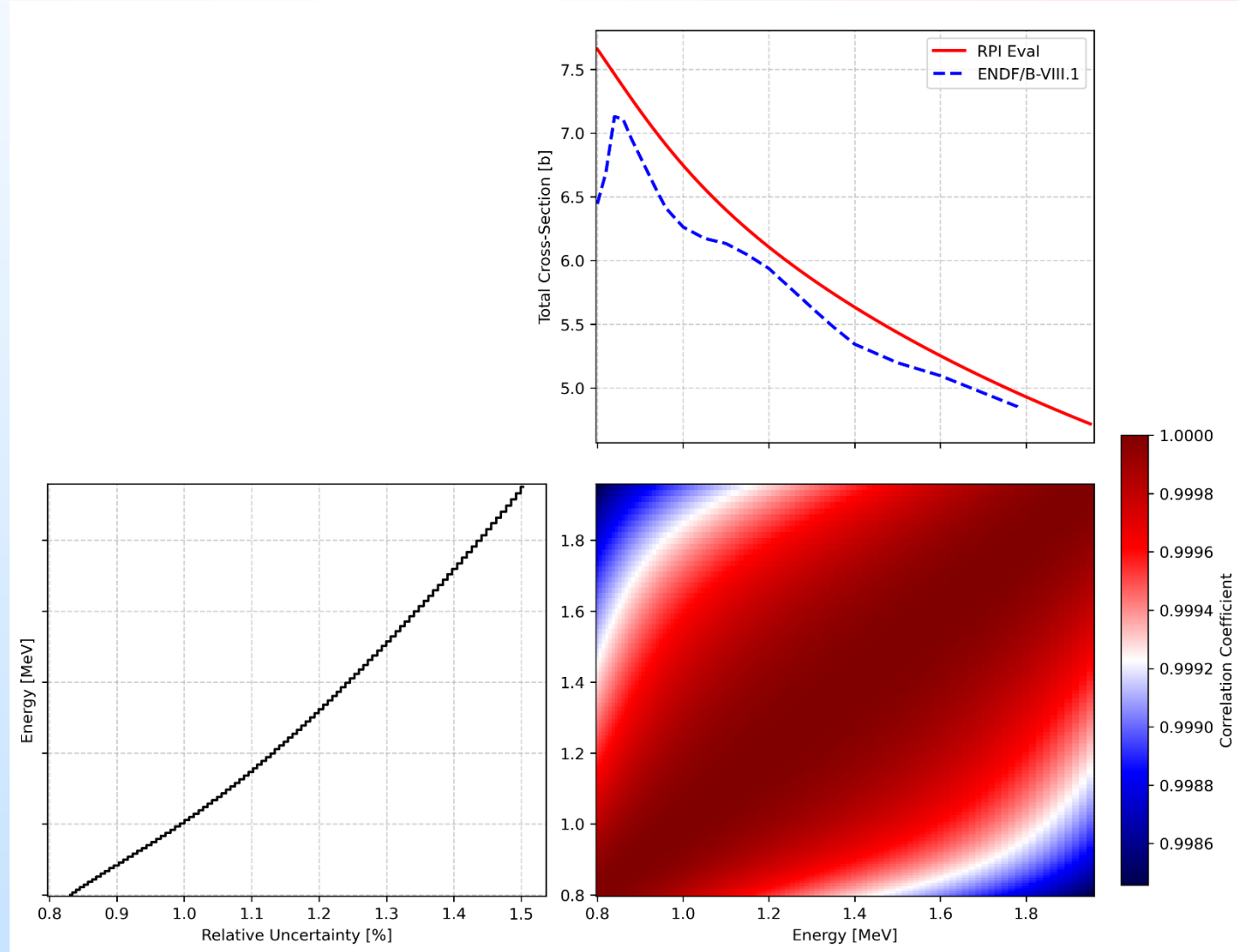


Nat-Zr Transmission for 10cm Sample (Rapp 2019)



^{90}Zr Total Cross-Section

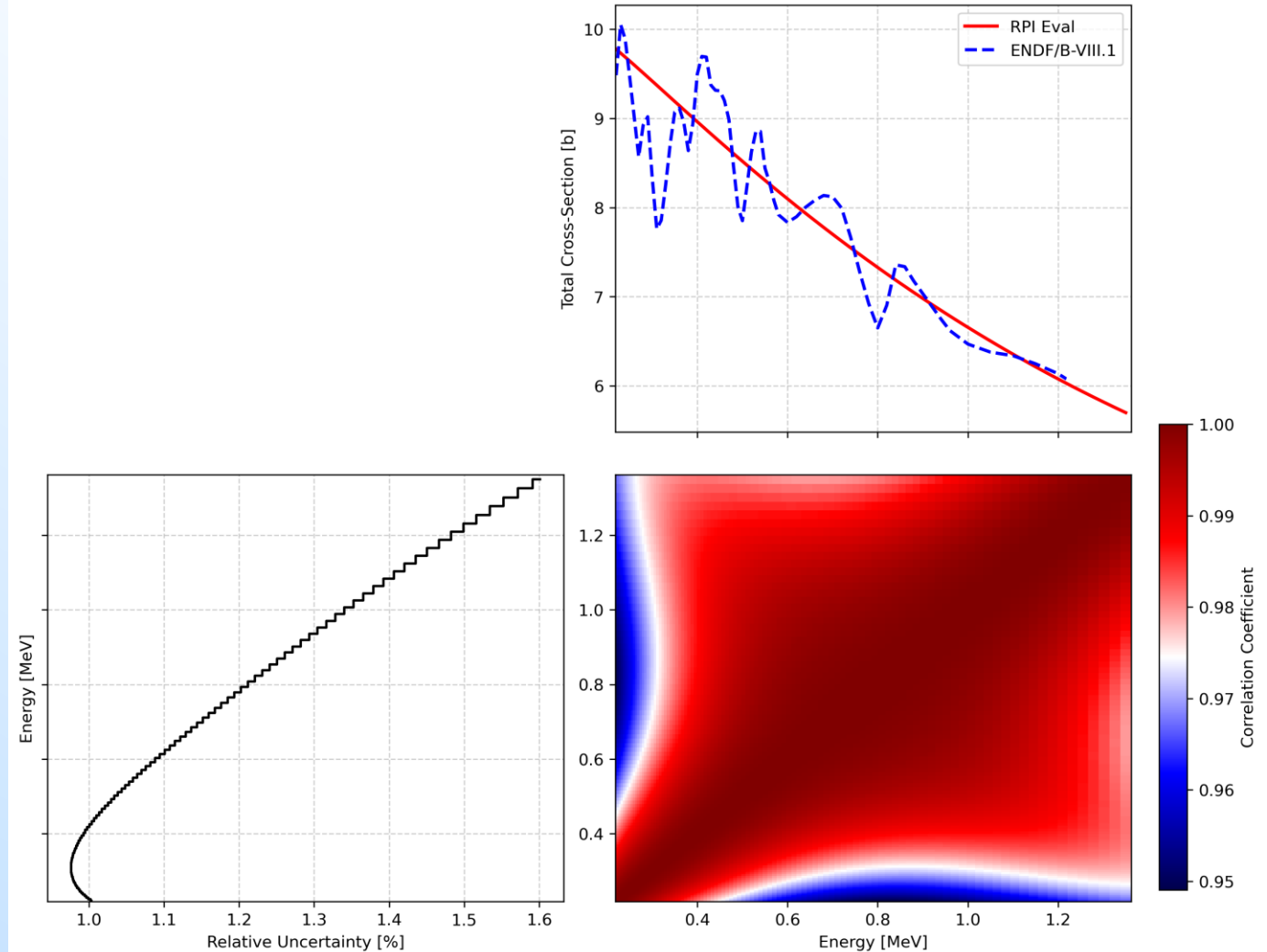
- Infinite dilute cross-section is ~5% higher in newer evaluation than 8.1
- Indicates that 8.1 File 3 cross-section was insufficiently corrected for self-shielding



^{91}Zr Total Cross-Section

- Significant fluctuations present in File 3 data, not represented by new represented cross-section.
- Need to determine effect this has on benchmarks, and how much of this is attributable to other Zr isotopes

