New Cross Section Measurements and Evaluations of Zirconium Isotopes

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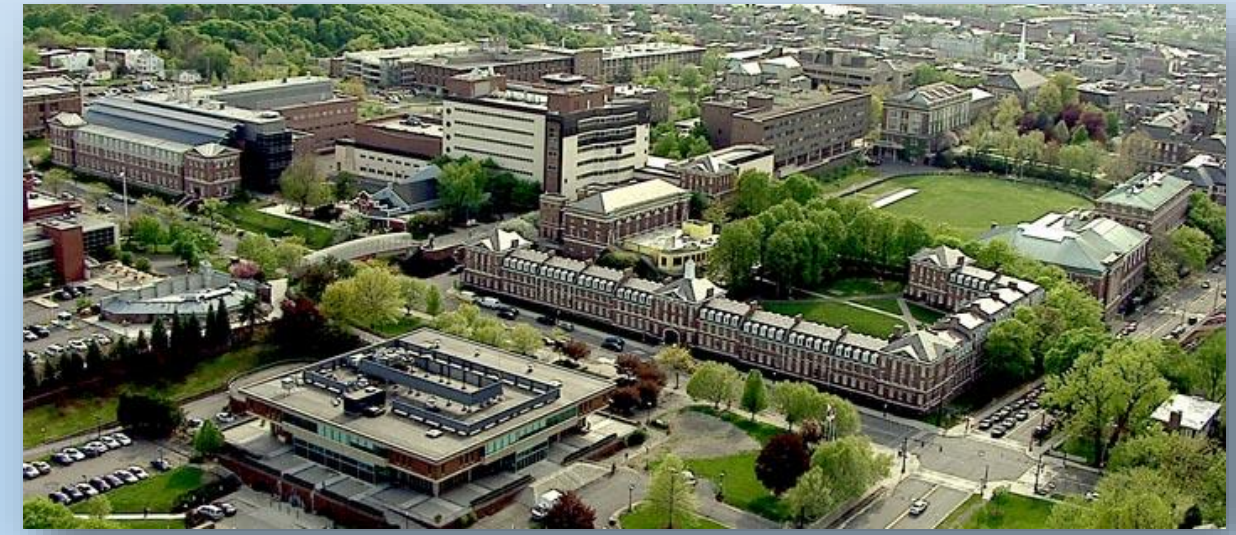

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Presentation Overview

1. Accomplishments Made in 2022
2. Motivation for investigation, new measurements, and re-evaluation of the Zr isotopes
3. Preliminary Evaluation Results from RPI ^{90}Zr Evaluation
4. Preliminary Results from Eigenvalue Sensitivity Study on Zr Sensitive Critical Benchmark Experiments

Major Accomplishments in 2022

Jan. – June

1. Completed data reduction of ^{90}Zr transmission data from 2021 ORNL/JRC-Geel experiment
2. Determined preliminary resonance parameters for ^{90}Zr from 3.8 keV – 500 keV from ORNL/JRC-Geel 2021, and ORNL 1977 transmission experiments

June – Sept.

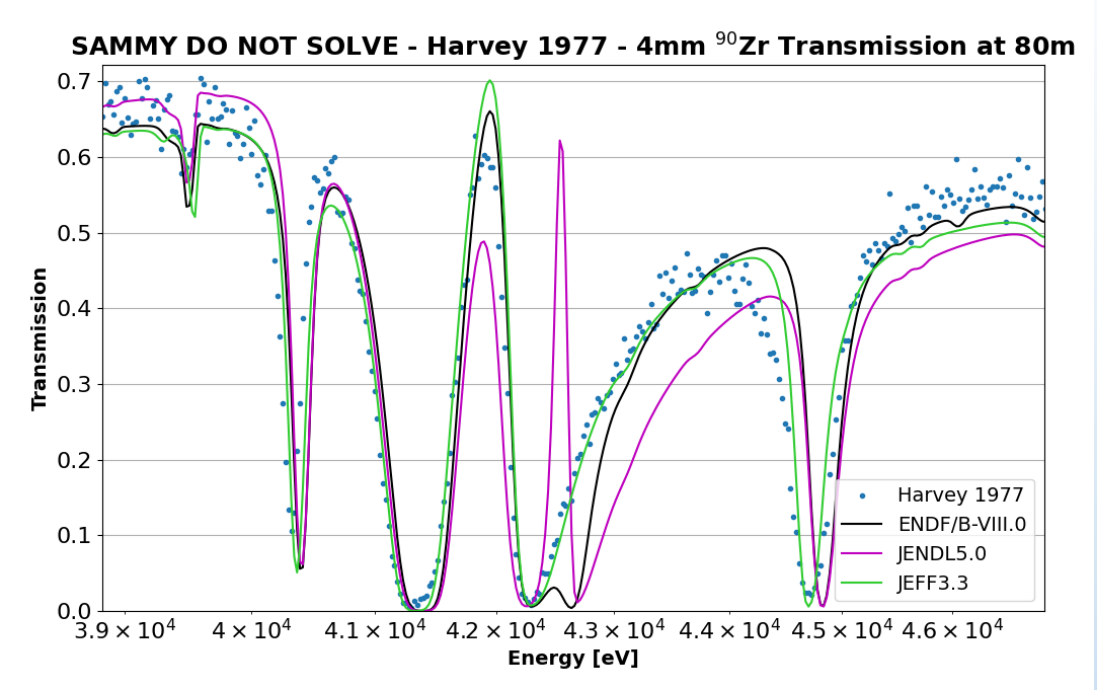
1. Fulfilled an internship with XCP-5 at LANL
   - Contributed to NJOY and ACEtk development
   - Developed software to verify proper nuclear data replication in MCNP6.3

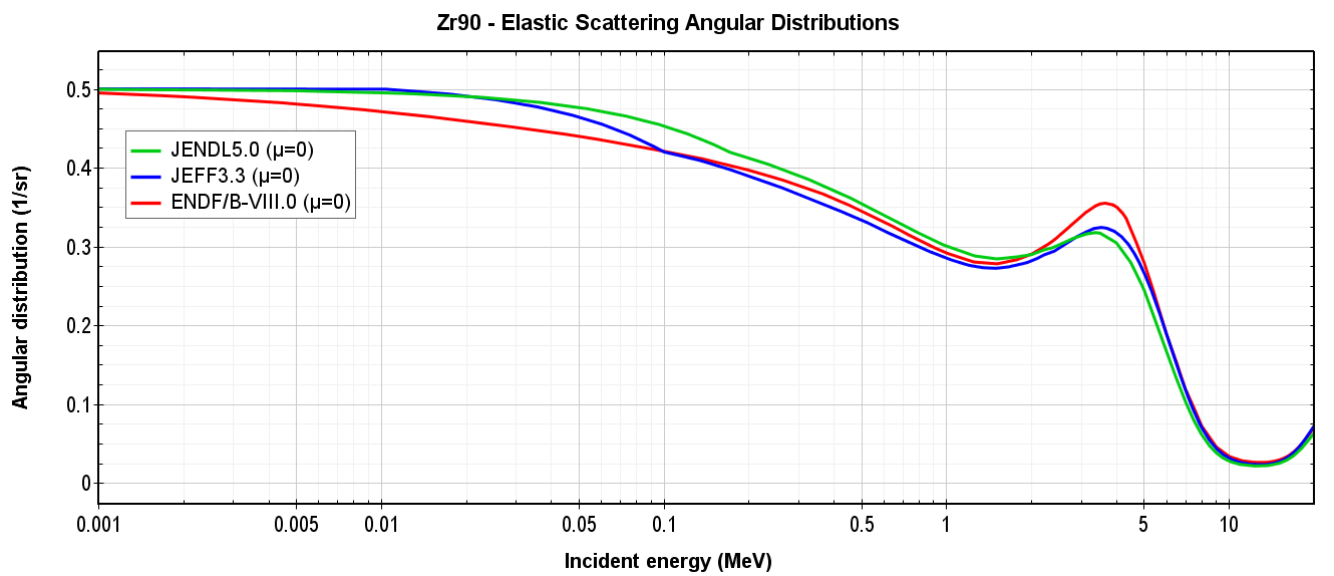
Sept. – Dec./Jan. 2023

1. Extensive eigenvalue sensitivity analysis performed on critical benchmark experiments with Zr
   - A more comprehensive methodology was employed to examine direct contributions to eigenvalue differences due to specific areas of an isotopic nuclear data evaluation
   - New knowledge of compensating errors in evaluated nuclear data libraries for Zr isotopes

