

New Zirconium Evaluations for ENDF/B-IX

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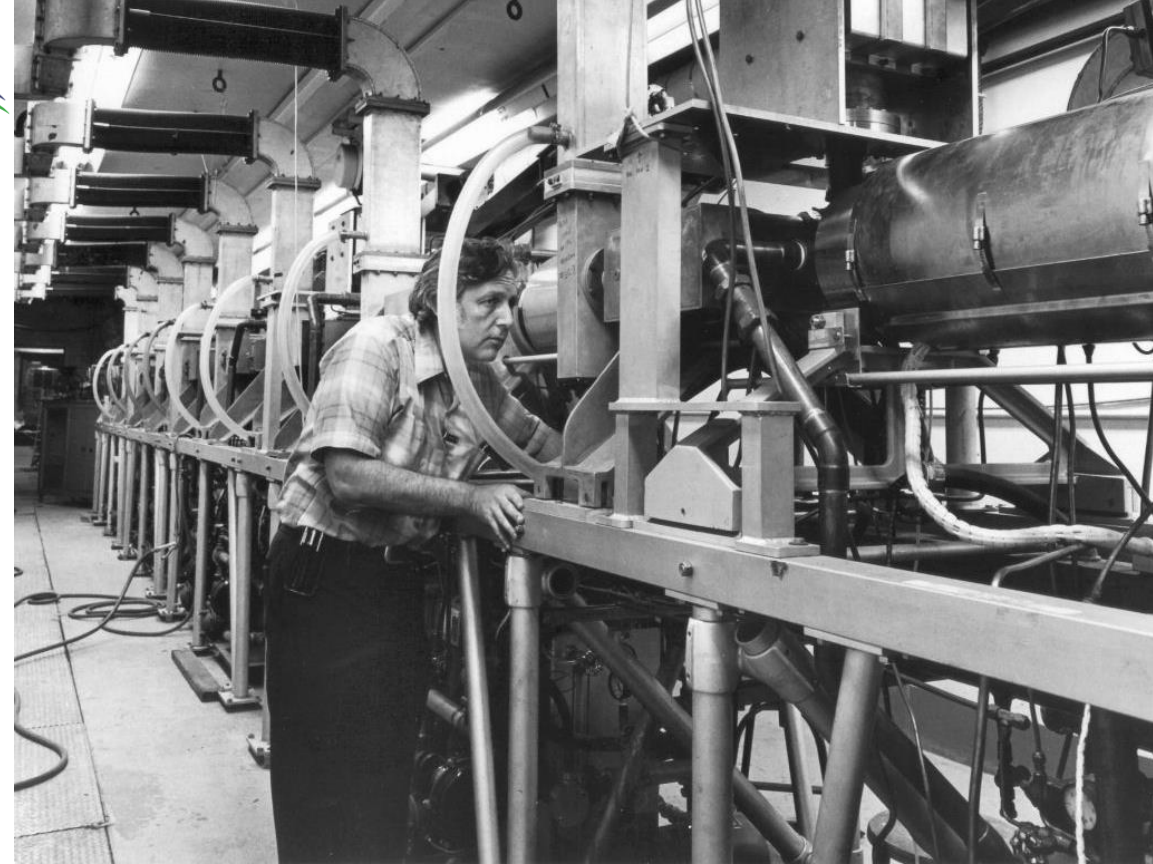
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Motivation for Stable Zirconium Isotope Evaluation

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 Zr data is lackluster despite widespread use.

Resolved Resonance Region

1. Resonances misassigned w.r.t transmission data
2. Large thermal cross section differences
3. Previous evaluations do not use R-Matrix formalism

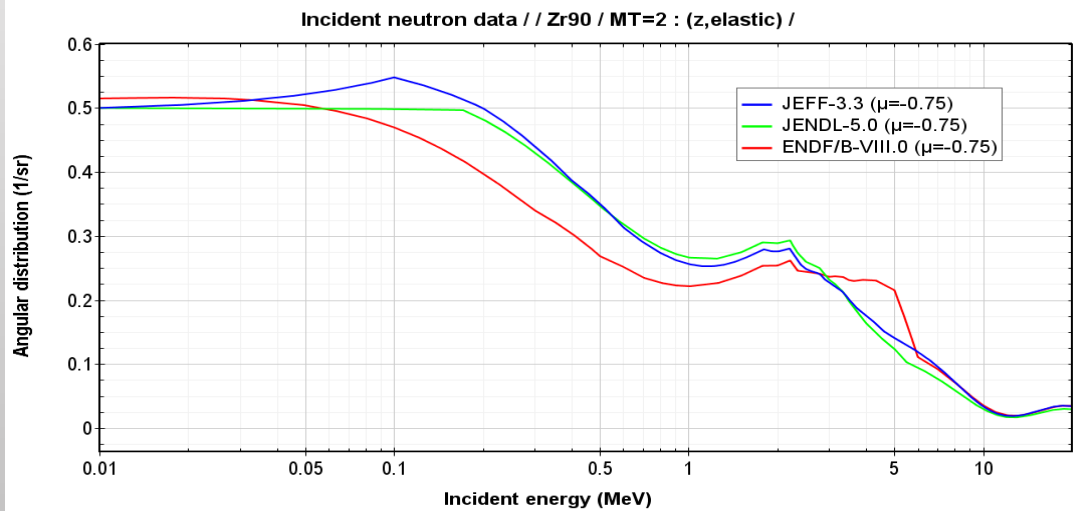
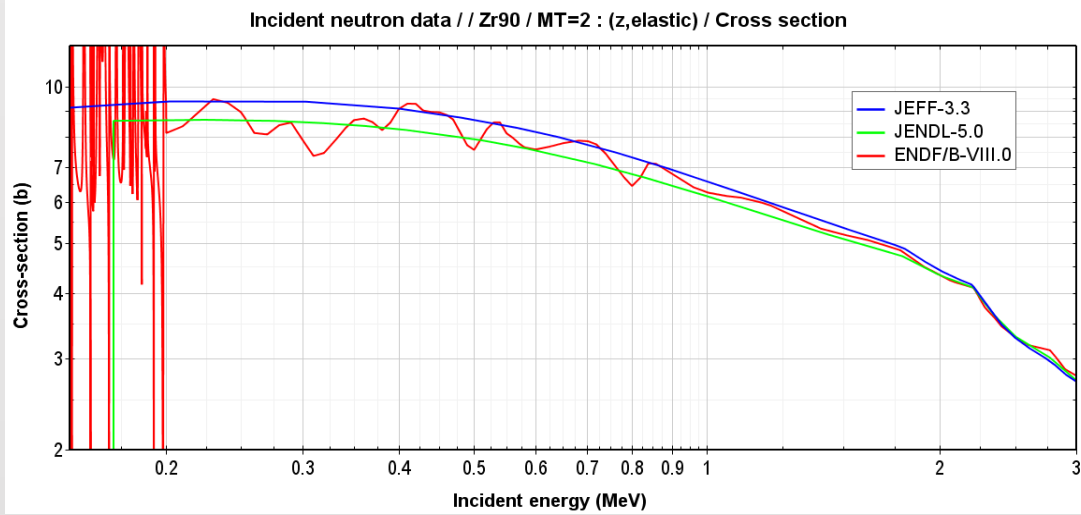
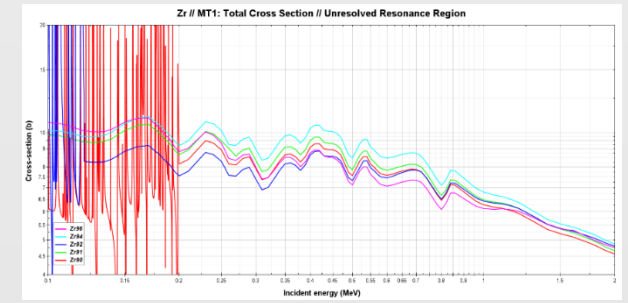
Unresolved Resonance Region

1. All isotopes possess same structure propagated from natural – unphysical
2. URR undocumented
3. Small cross sections differences observed cause significant differences in benchmarks