Zr-91 Total Cross-Section Comparison



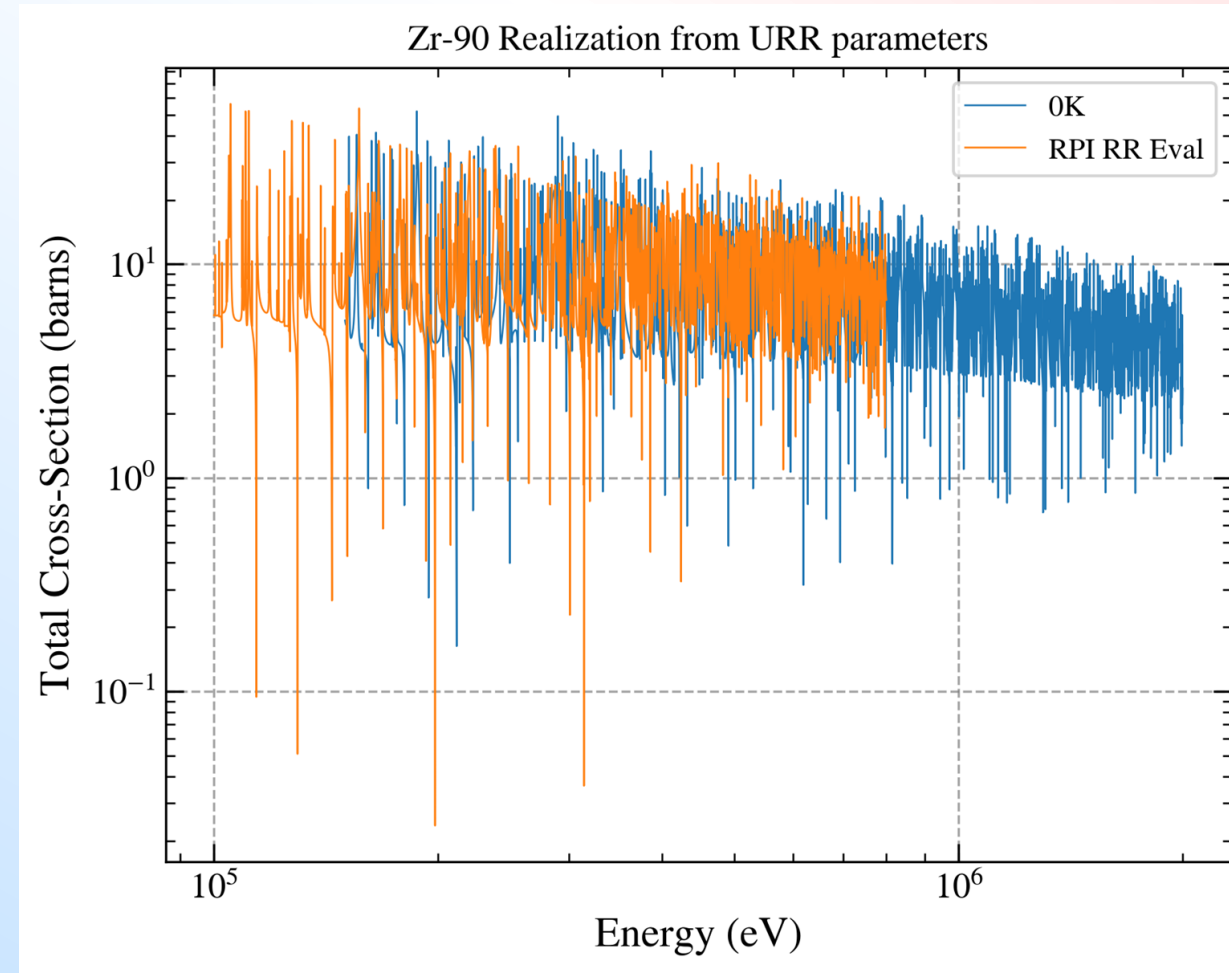
Calculating Self-Shielding Uncertainty

Determined the variance of C_T for each specific energy bin and thickness via Monte Carlo simulation.

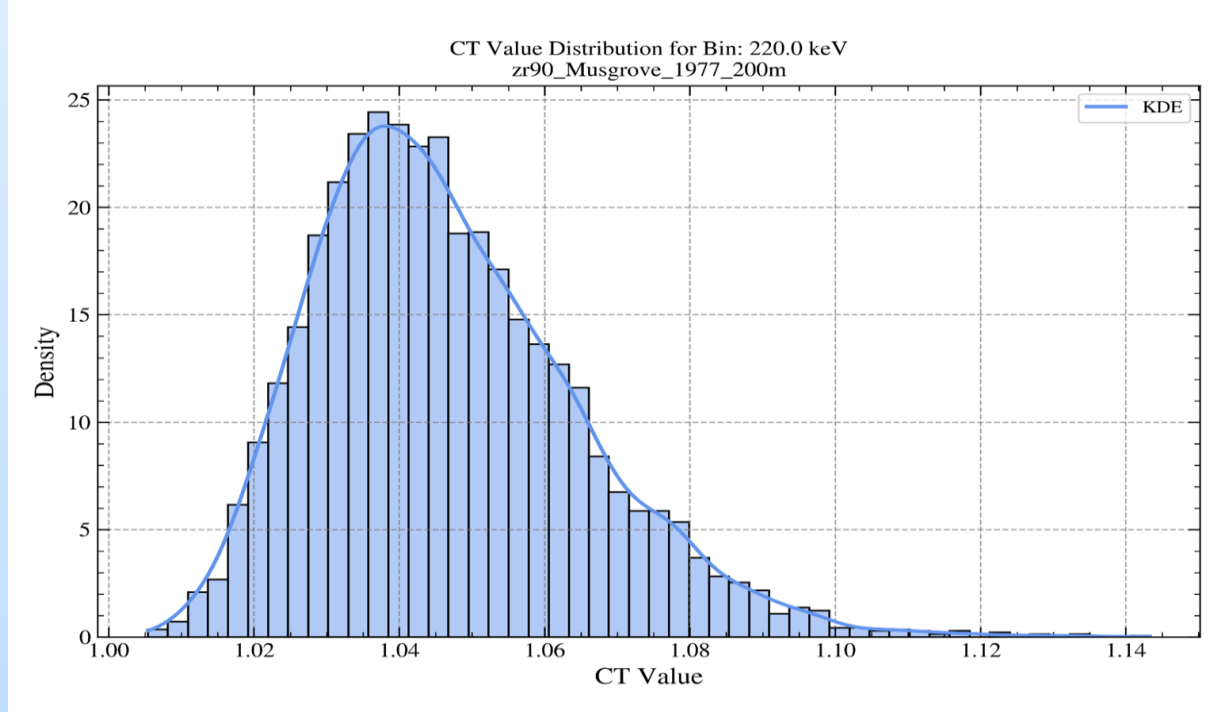
Method

- Generate thousands of unique resonance ladders from evaluated average parameters
- Calculated high-fidelity pointwise cross-sections for each ladder
- Calculate pointwise transmission based on experimental conditions and abundances
- Compute the exact self-shielding correction factor $C_{T,k}$ for each realization k
- Average results together to determine variance of