Motivation for Zirconium Investigation

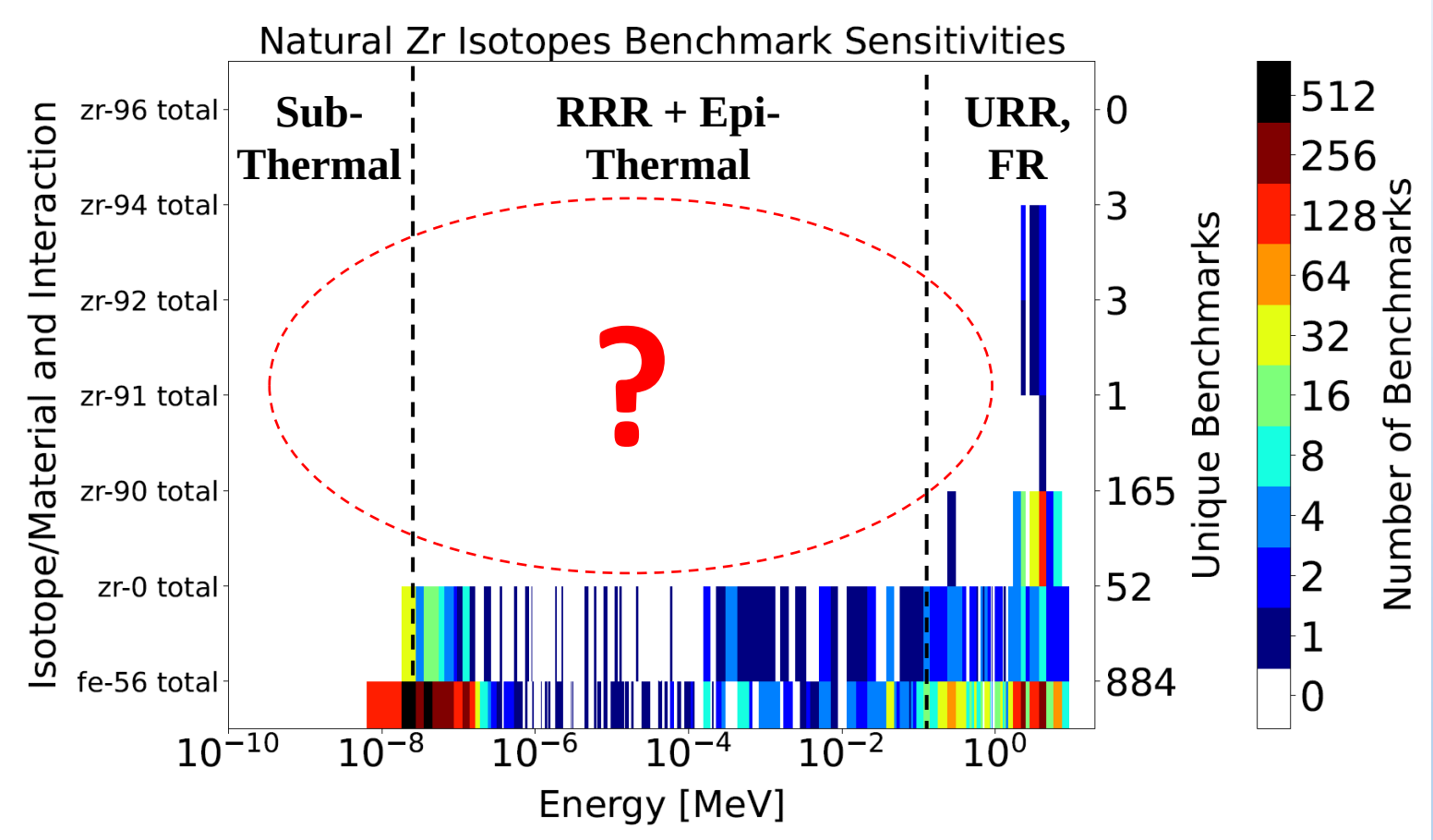
- Zirconium is **used in nearly all** commercial light water reactors in the US as fuel rod cladding and is being explored for advanced reactor concepts
- Conflicts in nuclear data evaluation between ENDF, JEFF, and JENDL exist in:
  - **Cross Sections**
    - Resolved and unresolved resonance parameters
    - High energy region
  - **Angular Distributions**
    - Elastic and inelastic scattering angular distributions





Current Zr Critical Benchmark Experiments

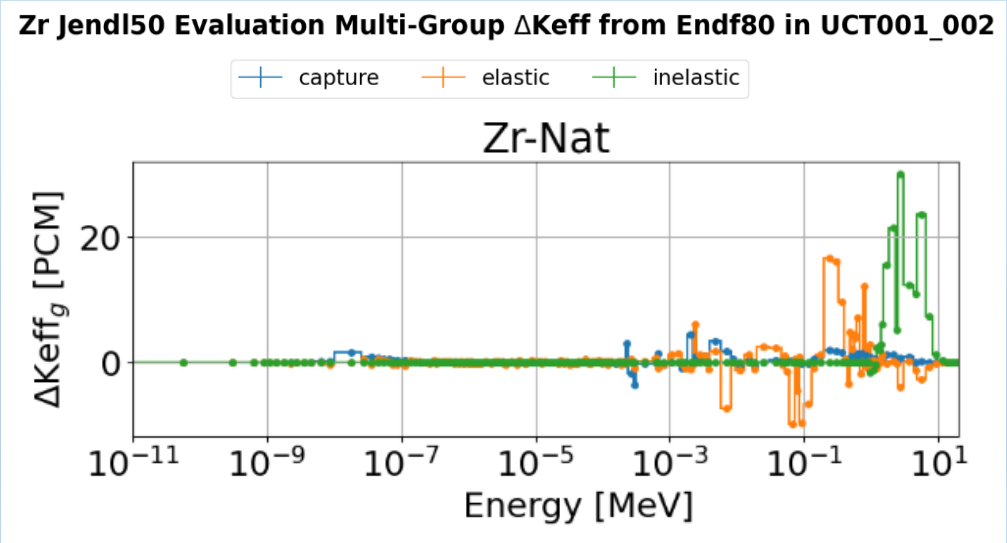
- High fidelity integral experiments are required to validate evaluation performance of Zr
  - Validation most important in energy range of fission neutron emission
  - Many Zr sensitive benchmark experiments are large thermal systems and/or do not meet modern evaluation standards
- Lack of differential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