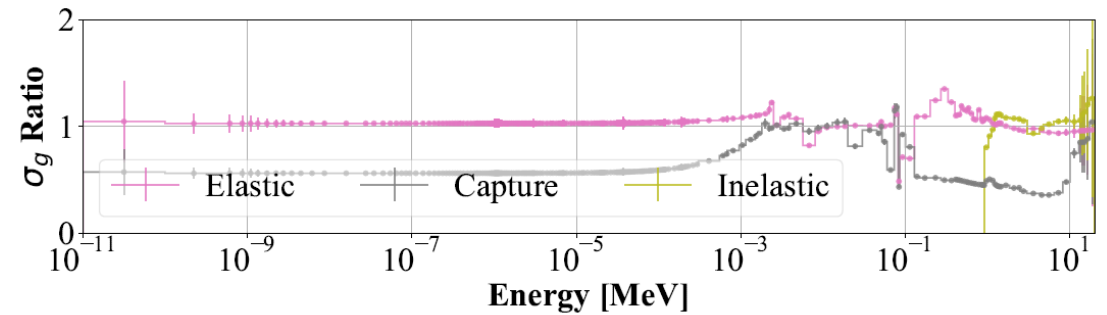
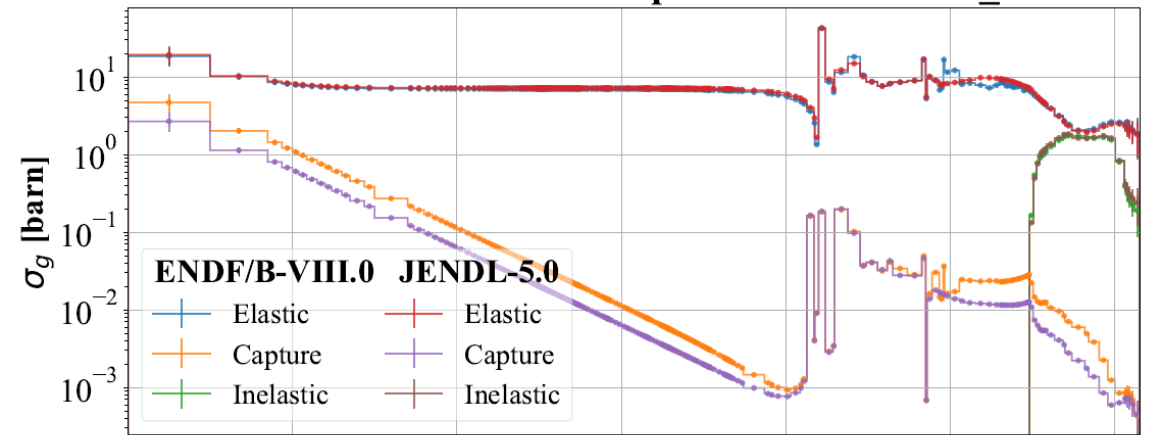
High Energy Region

1. New version of EMPIRE fixed bugs/more capabilities
2. New soft-rotor optical potential in RIPL developed for Zr
3. Elastic scattering angular distributions of utmost importance

Disagreement and Inconsistencies



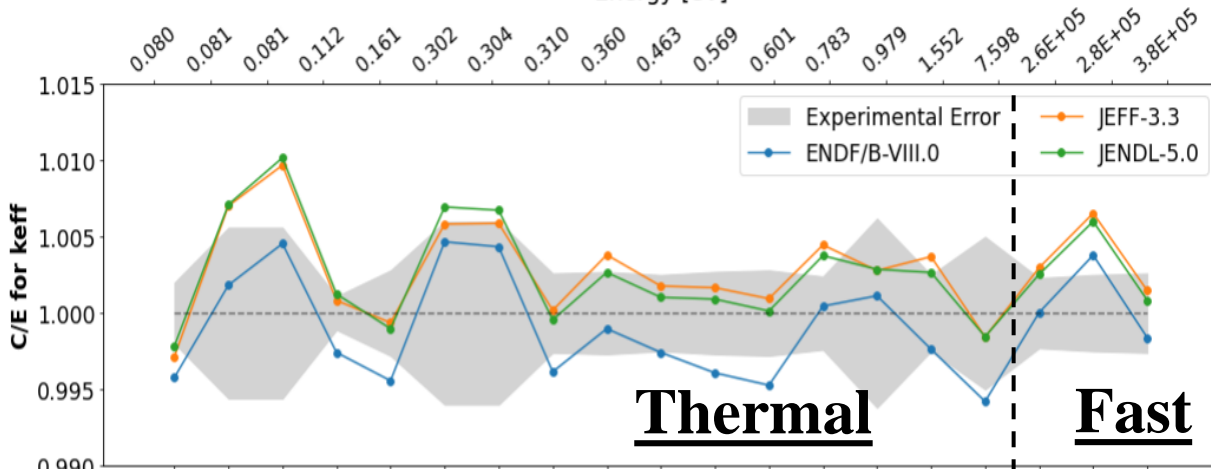
⁹²Zr Multi-Group Cross Sections For JENDL-5.0 and ENDF/B-VIII.0 Sampled From LCT074_005



Benchmark Sensitivity

C/E of Zirconium Sensitive Critical Benchmarks

Energy [eV]

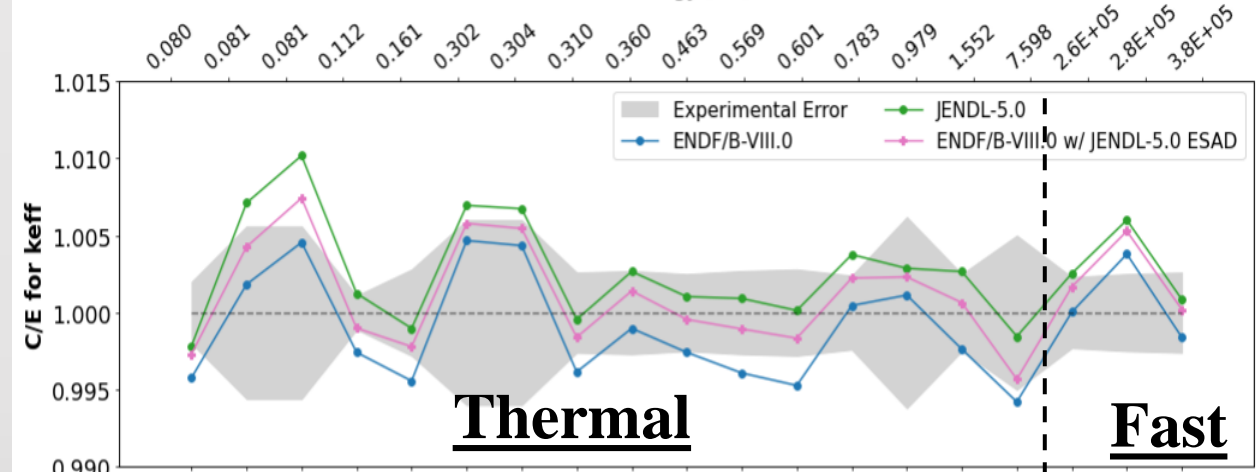


Thermal

Fast

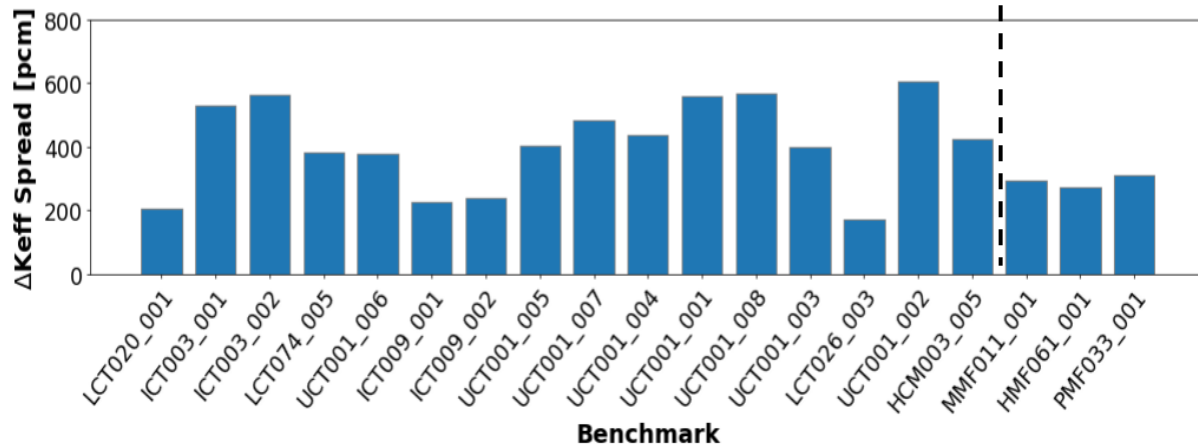
C/E of Zirconium Sensitive Critical Benchmarks with ESAD Perturbation

Energy [eV]