C_T

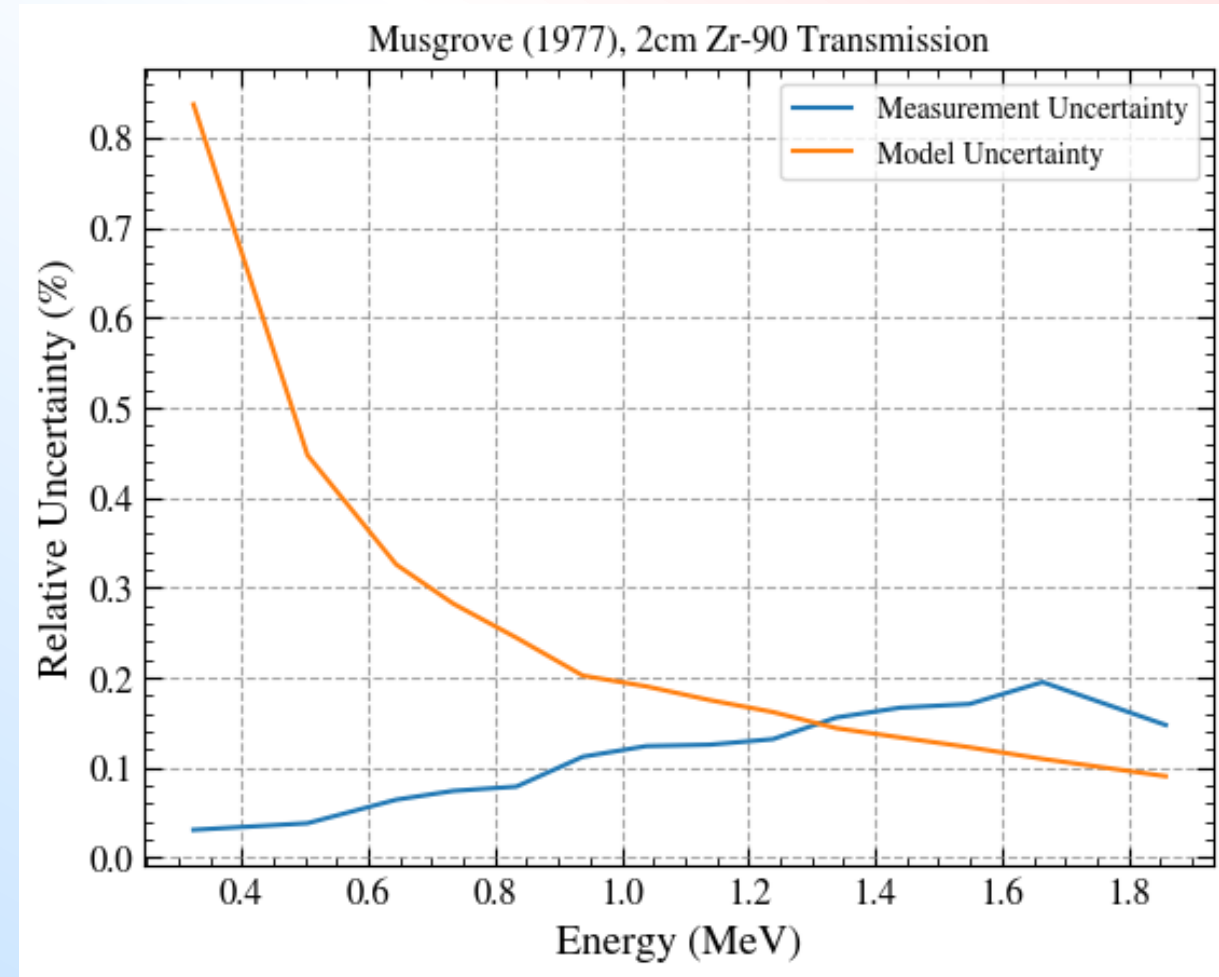


Propagating Self-Shielded Uncertainty



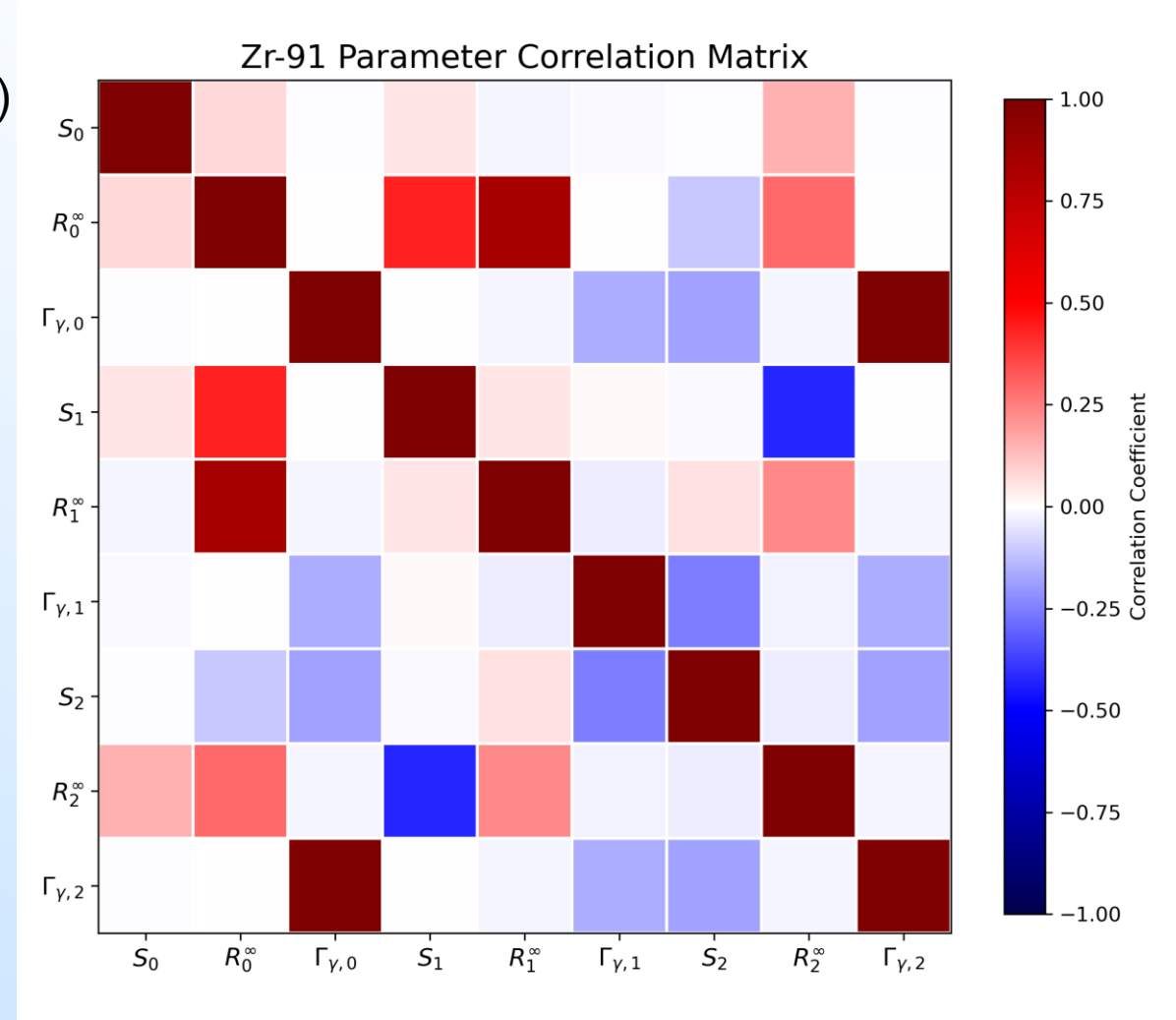
$$\Delta SF_correction_i = \Delta C_{T,i} e^{-n\langle\sigma\rangle}$$

$$\Delta_i = \sqrt{\Delta_{i,stats}^2 + \Delta_{i,SF_correction}^2}$$



Fitting Results: Zr-91

	Strength (10^{-4})	R_{∞} (fm)	Avg Gamma (eV)
0	0.398 ± 0.021	-0.231 ± 0.017	0.151 ± 0.005
1	5.071 ± 0.162	-0.217 ± 0.050	0.194 ± 0.006
2	0.321 ± 0.080	-0.263 ± 0.041	0.151 ± 0.005



^{nat}Fe URR improvement attempts

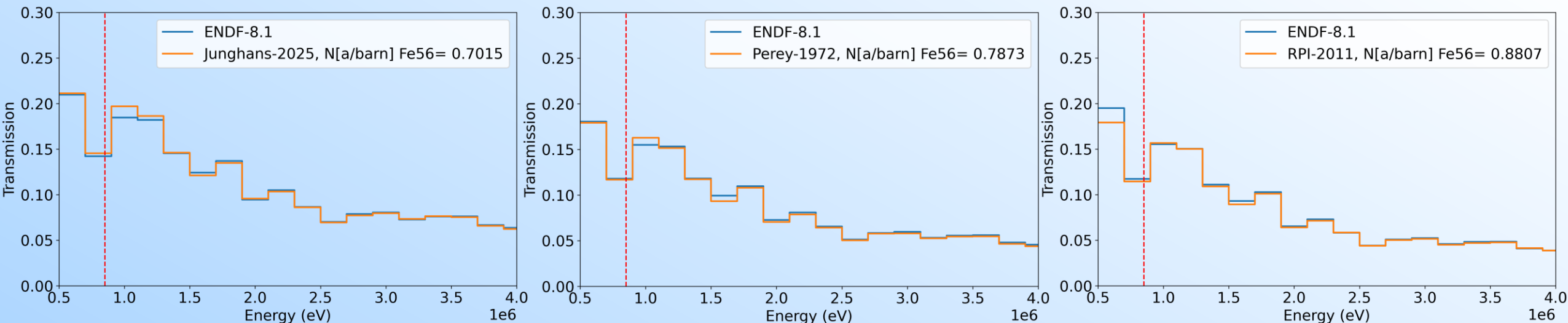
Comparison of URR evaluations to thick Iron transmission measurements

Experiment	Sample (% Fe-56)	N-Fe-56 [a/b]	Data Type
Junghans 2025	Fe-nat (91.75)	0.7015	Transmission
Perey 1972	Fe-nat (91.75)	0.7873	Cross section
RPI 2011	Fe-enriched (97.07)	0.8807	Transmission

- Analytical calculation, possible for ENDF 8.1 (no URR)
 - Experiment - If needed, convert data to transmission and group
 - Calculation - Calculate transmission from ENDF and group to same energy bins.
- MCNP calculate transmission in given energy bins
 - Includes shelf shielding if defined in ACE file

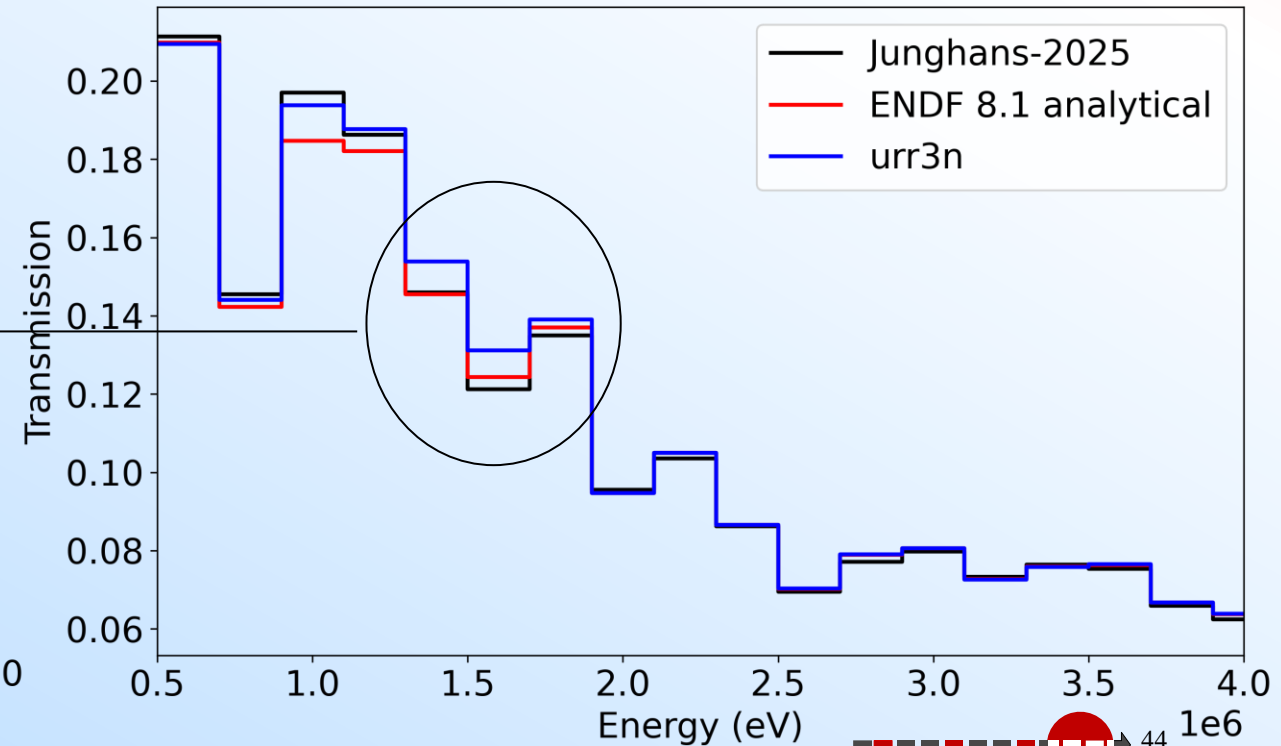
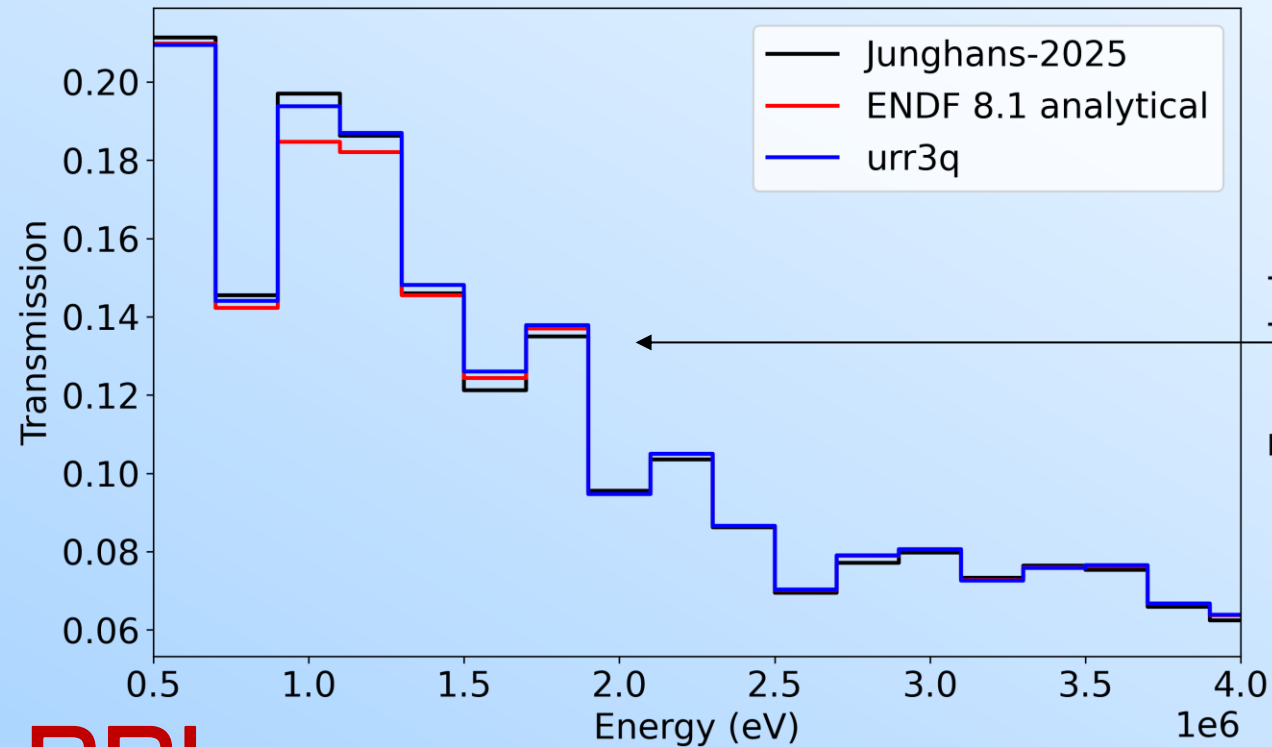
Experiments with three thick samples