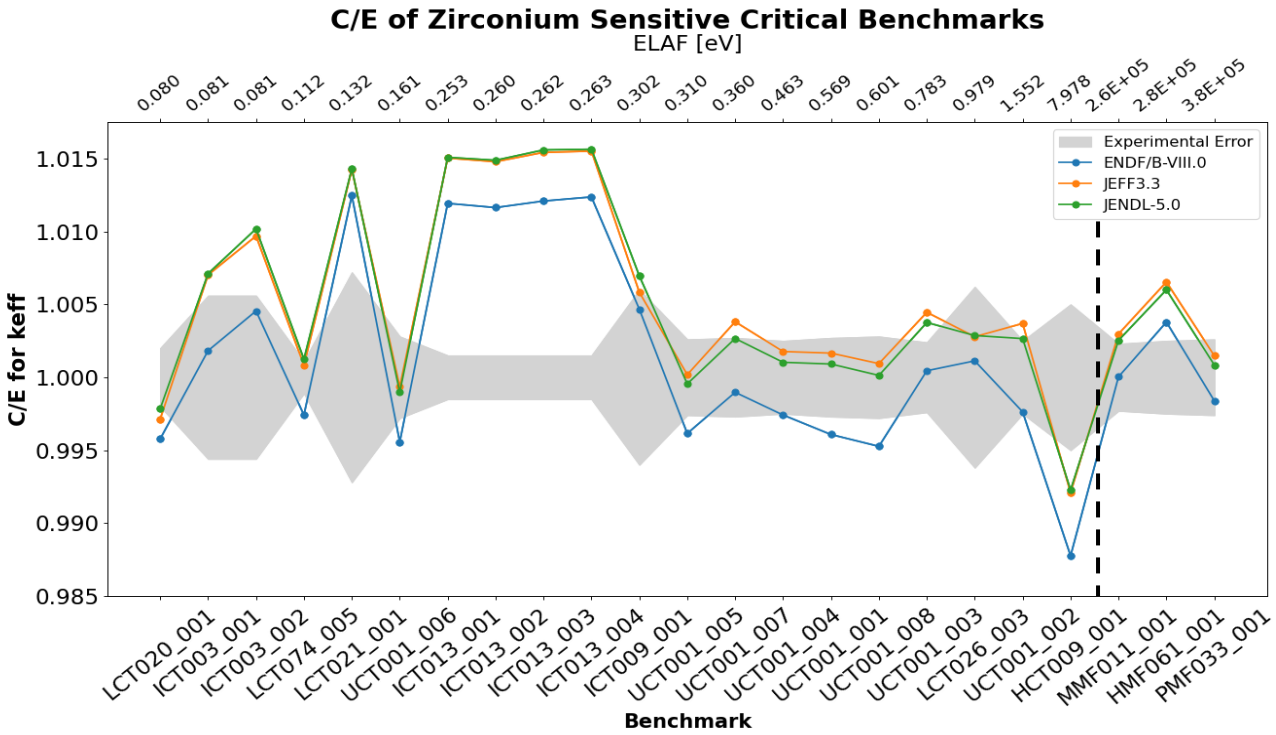


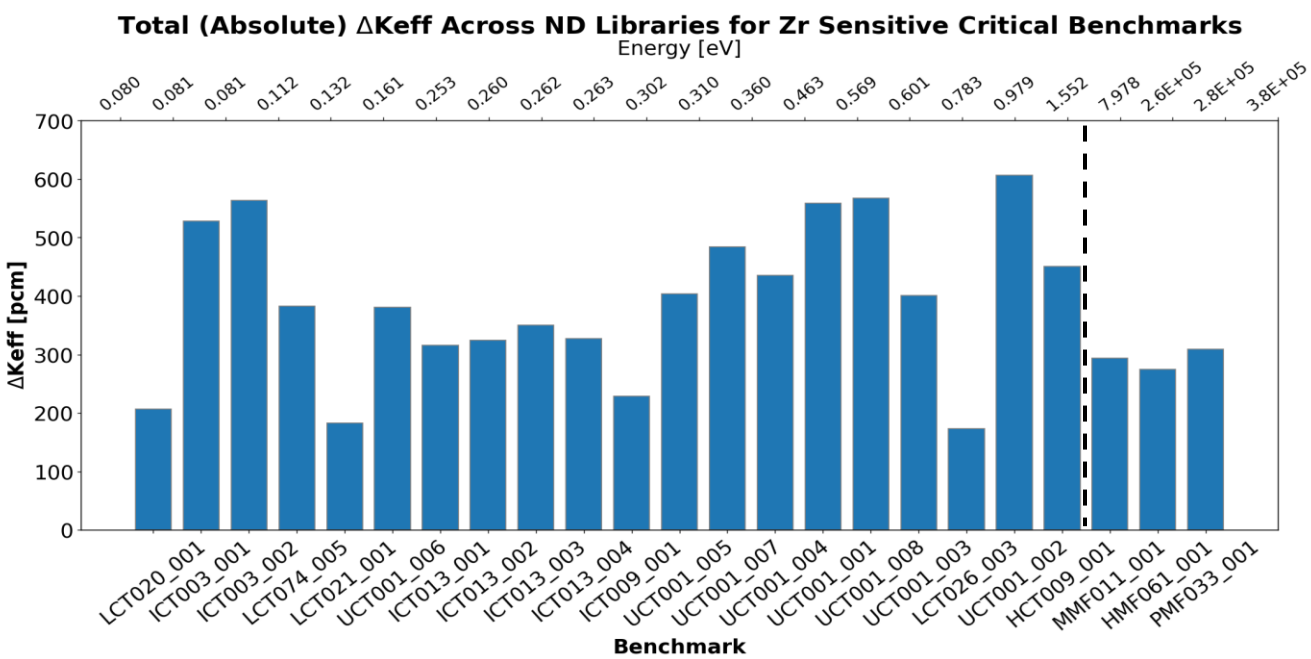
A score on this point corresponds to a sensitivity coefficient greater than or equal to 1e-3 at a given energy

Current Zr Integral Benchmark Experiments

- Lacking high fidelity fast integral experiments to validate Zr evaluations
- ΔK_{eff} of current thermal systems is mostly attributed to high energy neutron interactions