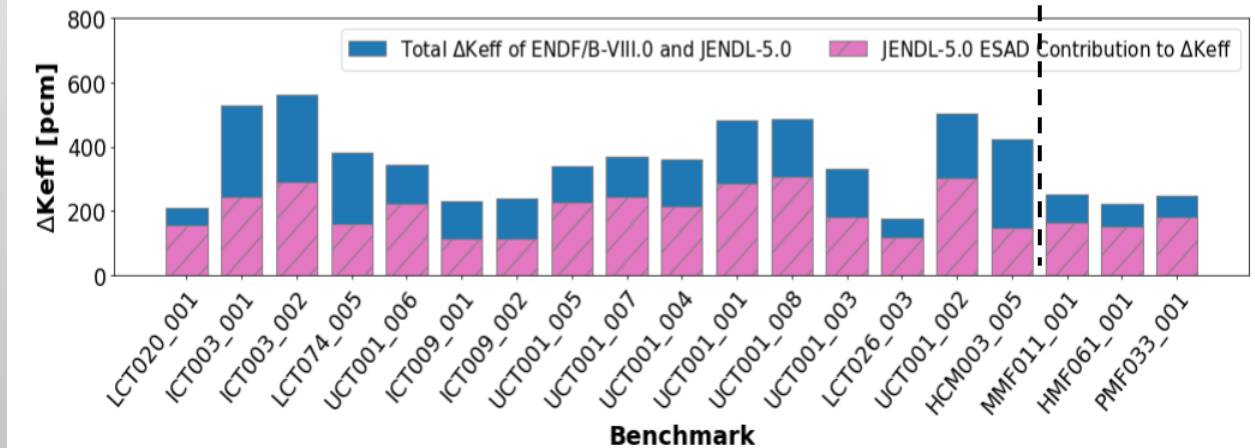


Thermal

Fast



Benchmark



Benchmark

NCSP Plan for Zirconium Nuclear Data

Measurements

Compilations

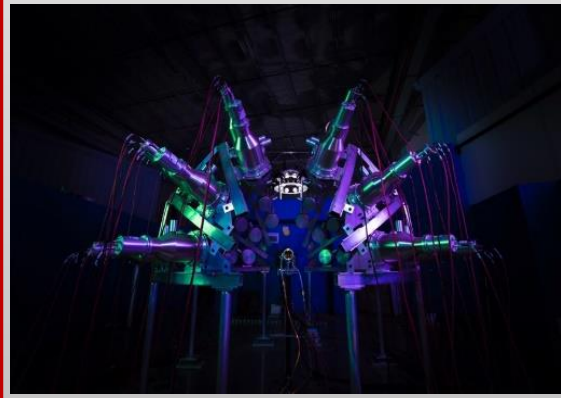
Evaluations

Processing

Validation

Applications

Zirconium (^{90,91,92,94,96} Zr)	ORNL	ORNL	ORNL				
Basis	Neutron capture and possibly transmission measurements in resonance range at GELINA. Old ORNL transmission data on enriched isotopes are available for analysis. Isotopically enriched samples are required. Zirconium is a key structural element that is primarily used in cladding for fuel rods and is currently in consideration for use with advanced nuclear fuel matrices in the form of zirconium hydride. The main application is reactor fuel cladding. ⁹⁰ Zr transmission and capture measurements were recently completed by ORNL. NR continues to be unsatisfied with Zr evaluations in ENDF. Inelastic scattering measurements at least on ⁹² Zr, ^{90,91} Zr measurement completed. ^{92,94} Zr samples to be ordered in FY2023 and shipped to GELINA in FY2024. ⁹² Zr measurement to be completed and ⁹⁰ Zr measurement started in FY2024.						



EMPIRE
Nuclear Reaction Model Code

SAMMY

Zirconium (^{90,91,92,94,96} Zr)	ORNL	ORNL	ORNL	ORNL		
	NNL	NNL	NNL	NNL		
	RPI	RPI	RPI	RPI		
	BNL	BNL				

Basis
Resonance evaluations. Zirconium is a key structural element that is primarily used in cladding for fuel rods and is currently in consideration for use with advanced nuclear fuel matrices in the form of zirconium hydride. The latest ENDF/B-VII.1 resonance evaluation relies on JENDL-4 data and resonance parameters from the Atlas of Neutron Resonances. As a result, the evaluated resonance parameters are not based on detailed R-matrix analyses. In addition, newer RPI total cross-section measurements on natural zirconium indicate that the older ENDF/B-VI.8 data match the recent RPI measurements better than the newer isotopic evaluations. Furthermore, improved differential measurements of the zirconium isotopes have been identified on the OECD/NEA nuclear data High Priority Request List (HPRL). Differential measurements are needed in the resonance region to accurately predict the neutron resonances for the zirconium isotopes, and corresponding resonance evaluations are needed to provide detailed resonance parameters and covariance data. In addition, the SAMMY evaluation software has the capability to generate angular scattering distributions from the resonance parameters thereby providing detailed resonance scattering structure that will improve the elastic scattering modeling for the zirconium isotope evaluations. NR continues to be unsatisfied with Zr evaluations in ENDF. BNL will re-evaluate the fast and URR regions of all stable Zr isotopes to ensure that the elastic scattering angular distribution is consistent with the rest of the fast region, to improve the inelastic scattering cross sections and to correct issues with the URR evaluation implemented in ENDF/B-VIII.0 (under DOE-SC funding).



New for ENDF/B-IX

RRR: New evaluations will use R-Matrix resonance parameterization determination over MLBW.
Evaluations will incorporate new ORNL isotopic transmission and capture measurements.

URR: New evaluations will leverage the new implementation of SESH in SAMMY.

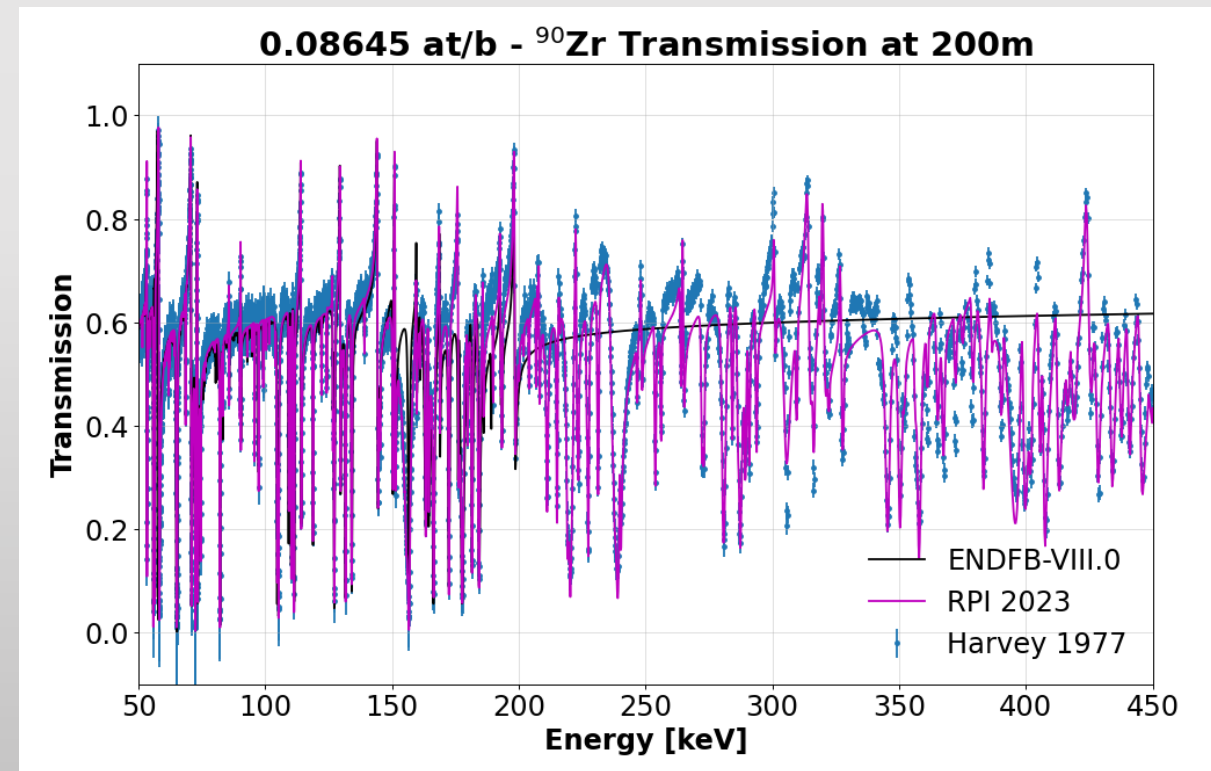
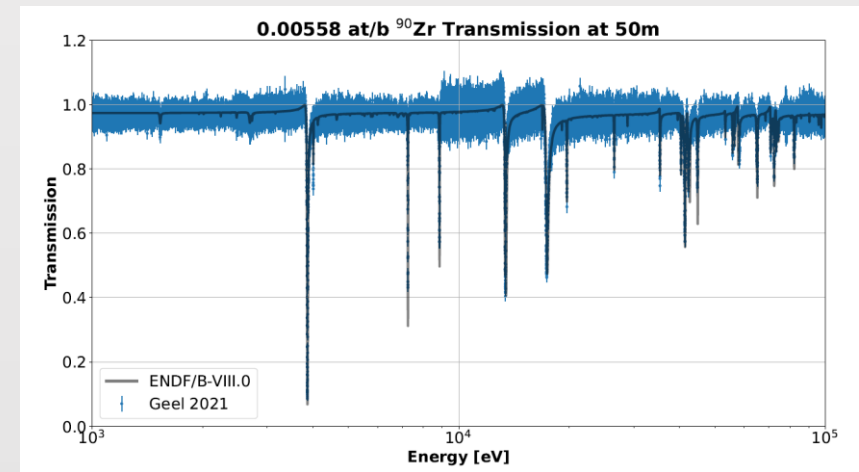
Fast: New evaluations with modern version of EMPIRE using new soft-rotor OMP developed for Zr. E
Evaluations will leverage new ^{nat}Zr transmission from RPI, DT validation data from China, and others.