- The plots are arranged by increasing Fe-56 thickness from left to right.
- There seems to be a trend:
 - The thickest sample seems to agree best above the RRR but not so good in RRR.
- In URR in general, a lower transmission in a calculation relative to experiment means that the calculation is missing self shielding.



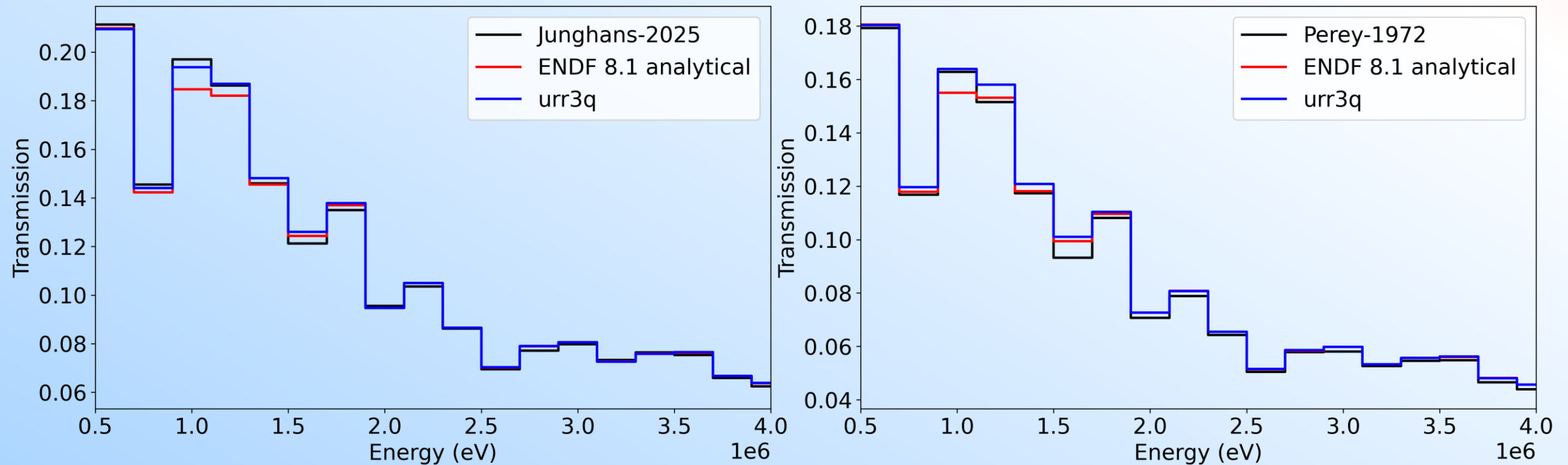
URR3q

- Use MCNP with ACE files provided by Andrej Trkov
- URRq compares better to Junghans experimental data in between 1-1.5 MeV.
 - Some degradation between 1.5-1.7 MeV
- Not so good agreement with the thicker Perey sample.



URR3q

- Several differences with the thicker Perey sample.



Neutron-Induced γ -ray Spectra Measurements at the RPI LINAC

K. Keparutis and I. Parker

This work was partially performed under appointment to the Rickover Fellowship Program in Nuclear Engineering sponsored by Naval Reactors (NR) Division of the National Nuclear Security Administration (NNSA).

This material is partially based upon work supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics, under Award Number DE-SC0024679.

RPI Neutron-Induced γ -ray Spectra Measurements

Measurements coupled with updated simulation methods provide a tool that can be used to **assess the accuracy of γ -ray production data** stored in nuclear data libraries

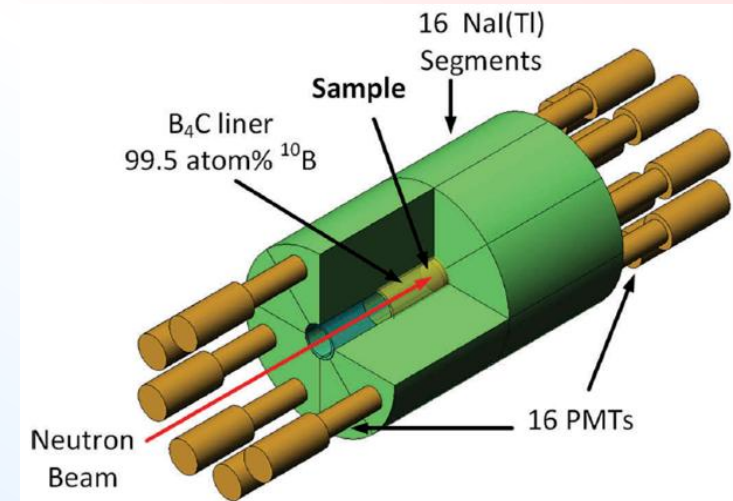
- Samples measured at RPI with **incident neutron energies of 0.01-100 eV**:
 ^{56}Fe , ^{55}Mn , ^{59}Co , $^{\text{nat}}\text{Ta}$, $^{\text{nat}}\text{U}$, ^{235}U , $^{\text{nat}}\text{Cd}$, $^{\text{nat}}\text{Au}$, $^{\text{nat}}\text{In}$, and NaCl
- Updated simulation method: **mod-MCNP6.2/DICEBOX**
 - γ -ray cascades generated using DICEBOX and transported through the detector geometry
 - Writes an output file that saves γ -ray energy deposition in detector segments (enables event-by-event analysis including coincidence)

Motivation: improving γ -ray production data

- Increase the accuracy of **reactor and shielding calculations**
- Understand the effects of **γ -ray heating** in nuclear reactors
- Improve **isotope identification** for active neutron interrogation