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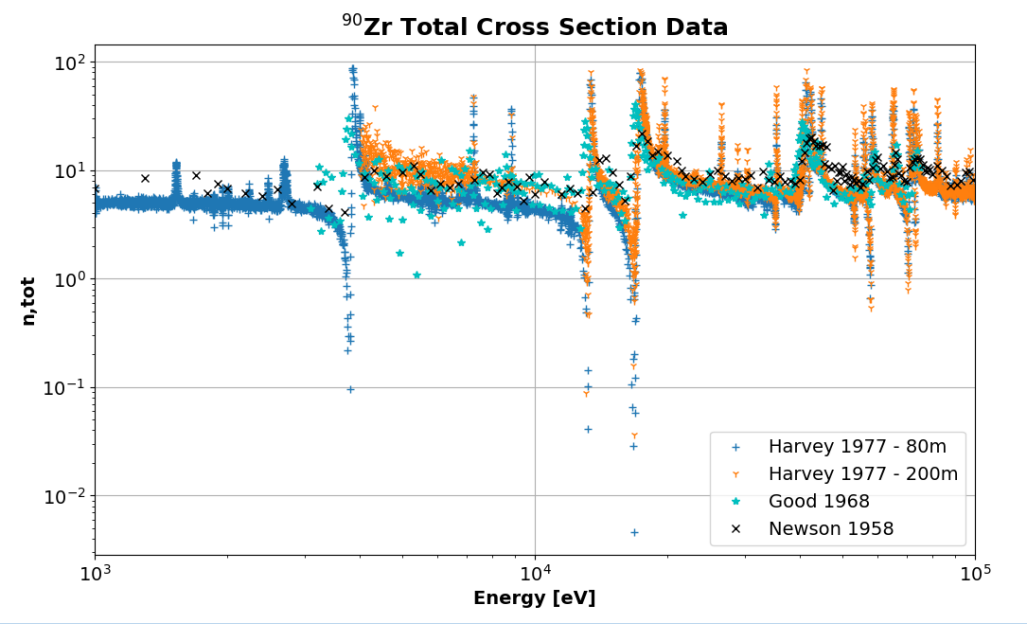
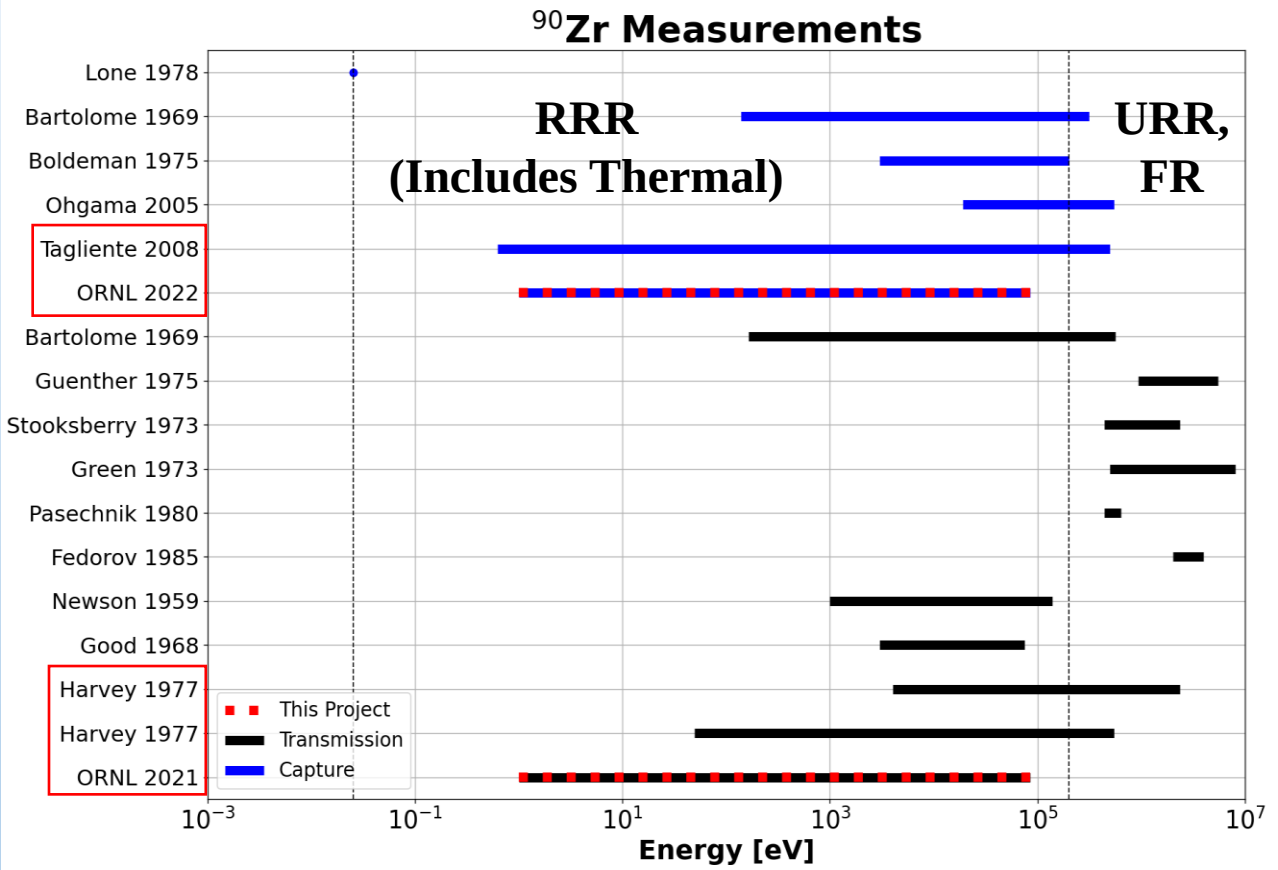
Current ^{90}Zr Differential Cross Section Data

- Lacking high resolution transmission (E > 85 keV) data to verify Harvey, et al. 1977 measurements
- Disagreement between Harvey and Good + Newson transmission
- Good, Newson, and (raw) Bartolome data have poor energy resolution

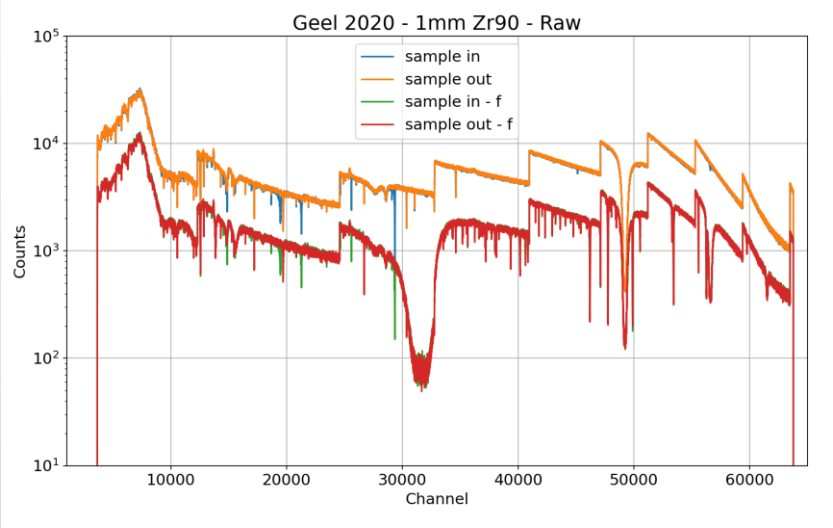


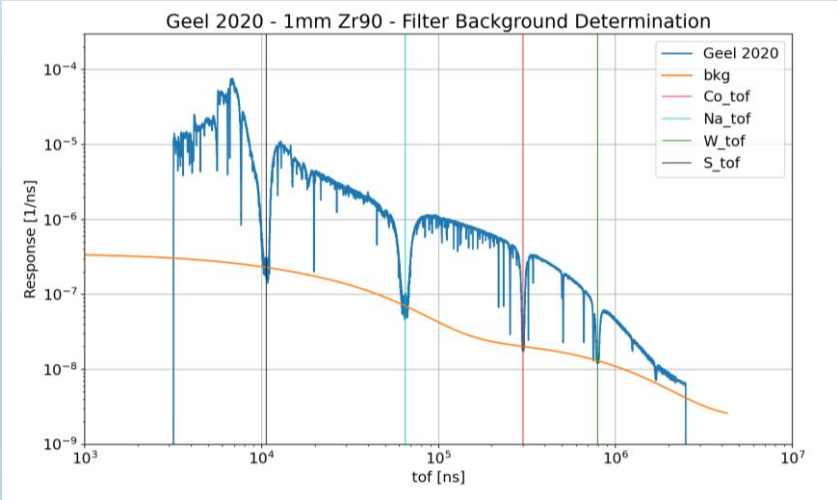


Energy region for new ORNL measurements only verified for ^{90}Zr transmission

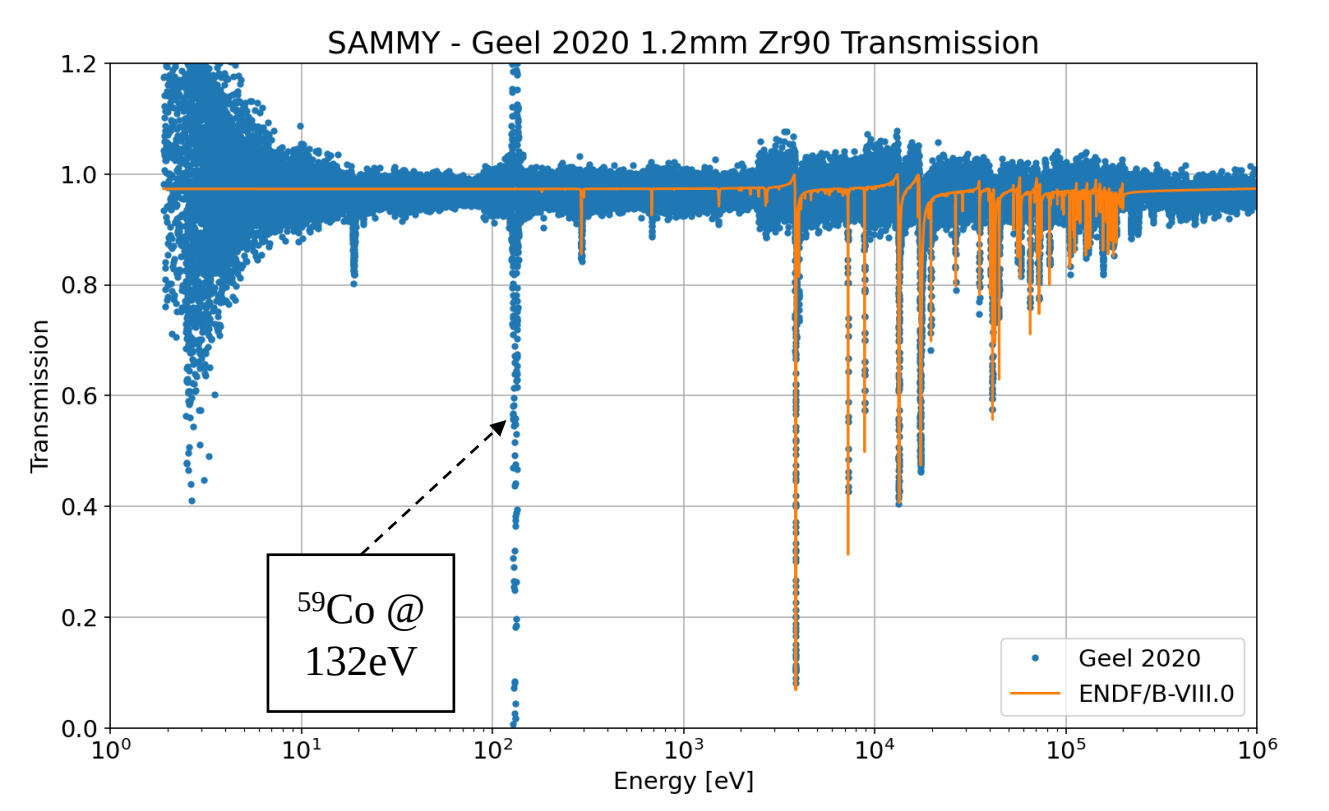
Data Reduction and Evaluation of ORNL/JRC-Geel ^{90}Zr Transmission Measurements