Isotope	New ORNL/GEEL Measurement Status	RRR Evaluation	URR Evaluation	Fast Evaluation
Zr-90	Complete	RPI – NNL - ORNL	RPI – NNL - ORNL	RPI – BNL
Zr-91	Complete	RPI – NNL - ORNL	RPI – NNL - ORNL	RPI – BNL
Zr-92	2024/2025	ORNL	NNL - ORNL	BNL
Zr-94	2025/2026	ORNL	NNL - ORNL	BNL
Zr-96	N/A	ORNL	NNL - ORNL	BNL

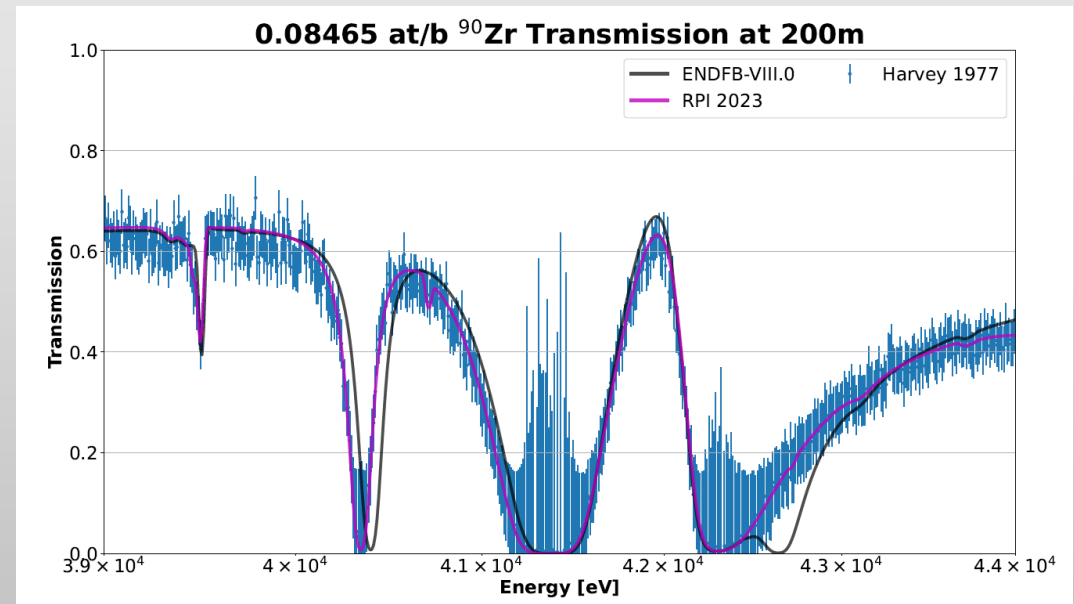
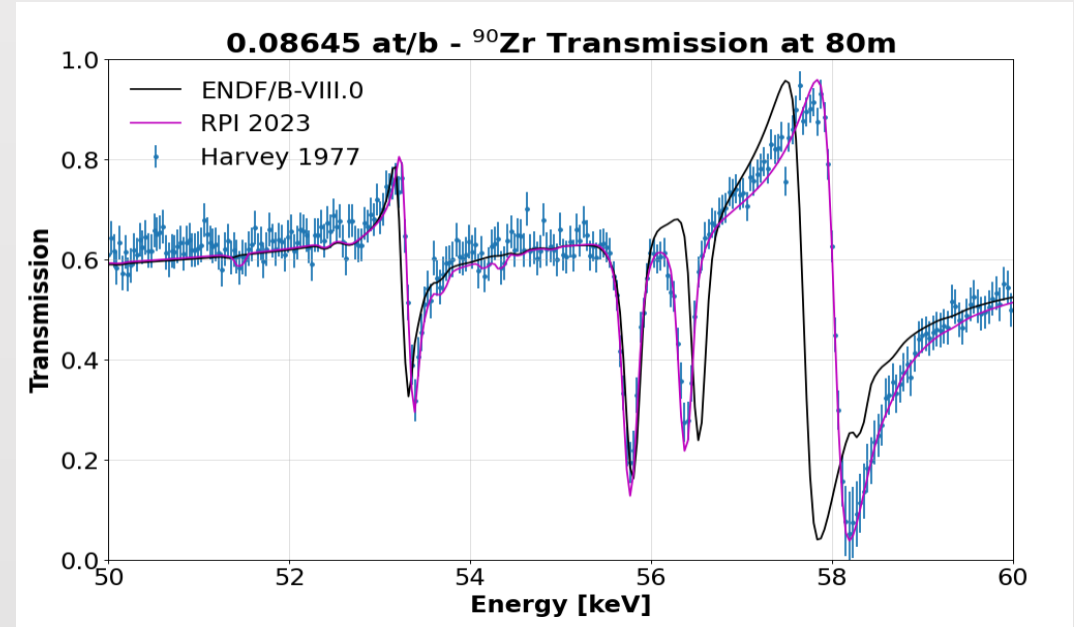
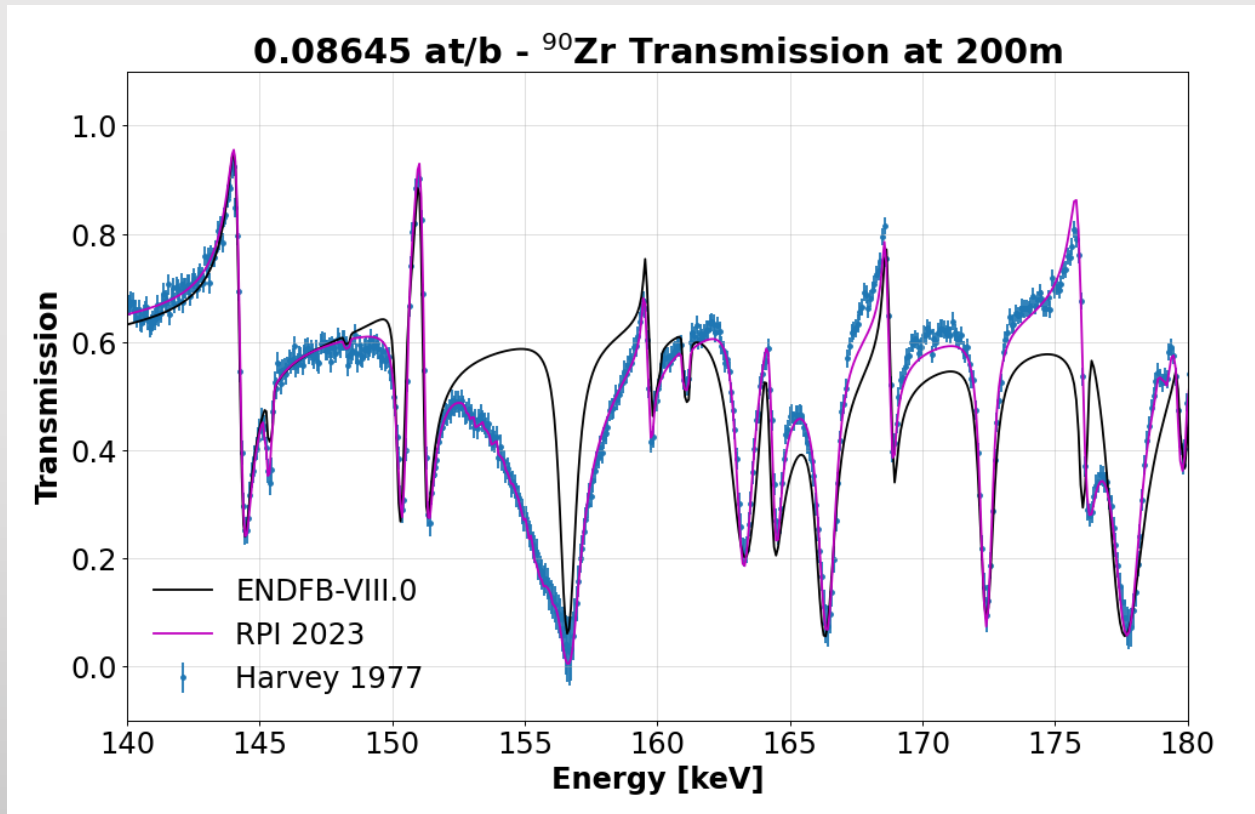


^{90}Zr Evaluation at RPI

- Metallic ^{90}Zr samples measured at ORELA (1977) and JRC-Geel (2021)
- Two high resolution transmission measurements of 0.08645 at/b sample from ORELA:
 1. 80m w/ 6Li (100 eV \rightarrow 500 keV)
 2. 200m w/ NE110 (30 keV \rightarrow 2.2 MeV)
- ORNL/JRC-Geel measurements used thin 0.00558 at/b capture sample
 - Large s-wave resonances don't black out
 - Deadtime limits use above 85 keV