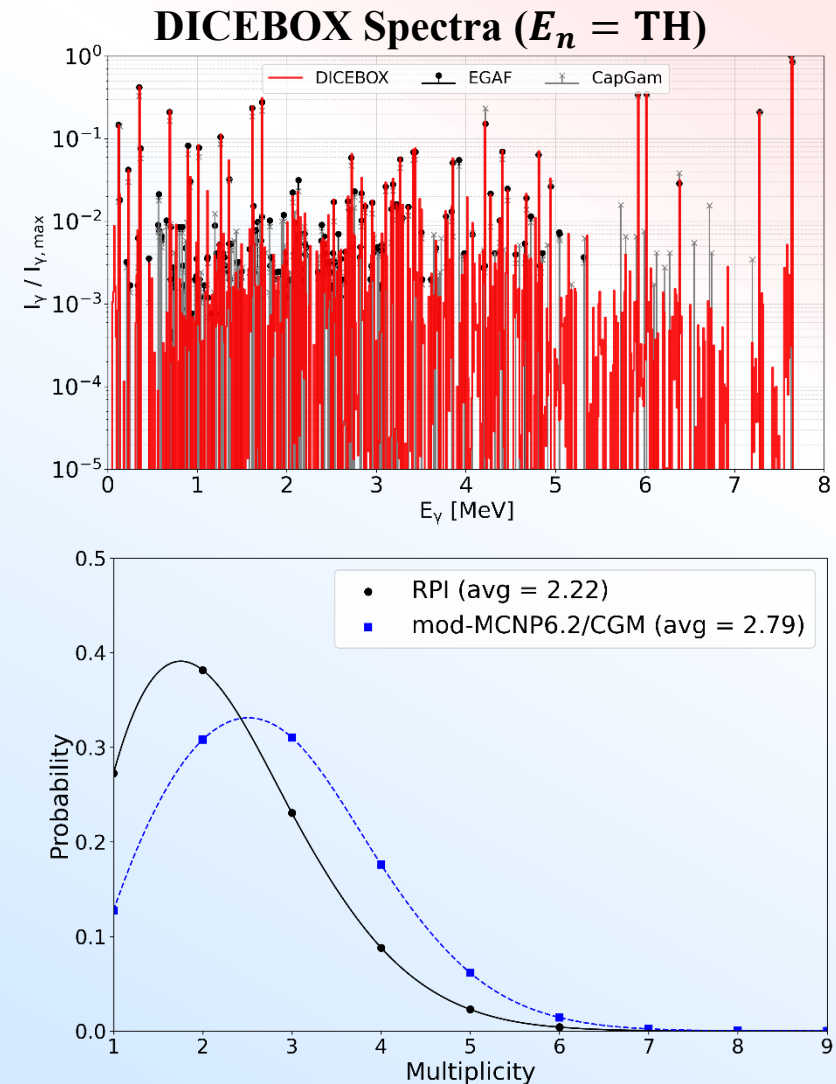
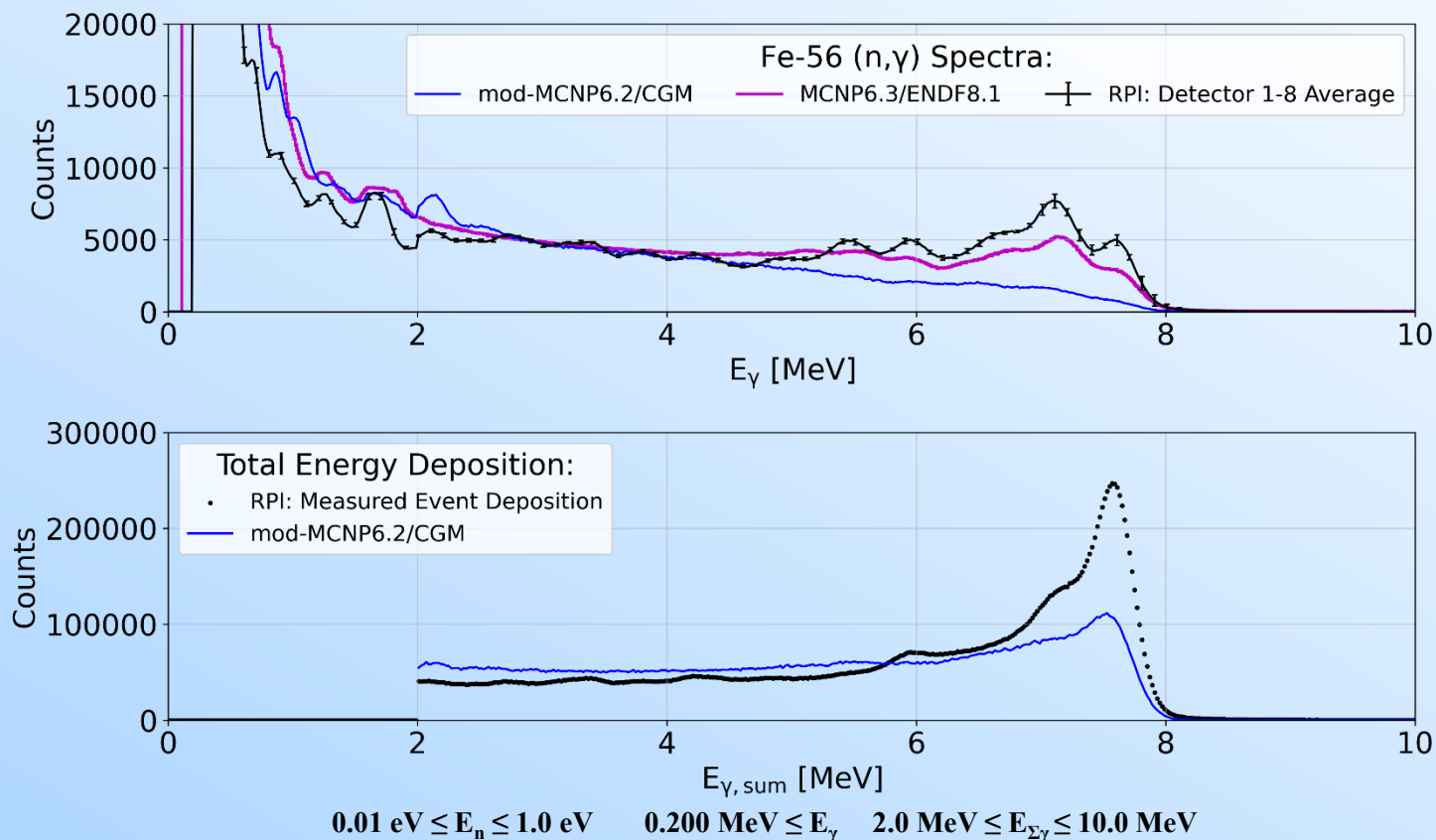
Awarded DOE Grant (FY23-25) as a follow-on project with the GRIN collaboration: **Development of Benchmark Measurements for Capture Gamma Cascades (DE-SC0024679)**

- Benchmark deliverables: measurement data, simulation tools, and benchmark template



Method Validation with ^{56}Fe (unmodified MCNP)

Using R.B. Firestone^[1] gamma-ray data as the cascade generator input, simulations match experimental data collected at RPI.



^[1]R. B. Firestone et. al., Phys. Rev. C **95**, 014328 (2017).

Simulation Capabilities:

Mod-MCNP6.2^{[1][2]}:

- Modifies MCNP6.2 Cascading γ -Ray Multiplicity (CGM) module used to produce correlated secondary emissions.
- Implements the ability to read externally made γ -ray cascade files in place of CGM generated gamma-ray cascades.
- Adds an event-by-event output energy deposited for each detector segment per neutron history.
 - Enables simulation and measurements to be processed identically.
- Cascades files are generated with DICEBOX^[3], GIDI⁺^[4], or other cascade generation codes.

¹Werner, C. J., (2018). *MCNP version 6.2 release notes* (LA-UR-18-20808). Los Alamos National Laboratory.

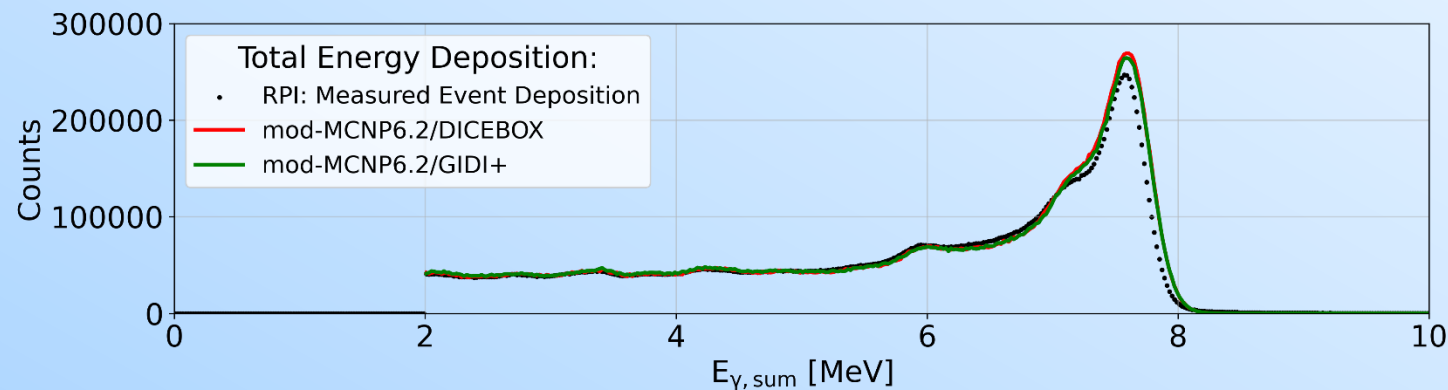
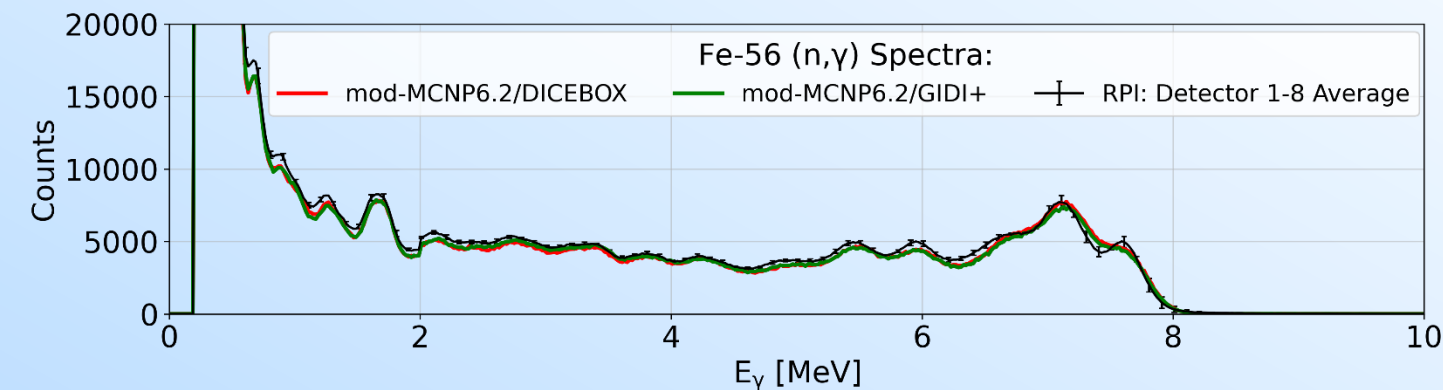
²Y. Danon et al., EPJ Web of Conferences 294 01001 (2024)

³Bečvář, F. (1998). Simulation of γ cascades in complex nuclei with emphasis on assessment of uncertainties of cascade-related quantities. *Nuclear Instruments and Methods in Physics Research Section A*, 417(2-3), 434-449. [https://Laboratorydoi.org/10.1016/S0168-9002\(98\)00787-6](https://Laboratorydoi.org/10.1016/S0168-9002(98)00787-6).