Reduction of Geel 2021 ^{90}Zr Transmission Experiment





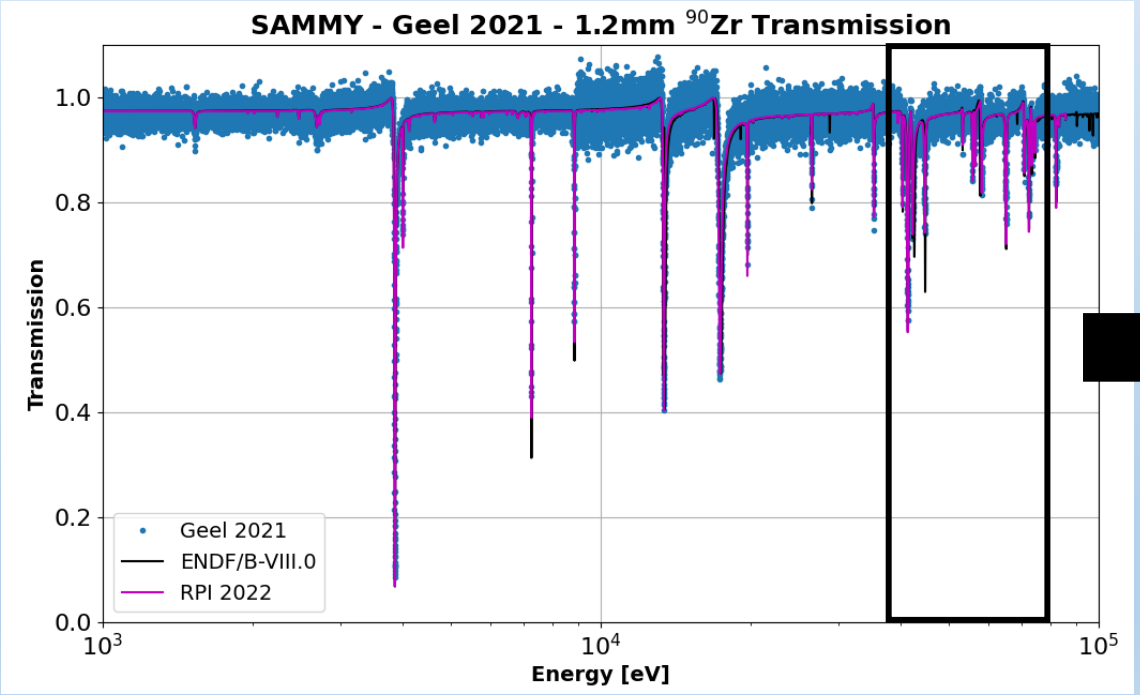
Data processed using Geel AGL reduced and verified to production level at RPI using AGS

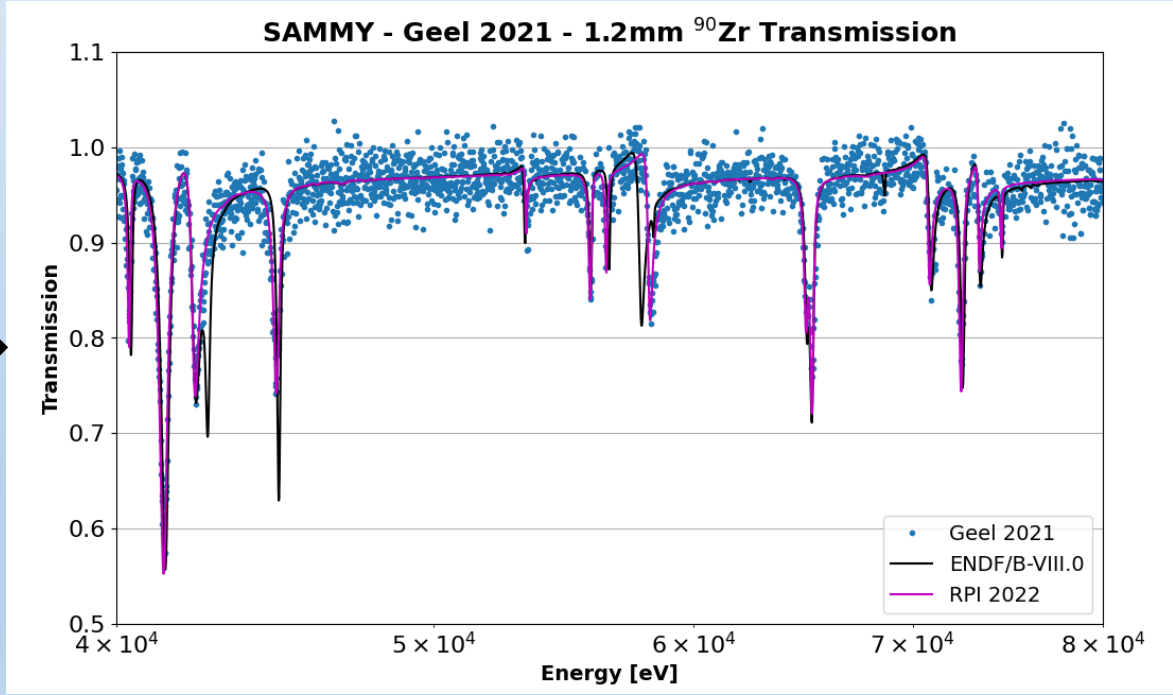


R-Matrix Resonance Analysis – ORNL/Geel 2021

^{90}Zr transmission measured by ORNL at JRC-Geel in 2021 at 45m

- Deadtime correction ratio issues with this experiment limit resonance parameter determination at ~86 keV