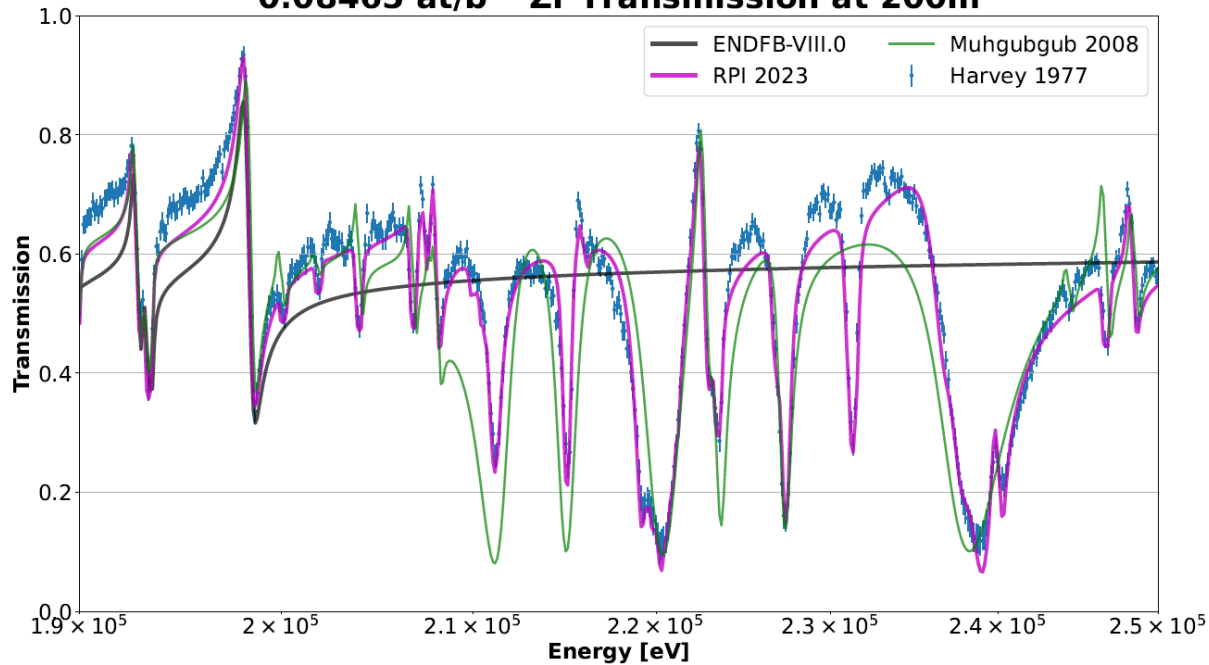


^{90}Zr Transmission

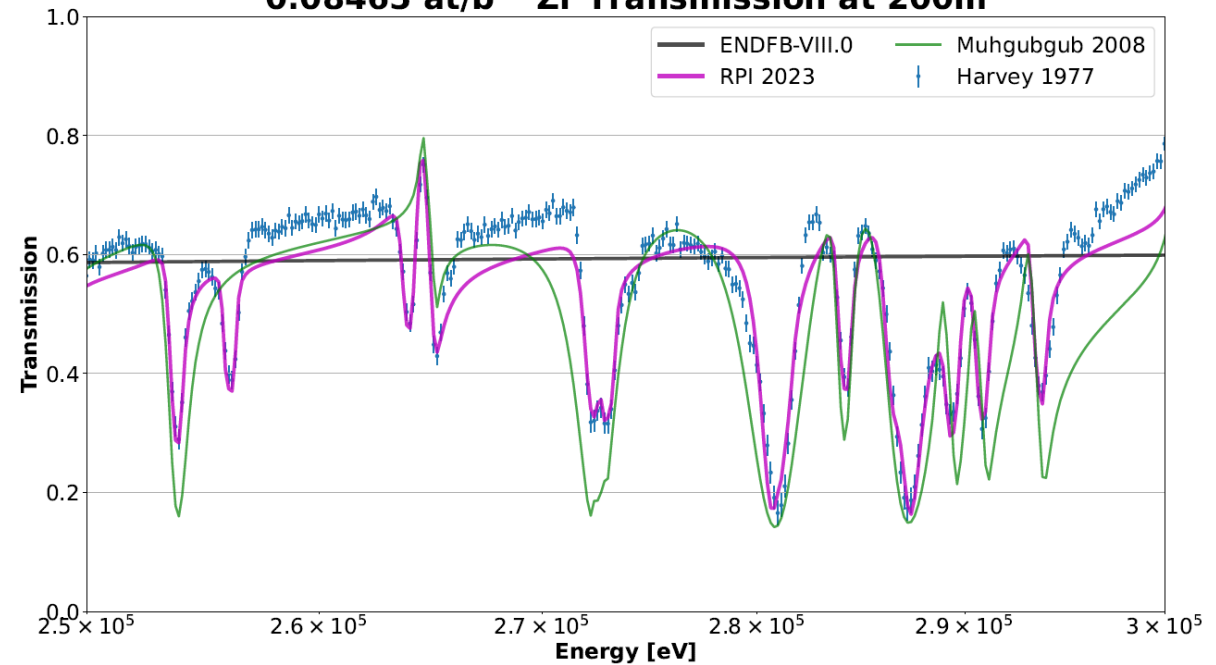


Progress on ^{90}Zr RRR Extension

0.08465 at/b ^{90}Zr Transmission at 200m



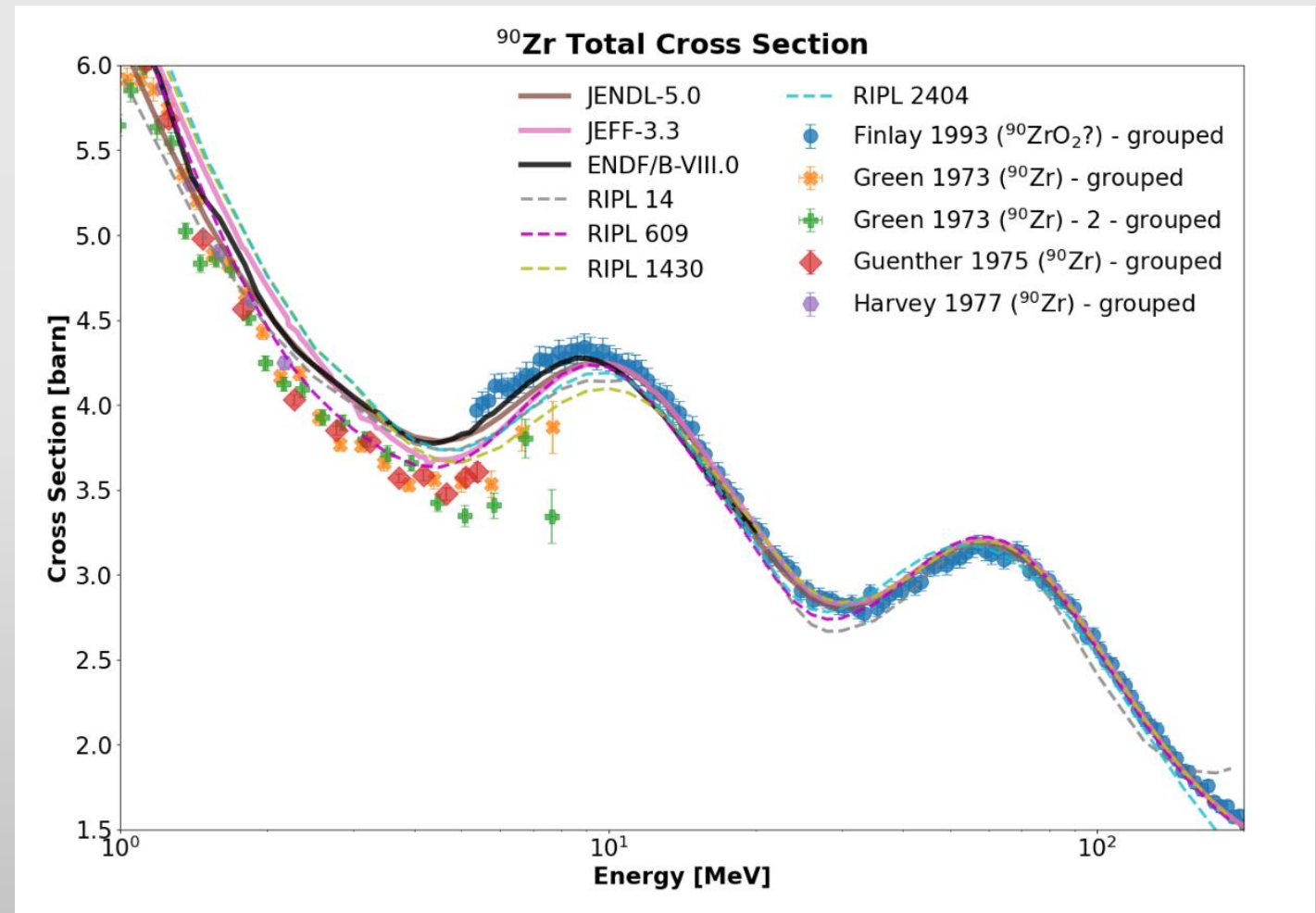
0.08465 at/b ^{90}Zr Transmission at 200m



Initial fitting is being performed to extend the resolved resonance region of ^{90}Zr above the current limit of 200 keV present in ENDF/B-VIII.0. More fitting and work with external levels is required.