⁴Lawrence Livermore National. (n.d.). *GIDI+ (General Interaction Data Interface Plus)* [Computer software]. GitHub. <https://github.com/LLNL/gidiplus>

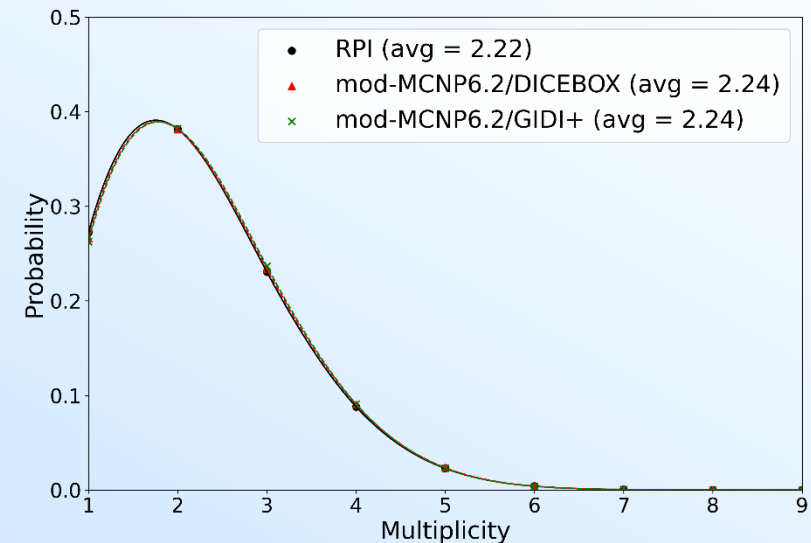
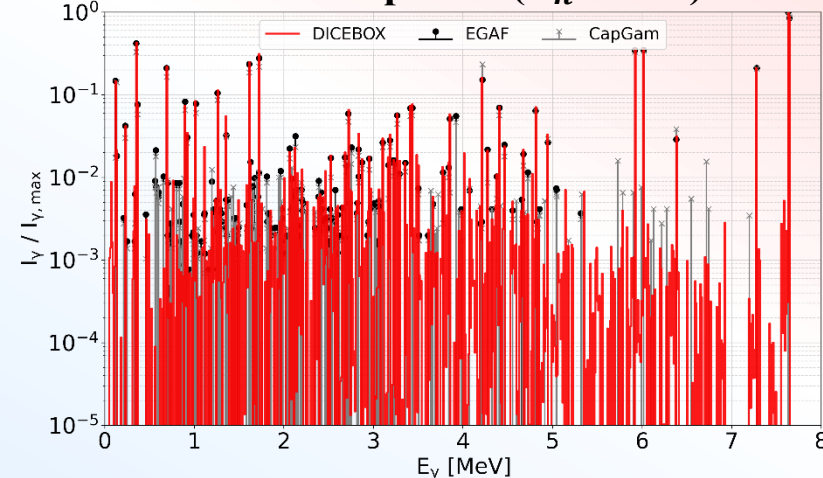
Method Validation with ^{56}Fe :

Using R.B. Firestone^[1] gamma-ray data as the cascade generator input, simulations match experimental data collected at RPI.



$0.01 \text{ eV} \leq E_n \leq 1.0 \text{ eV}$ $0.200 \text{ MeV} \leq E_\gamma$ $2.0 \text{ MeV} \leq E_{\Sigma\gamma} \leq 10.0 \text{ MeV}$

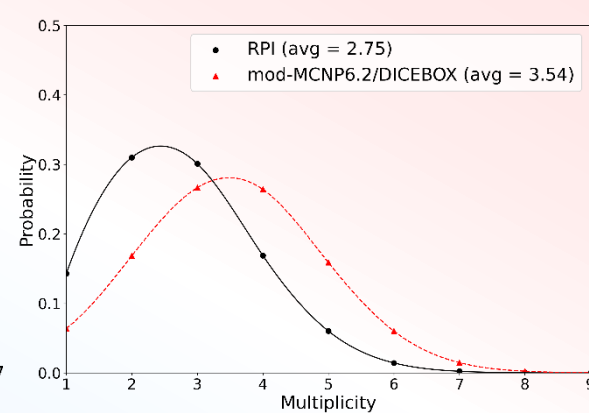
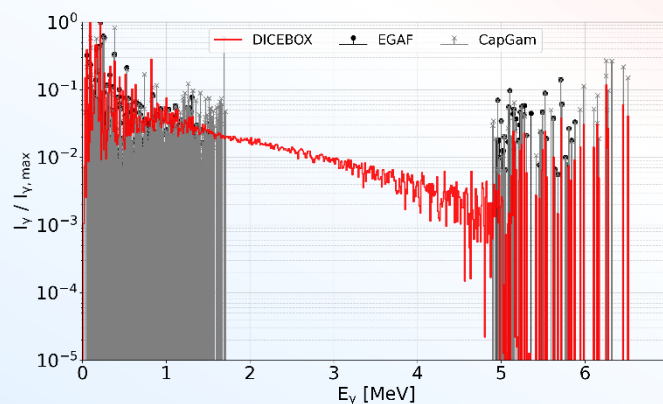
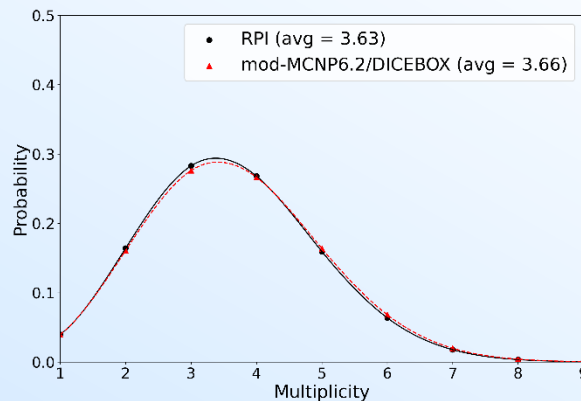
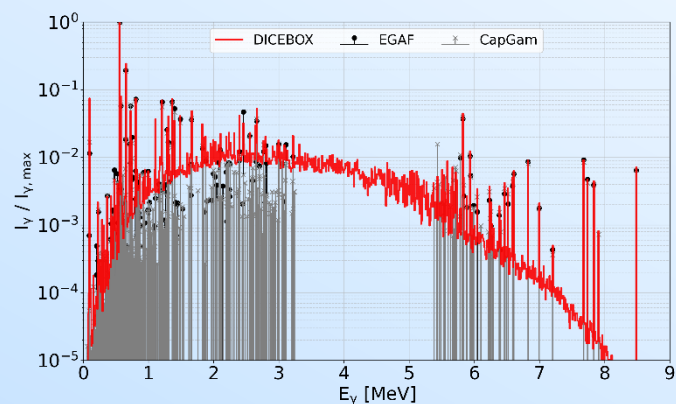
DICEBOX Spectra ($E_n = \text{TH}$)



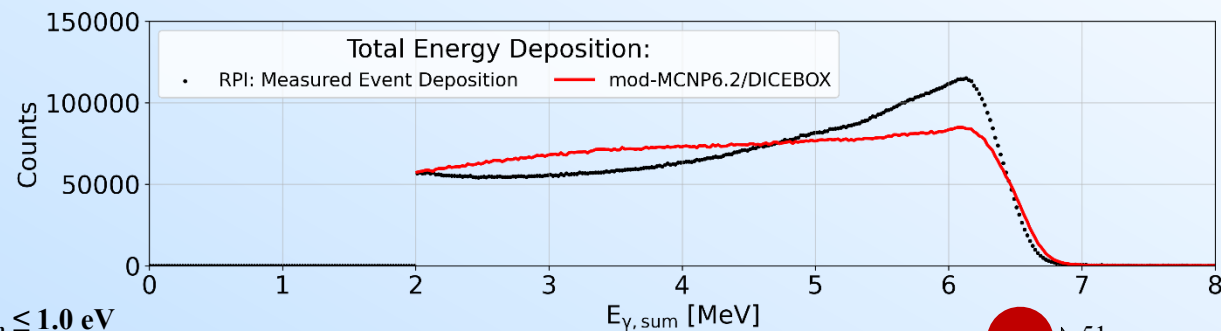
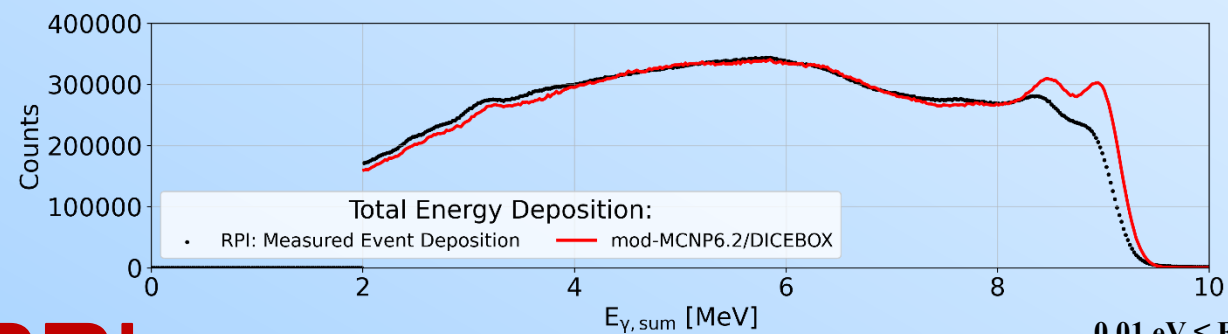
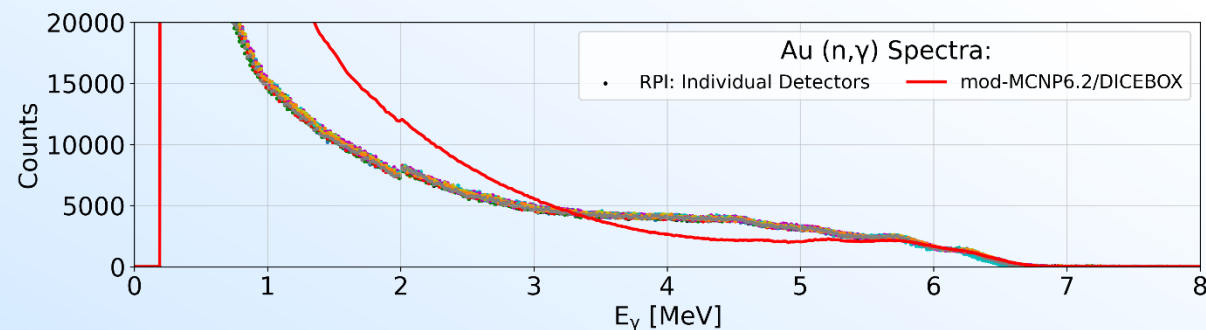
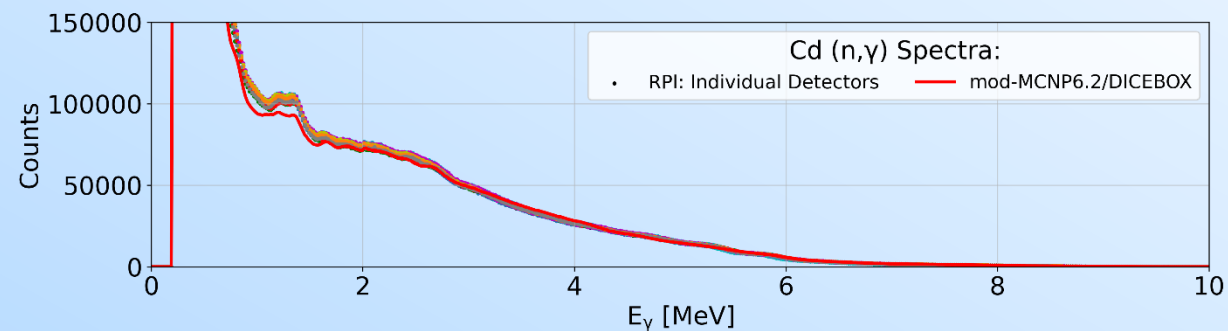
^[1]R. B. Firestone et. al., Phys. Rev. C **95**, 014328 (2017).