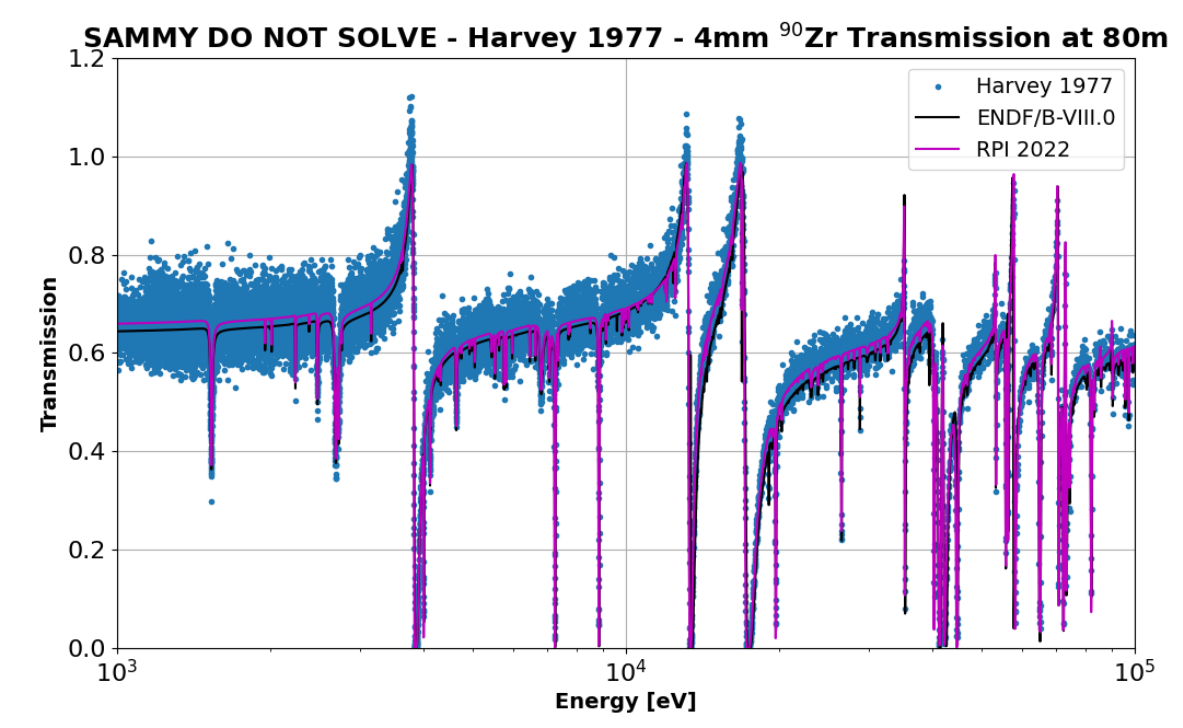


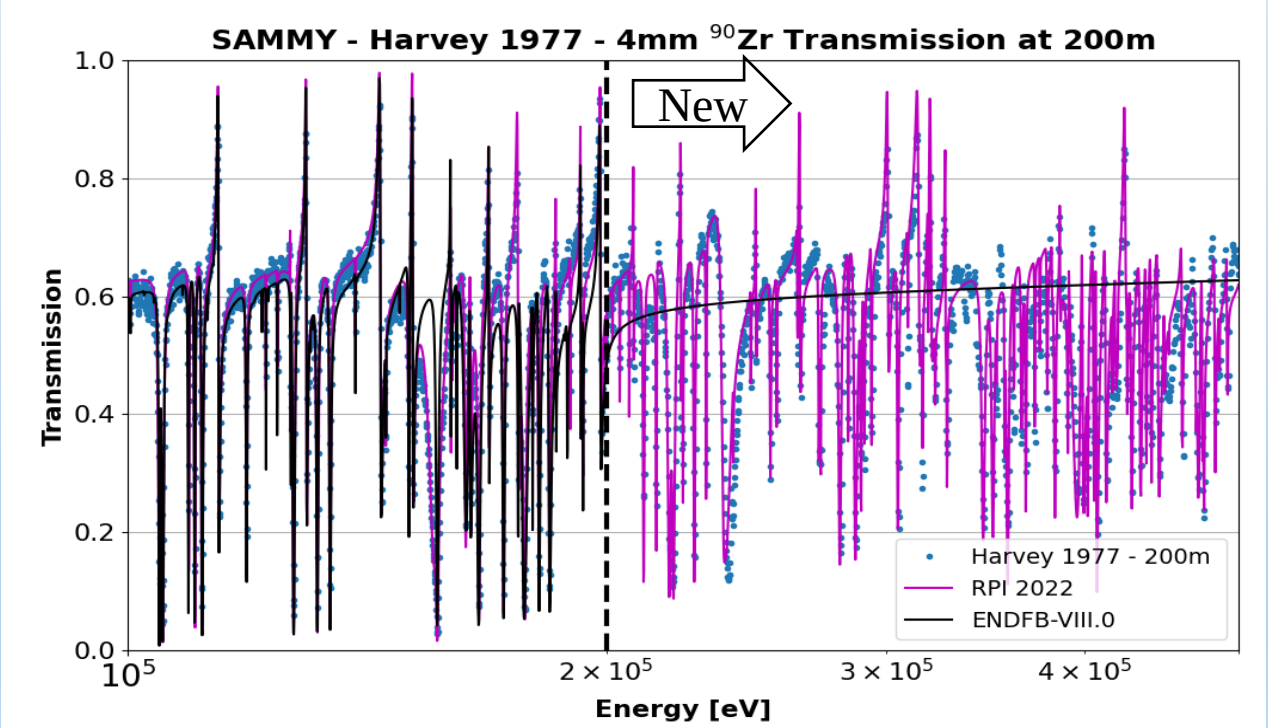


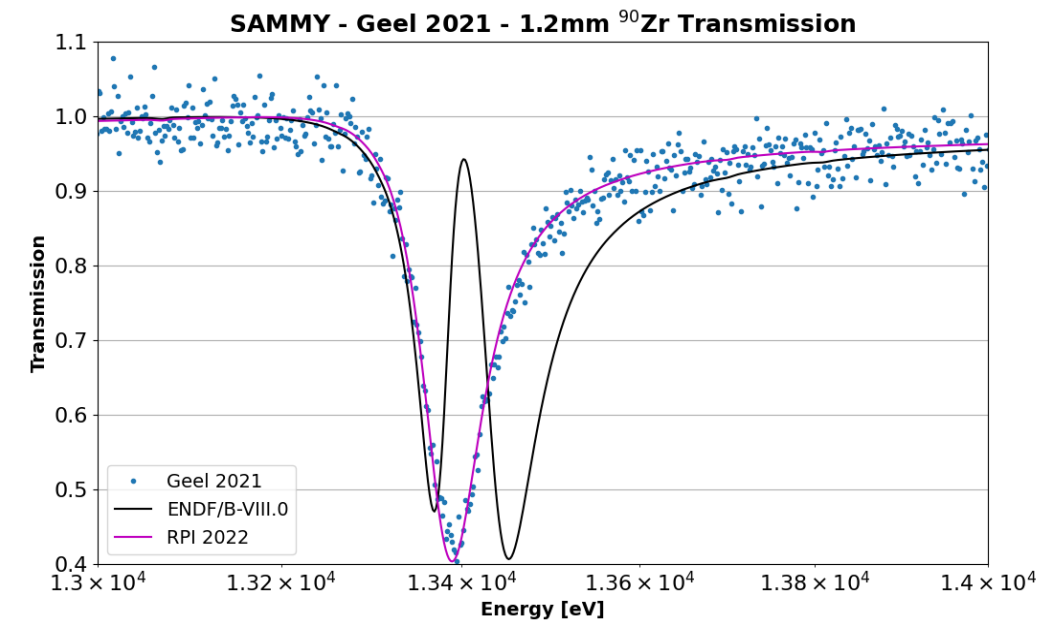
R-Matrix Resonance Analysis – ORNL 1977

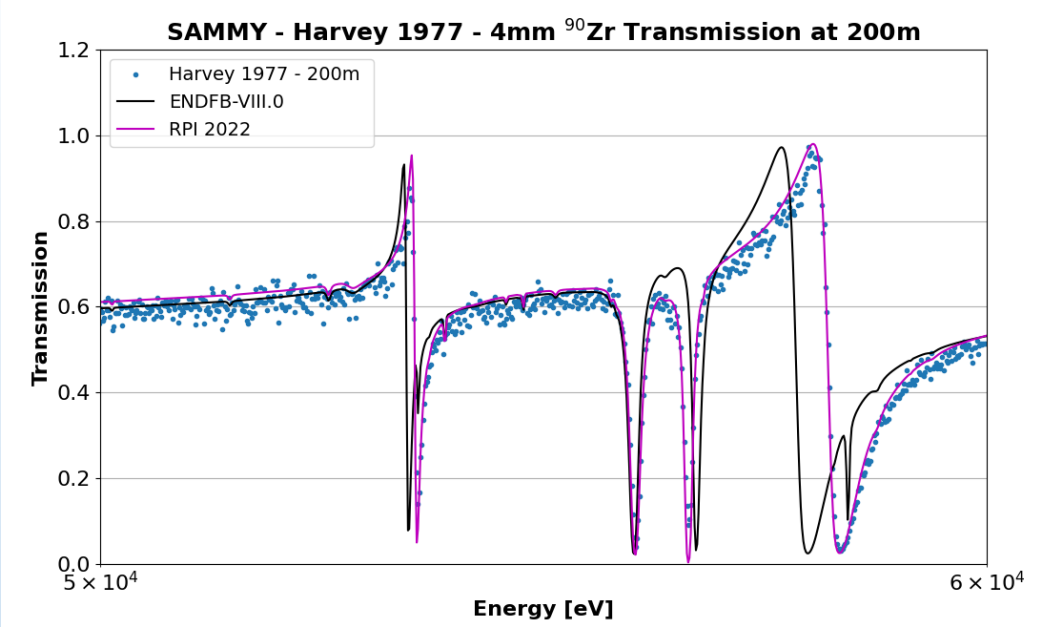
^{90}Zr transmission measured by Harvey, et. al at 80m and 200m in 1977 at ORELA

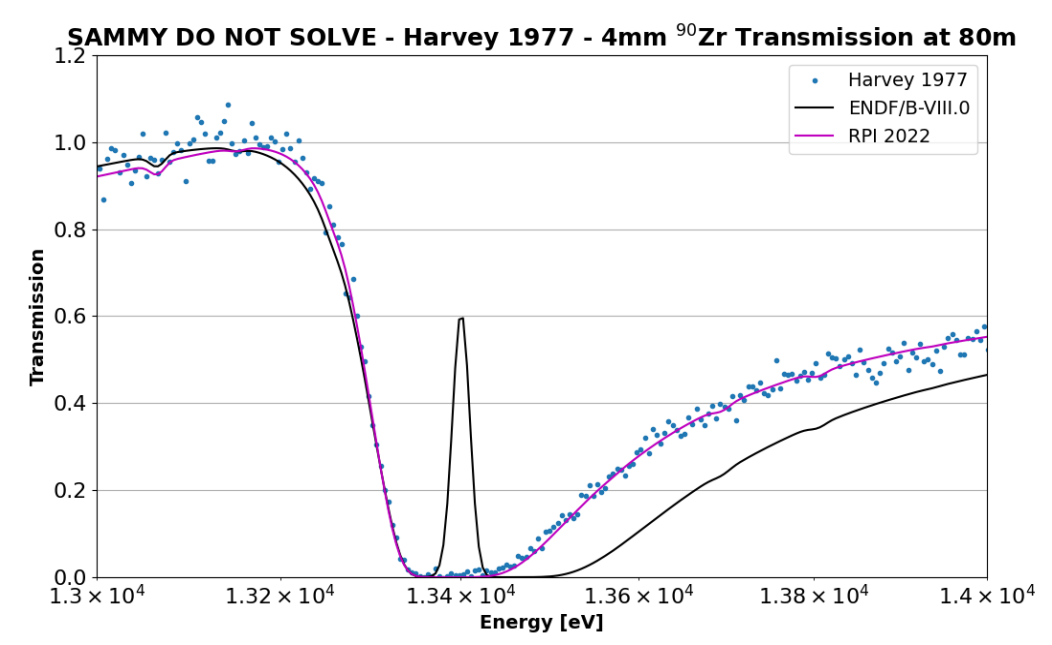
- 80m data used from first resonance (3.8 keV) to ~200 keV
- 200m data used from ~30 keV to 500 keV – (Preliminary)
  - **300 keV extension of RRR over current ENDF/B-VIII.0 evaluation**

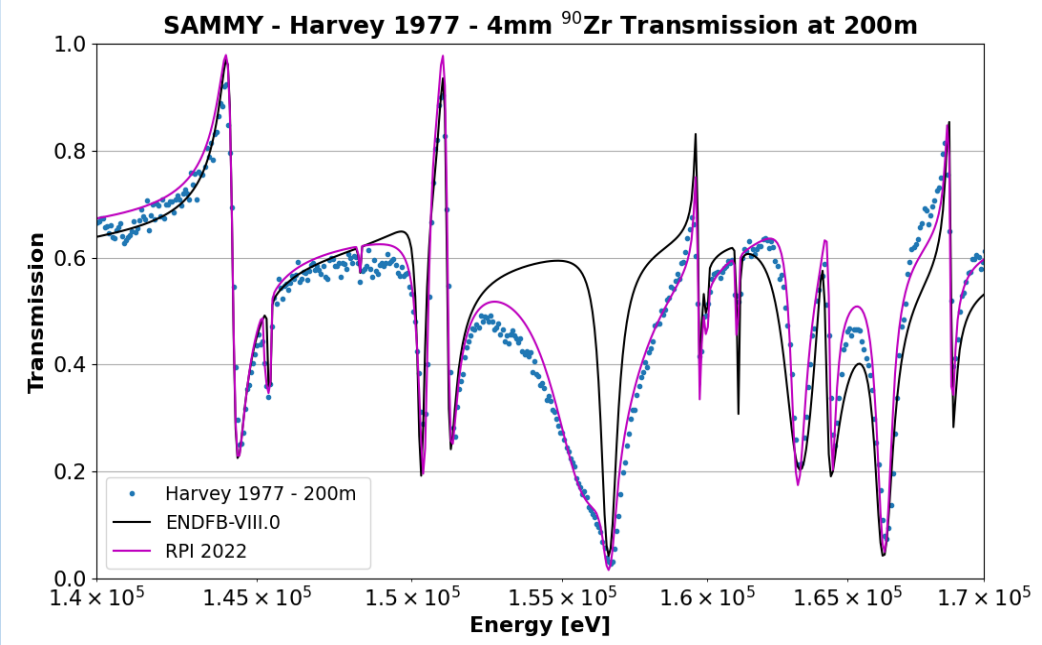