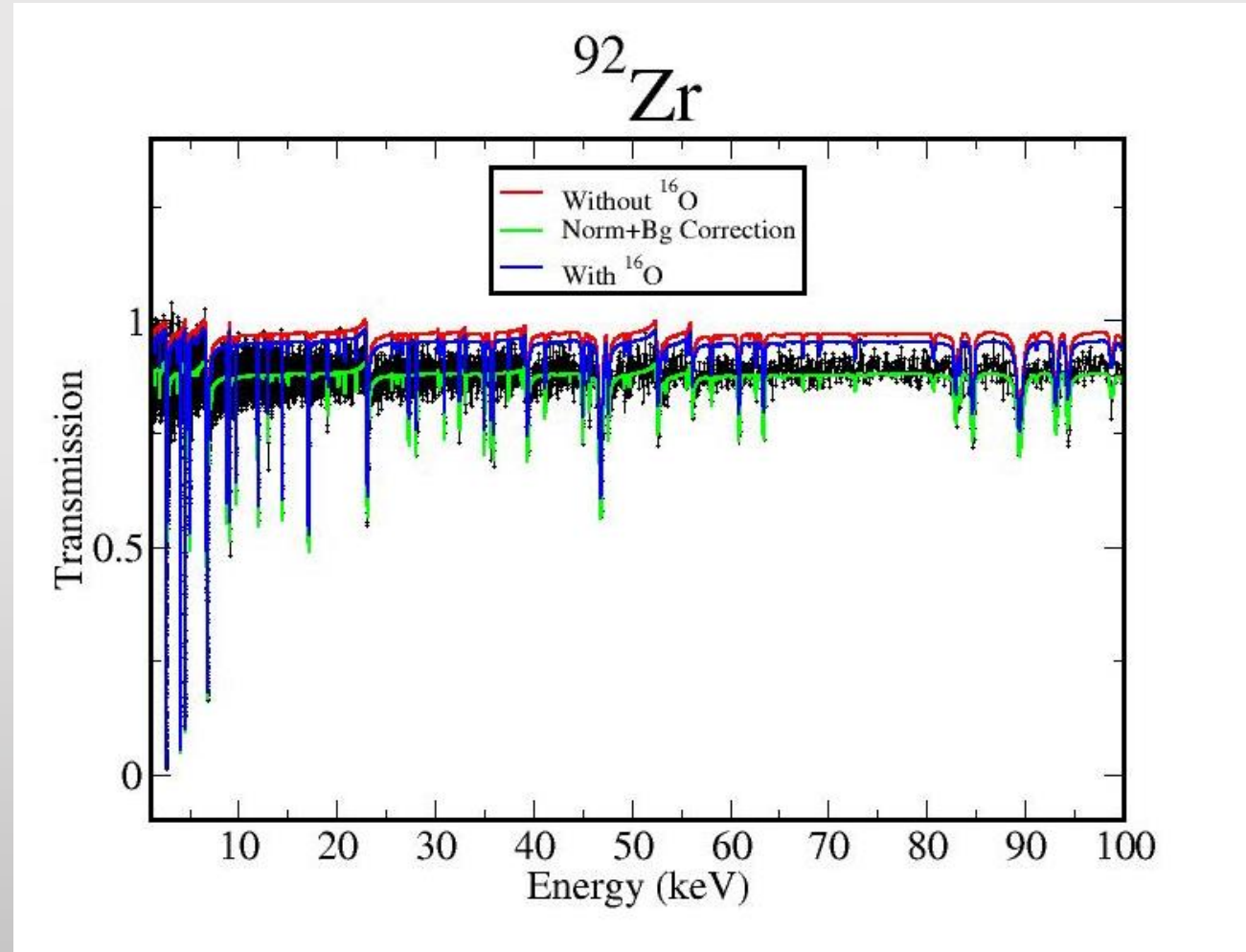
Beginnings of ^{90}Zr Fast

- Soft rotational coupled-channels optical model potential developed by Capote and Soukhovitskii specifically for Zr isotopes (RIPL 609)
- Investigation of different OMPs present in RIPL and elsewhere is first step
- Discontinuity at ~ 7 MeV between Finaly and all other measurements is observed

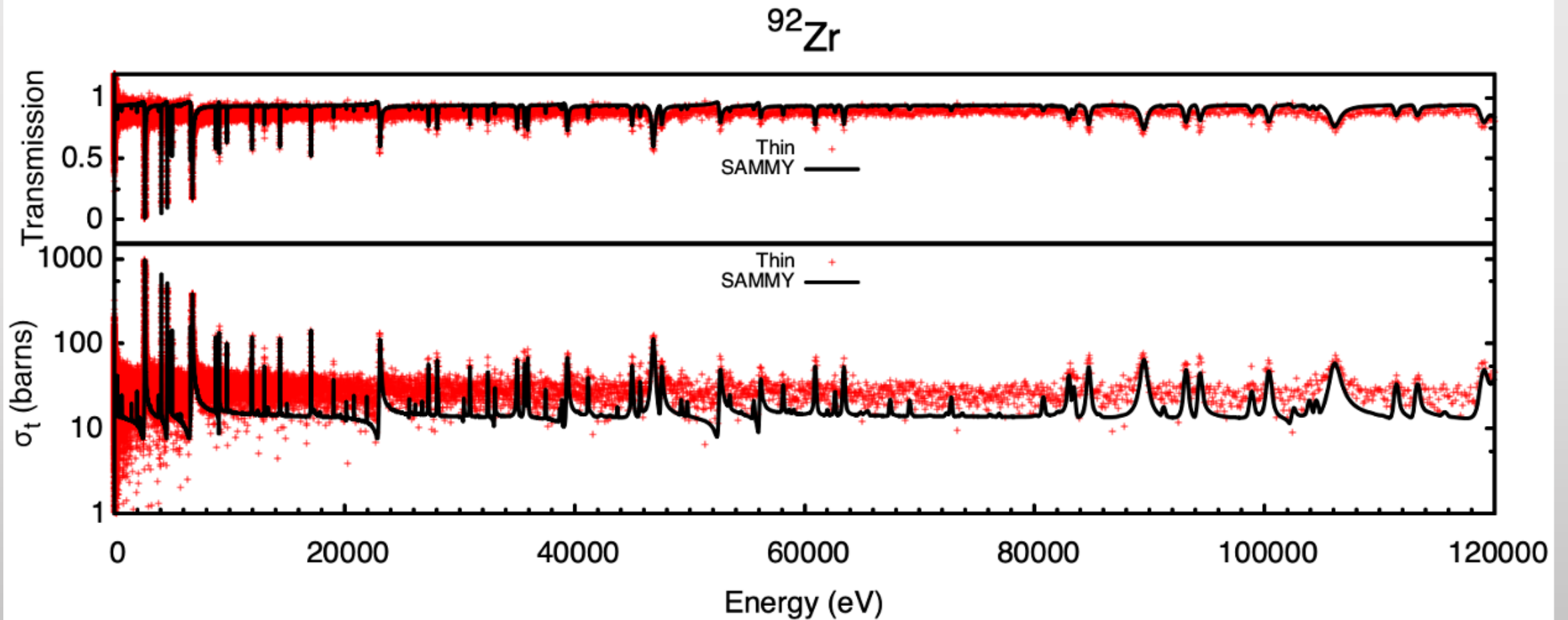


^{92}Zr and ^{94}Zr Evaluation at ORNL

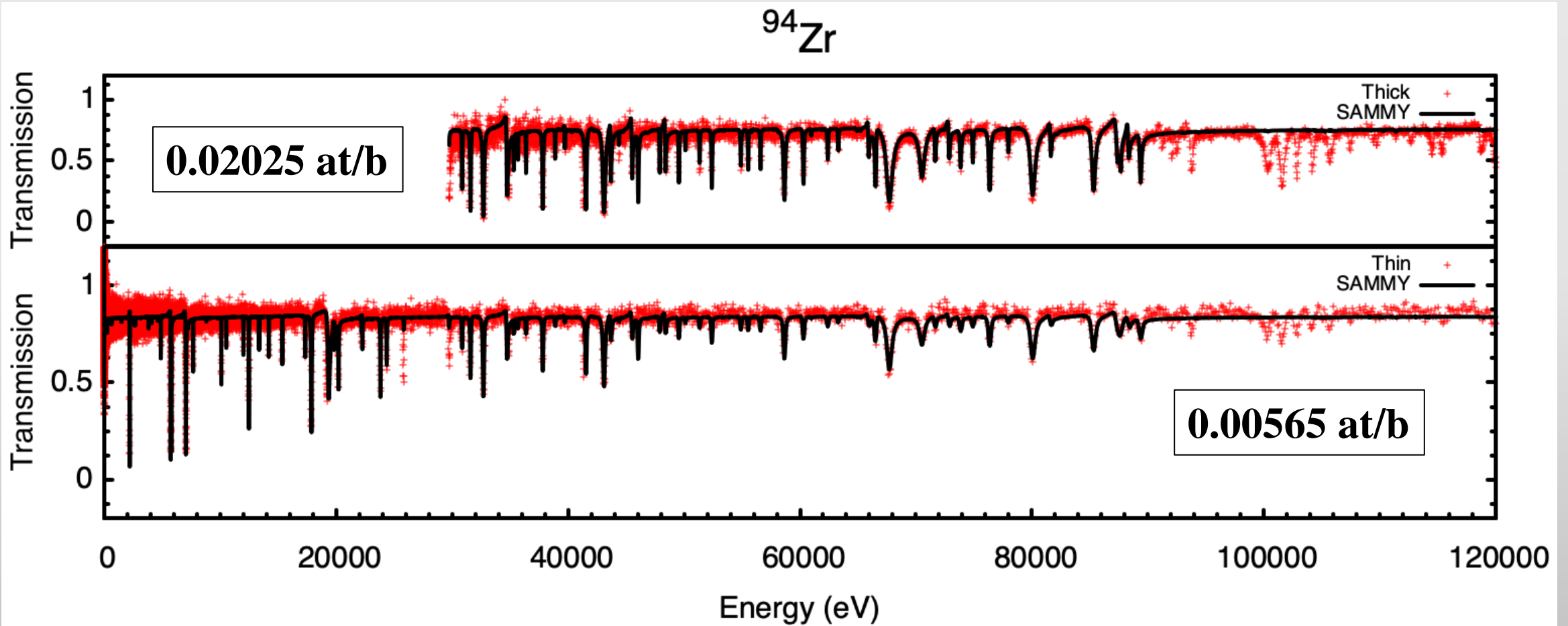
- 2 high resolution transmission measurements from ORELA
- 0.00455 at/b thin and 0.02245 at/b thick samples measured at distance of 78.2 meters
- ZrO_2 samples – EXFOR data uncorrected for oxygen content
- Background correction and re-normalization needed
- Similar story with ^{94}Zr



Fitted thin sample ^{92}Zr ORELA transmission data corrected for the normalization, background, and ^{16}O content.