Isotope	Abundance	$\sigma_t(0.0253 \text{ eV})$	$\sigma_v(0.0253 \text{ eV})$
Cd-113	0.1222	19994.01	19969.33
Rest	0.8778	55.9	22.36

Results: ^{nat}Cd , ^{nat}Au



^{113}Cd only in DICEBOX, all other Cd isotopes in CGM

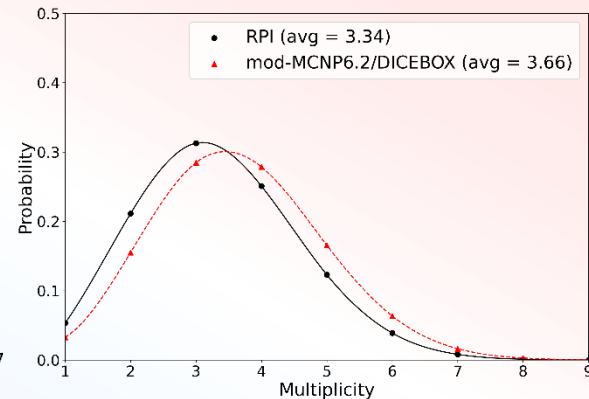
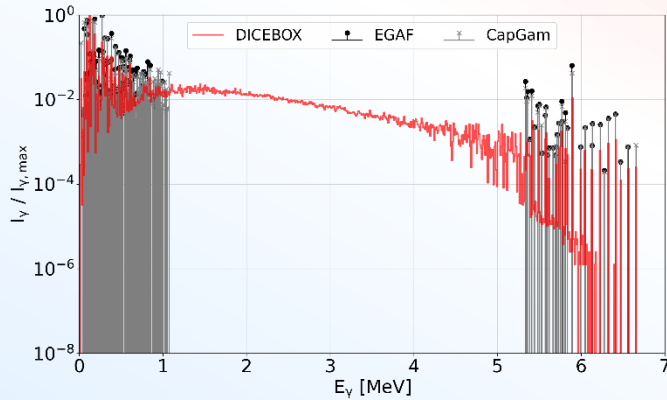
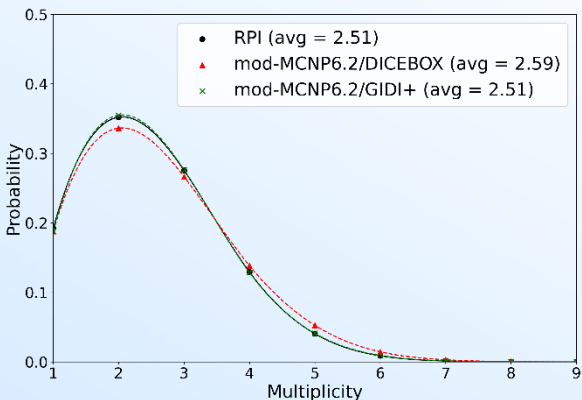
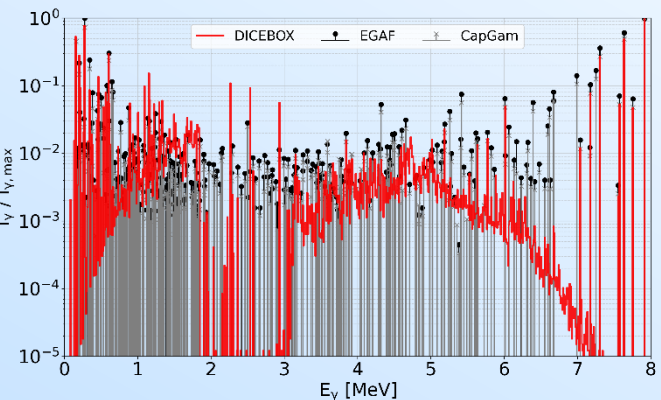


$0.01 \text{ eV} \leq E_n \leq 1.0 \text{ eV}$
 $0.200 \text{ MeV} \leq E_\gamma$
 $2.0 \text{ MeV} \leq E_{\Sigma\gamma} \leq 10.0 \text{ MeV}$

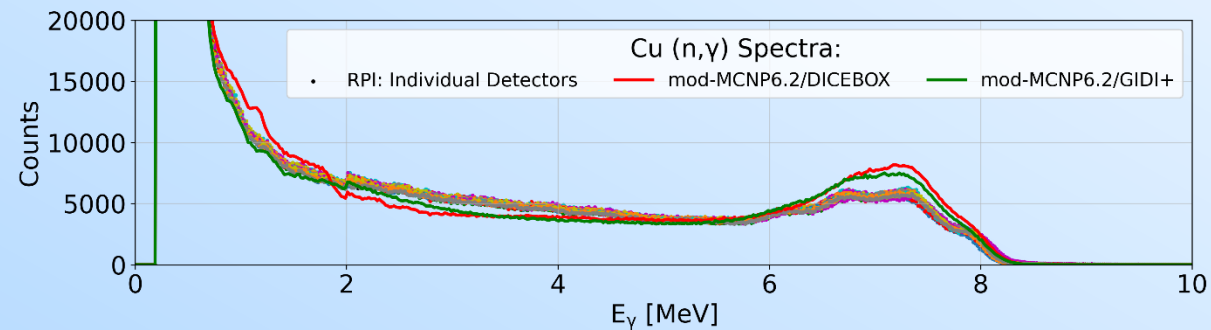
Isotope	Abundance	$\sigma_t(0.0253 \text{ eV})$	$\sigma_v(0.0253 \text{ eV})$
Cu-63	0.6915	6.61	4.47
Cu-65	0.3085	16.04	2.15

Results: natCu, natIn

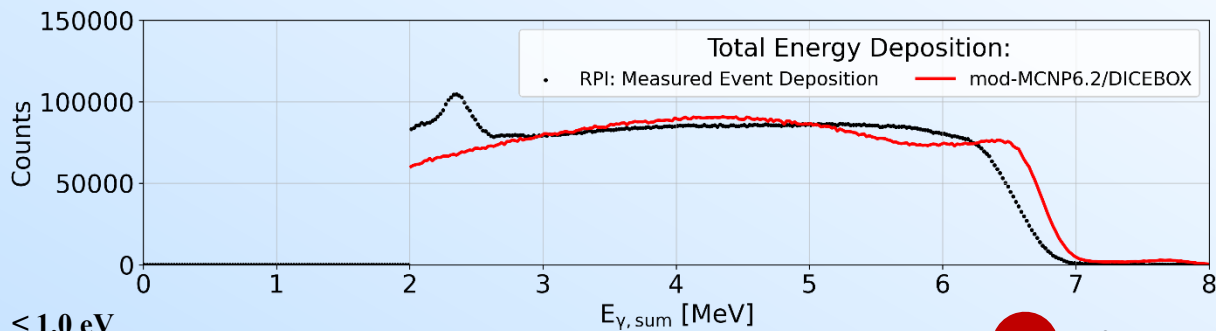
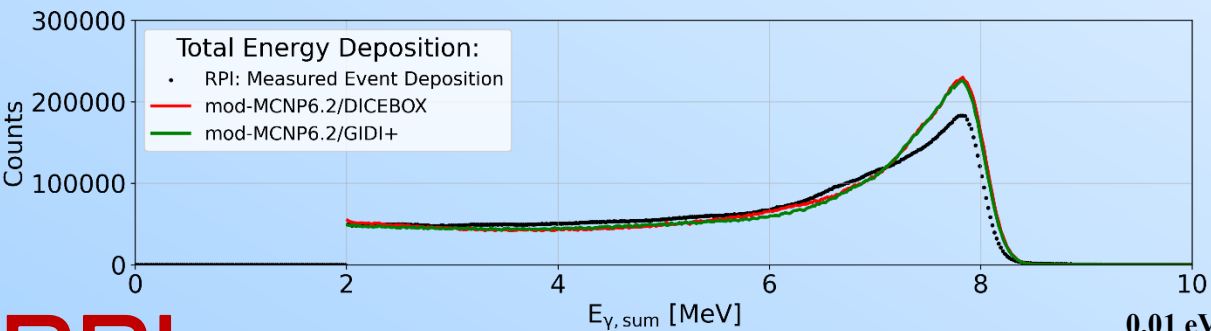
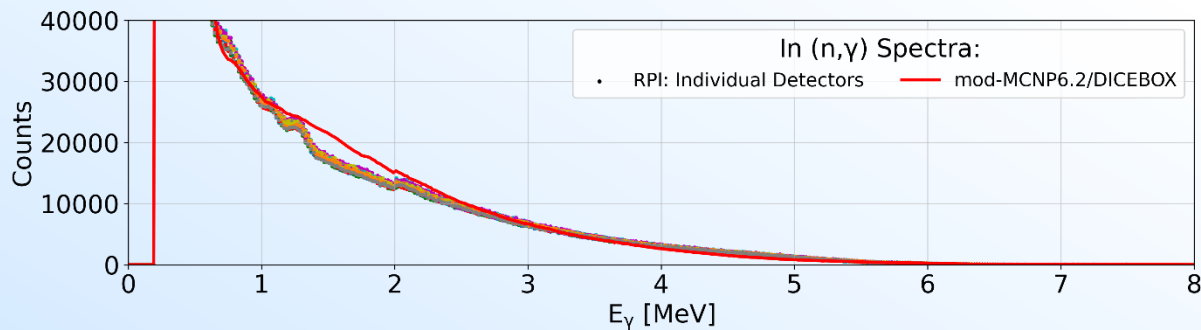
Isotope	Abundance	$\sigma_t(0.0253 \text{ eV})$	$\sigma_v(0.0253 \text{ eV})$
In-113	0.0429	15.82	12.13
In-115	0.9571	204.79	202.28