SAMMY - Geel 2021 - 1.2mm ^{90}Zr Transmission
Transmission
Energy [eV]
Geel 2021
ENDF/B-VIII.0
RPI 2022

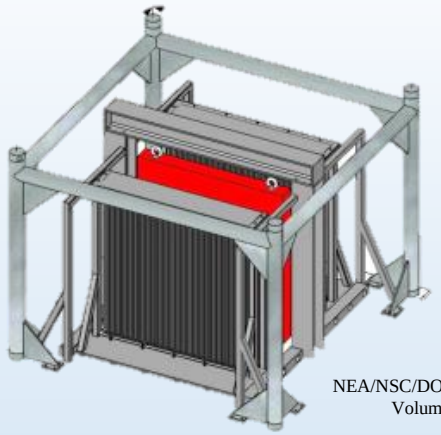

SAMMY - Harvey 1977 - 4mm ^{90}Zr Transmission at 200m
Transmission
Energy [eV]
Harvey 1977 - 200m
ENDFB-VIII.0
RPI 2022


SAMMY DO NOT SOLVE - Harvey 1977 - 4mm ^{90}Zr Transmission at 80m
Transmission
Energy [eV]
Harvey 1977
ENDF/B-VIII.0
RPI 2022


SAMMY - Harvey 1977 - 4mm ^{90}Zr Transmission at 200m
Transmission
Energy [eV]
Harvey 1977 - 200m
ENDFB-VIII.0
RPI 2022