Fitted thin and thick ^{94}Zr ORELA transmission data corrected for the normalization, background, and ^{16}O content.



Zirconium Evaluations Going Forward

RPI Evaluation Activities

- Finish ^{90}Zr resolved resonance region evaluation using new JRC-Geel (n, γ) data
- Extending ^{90}Zr resolved resonance region as far as reasonably achievable
- Decide on inclusion of URR in ^{90}Zr evaluation or use statistical model (fast) and perform evaluation(s)
- Repeat for ^{91}Zr

ORNL Evaluation Activities

- Examination whether extension of resolved resonance energy region is needed for $^{92,94}\text{Zr}$
- Inclusion of new JRC-Geel capture data in the fitting as they become available
- Inclusion of coherent and incoherent scattering in the resonance fitting
- Scope out ^{96}Zr
- Support NNL URR evaluations

BNL Evaluation Activities

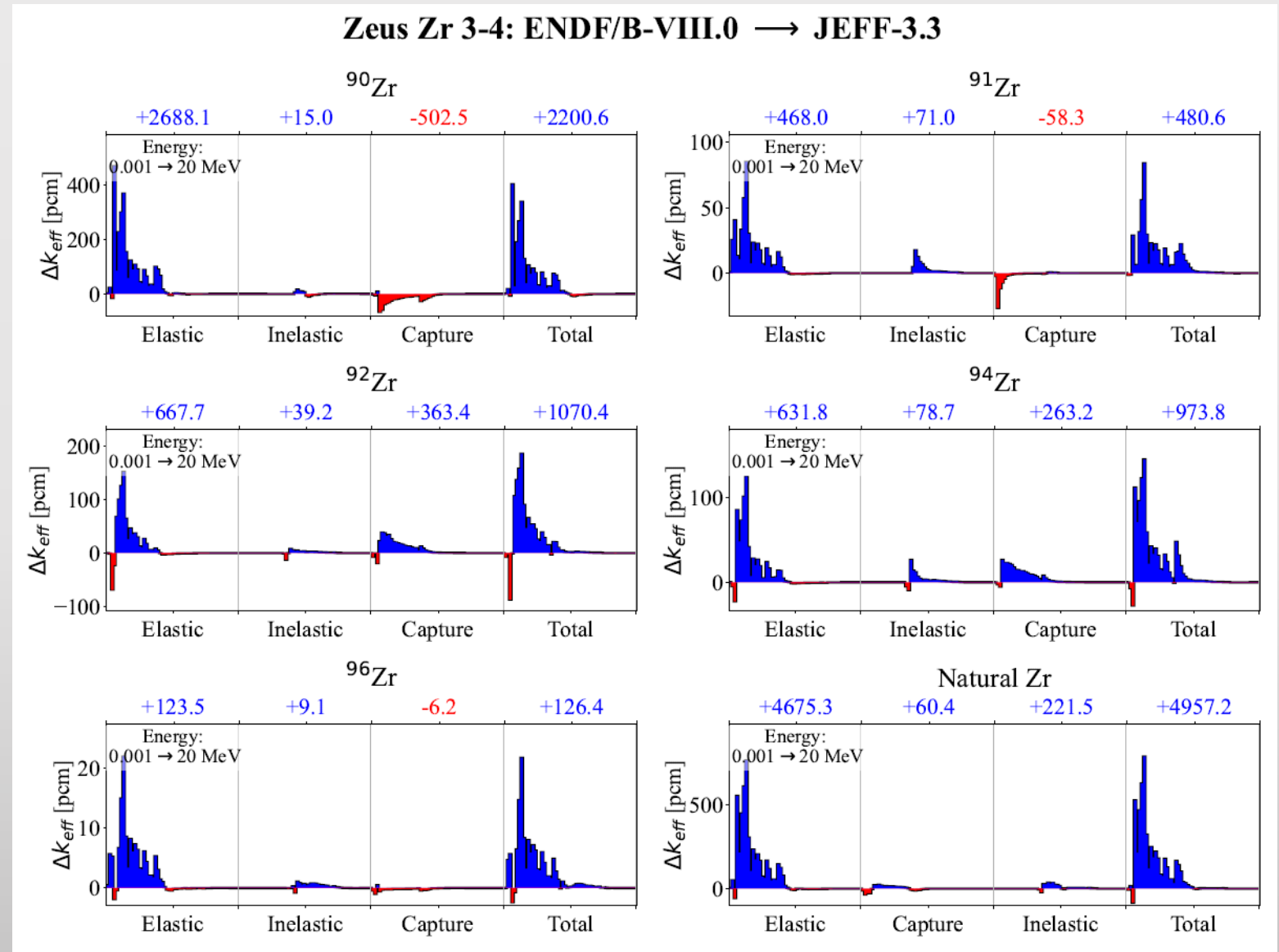
- Perform fast region evaluations of $^{92,94,96}\text{Zr}$
- Support RPI in performing $^{90,91}\text{Zr}$ fast region evaluation

NNL Evaluation Activities

- Perform unresolved resonance region evaluations of $^{92,94,96}\text{Zr}$
- Support RPI in performing $^{90,91}\text{Zr}$ RRR and URR evaluations

Sneak Peak at Future Validation

- IER 516: Zirconium Test Assembly in CED-1 (Preliminary design) at LANL
- Maximizing sensitivity to Zr nuclear data shows enormous differences in predicted system K_{eff} values of preliminary designs observed





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Extra Slides

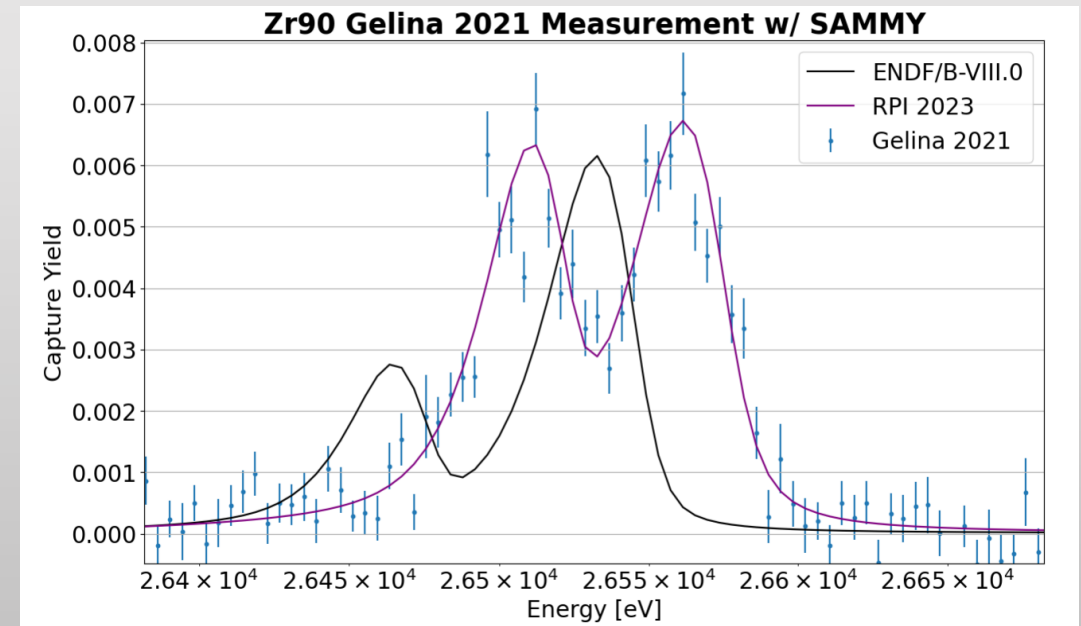
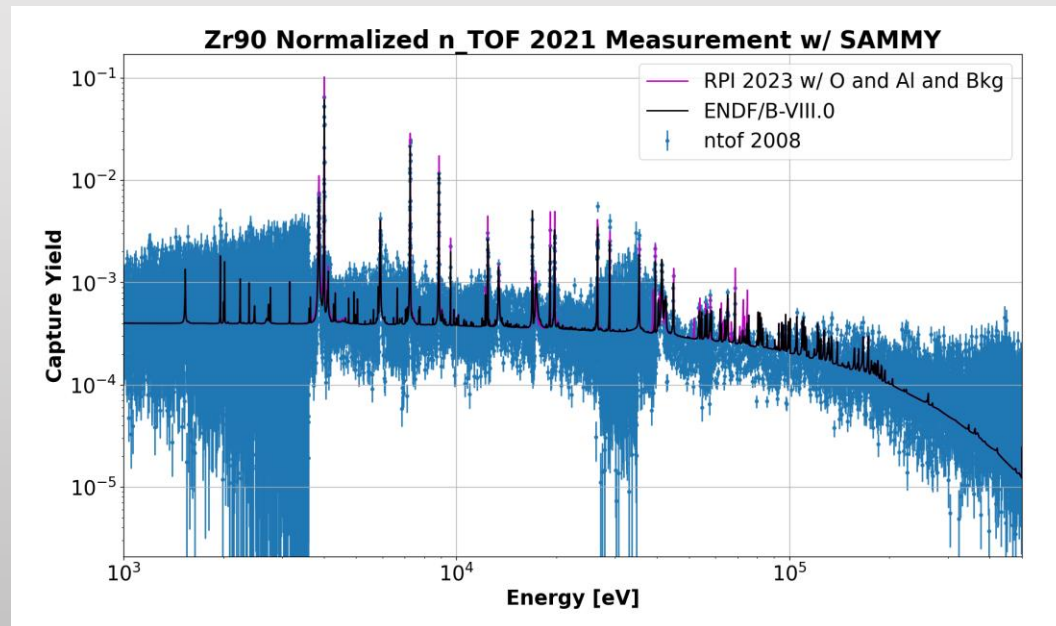