^{63}Cu only in DICEBOX & GIDI+, ^{65}Cu in standard CGM



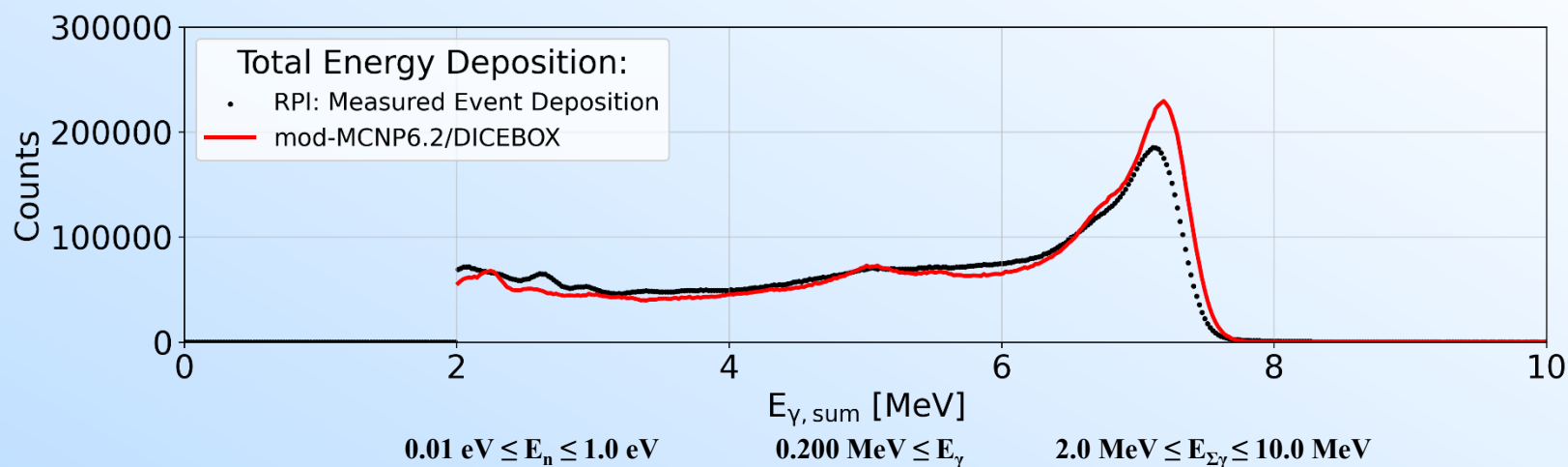
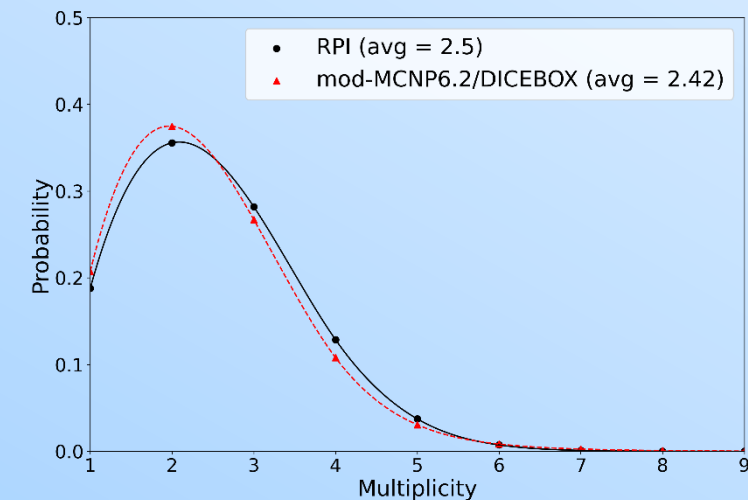
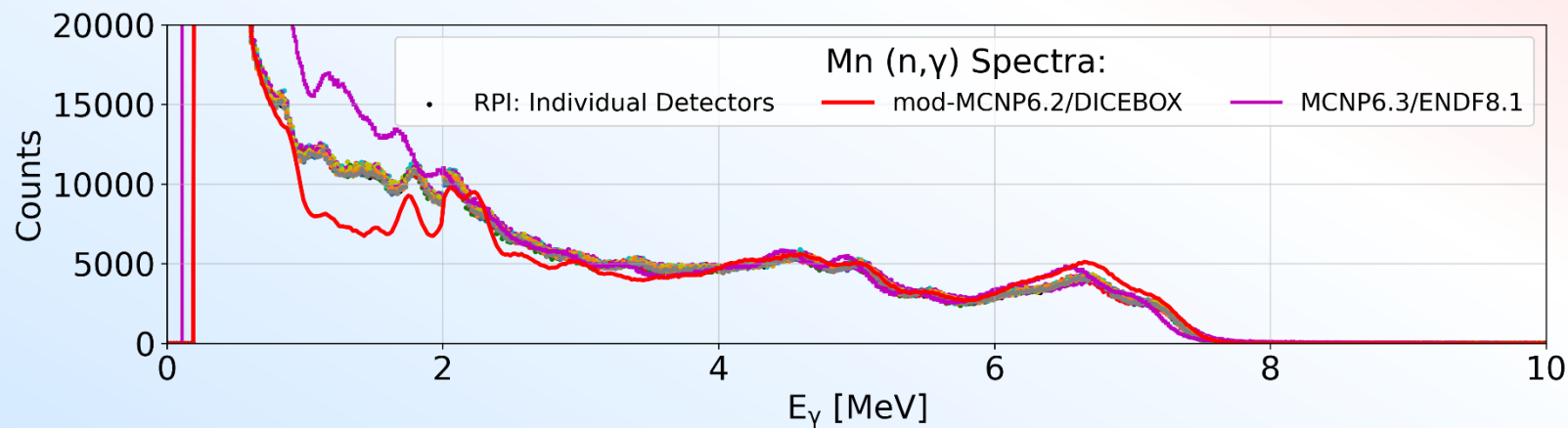
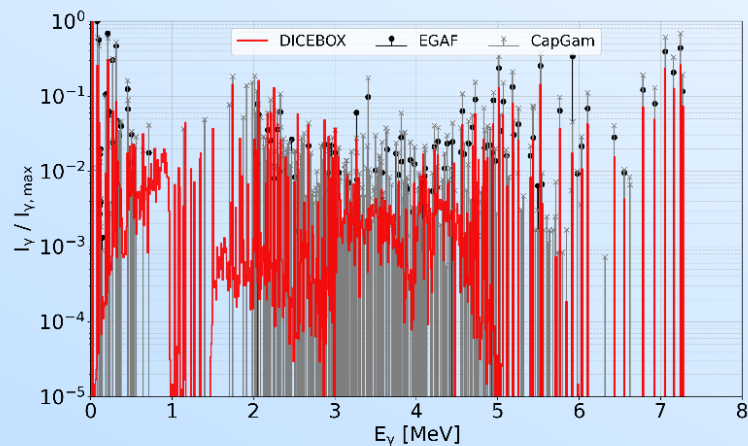
^{115}In only in DICEBOX, ^{115}In in standard CGM



$0.01 \text{ eV} \leq E_n \leq 1.0 \text{ eV}$
 $0.200 \text{ MeV} \leq E_\gamma$
 $2.0 \text{ MeV} \leq E_{\Sigma\gamma} \leq 10.0 \text{ MeV}$

Results: ^{nat}Mn

- ^{55}Mn updated thermal capture gamma-ray spectra in ENDF/B-VIII.1 unable to be used as a DICEBOX Input.
- ENDF Spectra agrees with RPI experimental data above 2 MeV.



Summary

- $^{90,91}\text{Zr}$ evaluation is progress
 - RRR energy was extended to higher energy for both isotopes.
 - Preliminary fast region calculation.
 - URR evaluation is on going
- URR in Fe-56 was considered and can provides some improvements but needs more work due to possibly discrepant the sample transmission experiments.
- RPI neutron-induced γ -ray spectra measurements and simulations
 - Several measurements were discussed (^{56}Fe , Cd, Au, Cu, In, Mn)
 - Methodology to compare the experiments to nuclear structure data was developed.
 - Observed differences between experiments and simulations indicate where capture gamma evaluations can be improved.
 - Working to develop a validation methods for neutron capture gamma production data and related transport methods.