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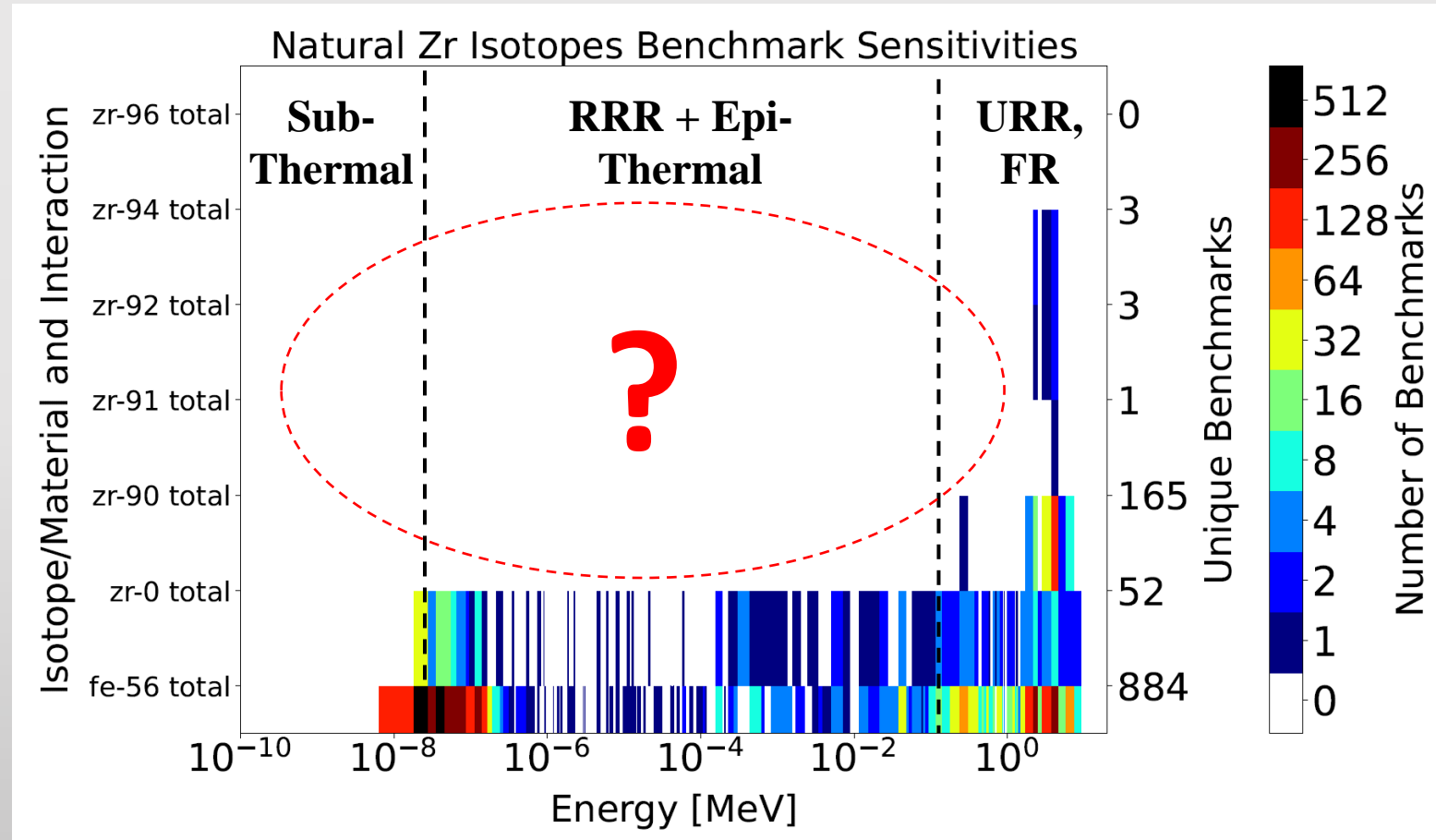
^{90}Zr Capture Preliminary Evaluation

- Capture measurement on same thin ^{90}Zr sample with C_6D_6 capture array at 60m at GELINA in 2021
 - Mistake found in flux normalization in data reduction after performing initial fitting with SAMMY
- nTOF measurement of ^{90}Zr capture at 185m with C_6D_6 using $^{90}\text{ZrO}_2$ sample
 - Background and encapsulation corrections made



Current Zr Critical Benchmark Experiments

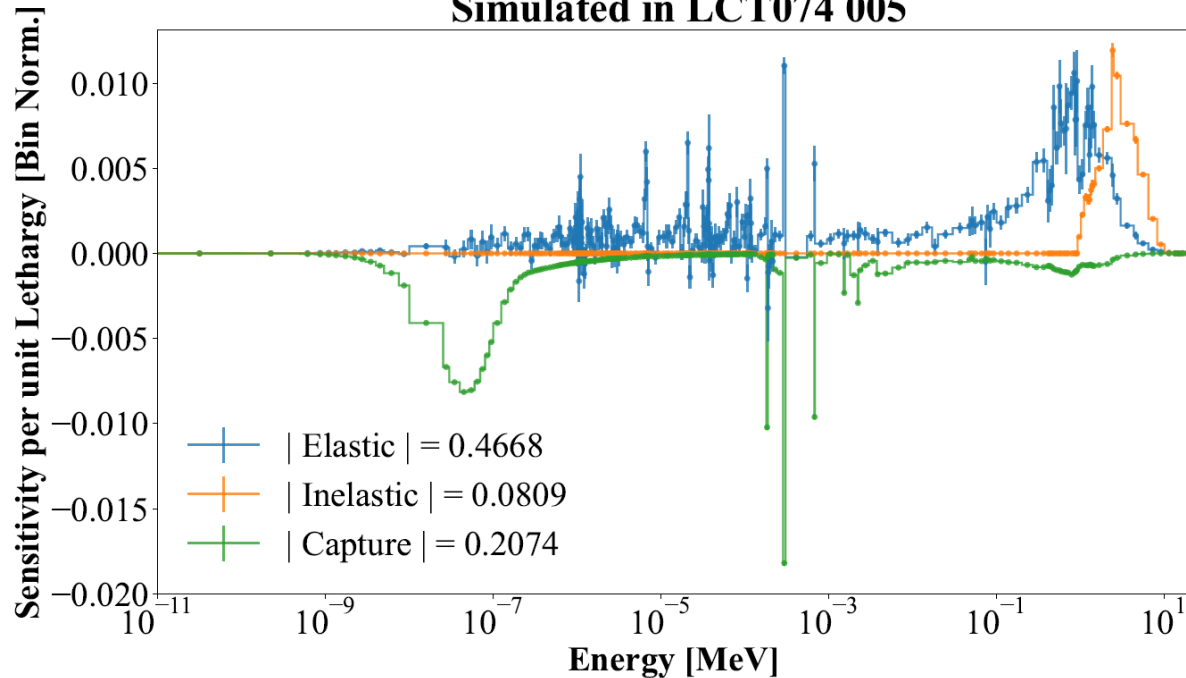
- High fidelity integral experiments are required to validate evaluation performance of Zr
 - Validation most important in energy range of fission neutron emission
 - Many Zr sensitive benchmark experiments are large thermal systems and/or do not meet modern evaluation standards
- Lack of differential and integral data can lead to non-physical evaluations



A score on this point corresponds to a sensitivity coefficient greater than or equal to $1e-3$ at a given energy

Some Sensitivity Profiles

ENDF/B-VIII.0 Natural Zr Sensitivity Profile
Simulated in LCT074 005



ENDF/B-VIII.0 Natural Zr Sensitivity Profile
Simulated in Zeus Zr 3-4