Time-Independent Eigenvalue Sensitivity Study

Critical Benchmark Eigenvalue Sensitivity Study Using Zr



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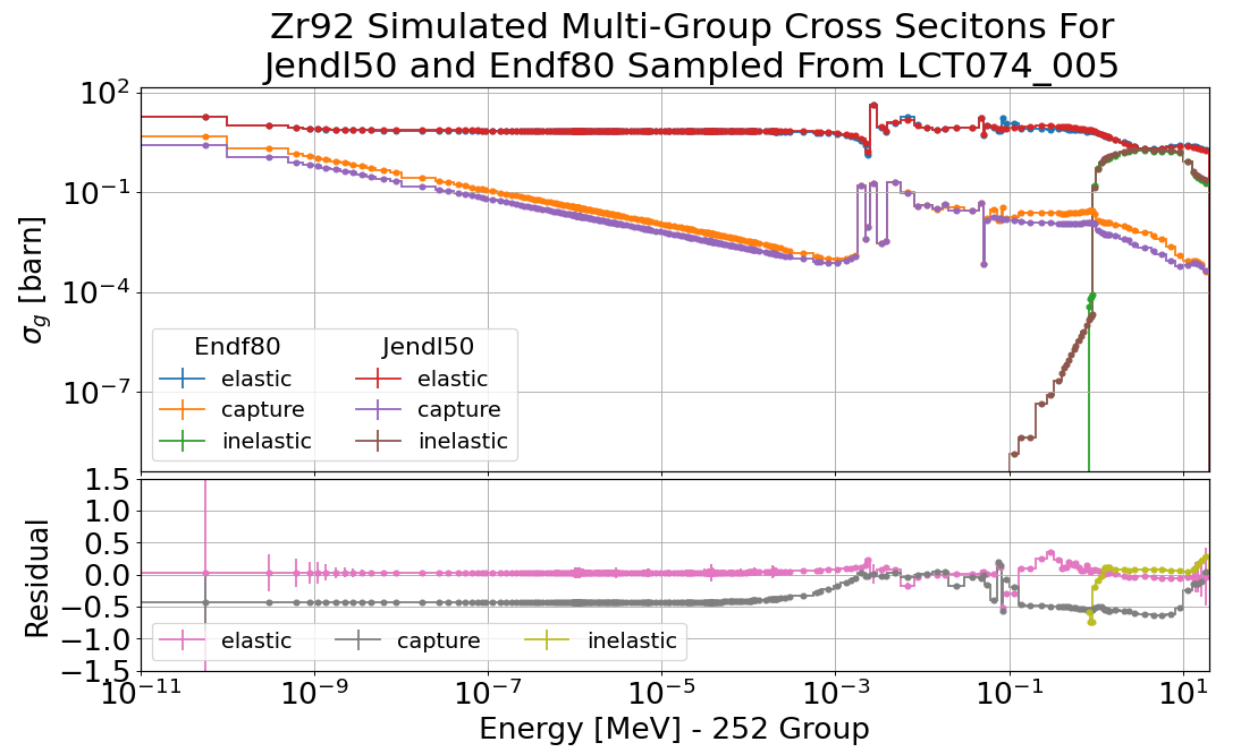
Methodology developed with MCNP KSEN to propagate differences in cross sections between nuclear data evaluations to differences in the eigenvalues of critical benchmark experiments.

$$\Delta keff\left(\Sigma_i\,(E)\right) = \left[S_{keff}\left(\Sigma_i^{E8}(E)\right) * \left(\frac{\Sigma_i^{E8}(E) - \Sigma_i^{J5}(E))}{\Sigma_i^{E8}(E)}\right)\right] * keff(\Sigma_i^{E8}(E))$$

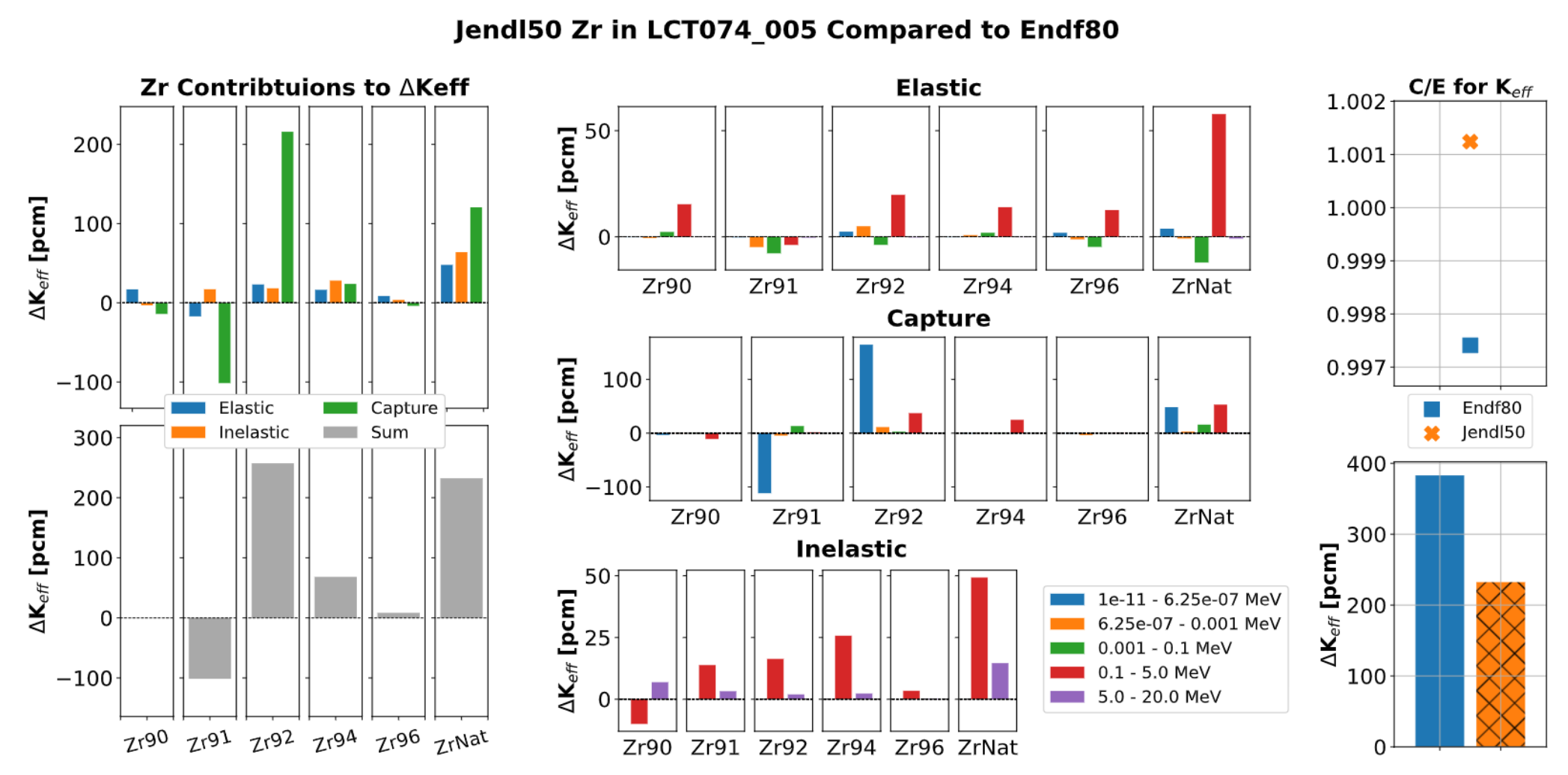
$\Delta keff\left(\Sigma_i\,(E)\right)$ - Difference in Eigenvalue from Cross Section for Reaction Channel *i* at Energy *E*

$S_{keff}(\Sigma_i^{E8}(E))$- Eigenvalue sensitivity to ENDF/B-VIII.0 Cross Section at Energy *E*

$\Sigma_i^x(E)$ – Evaluation *x* Cross Section for Reaction Channel *i* at Energy *E*

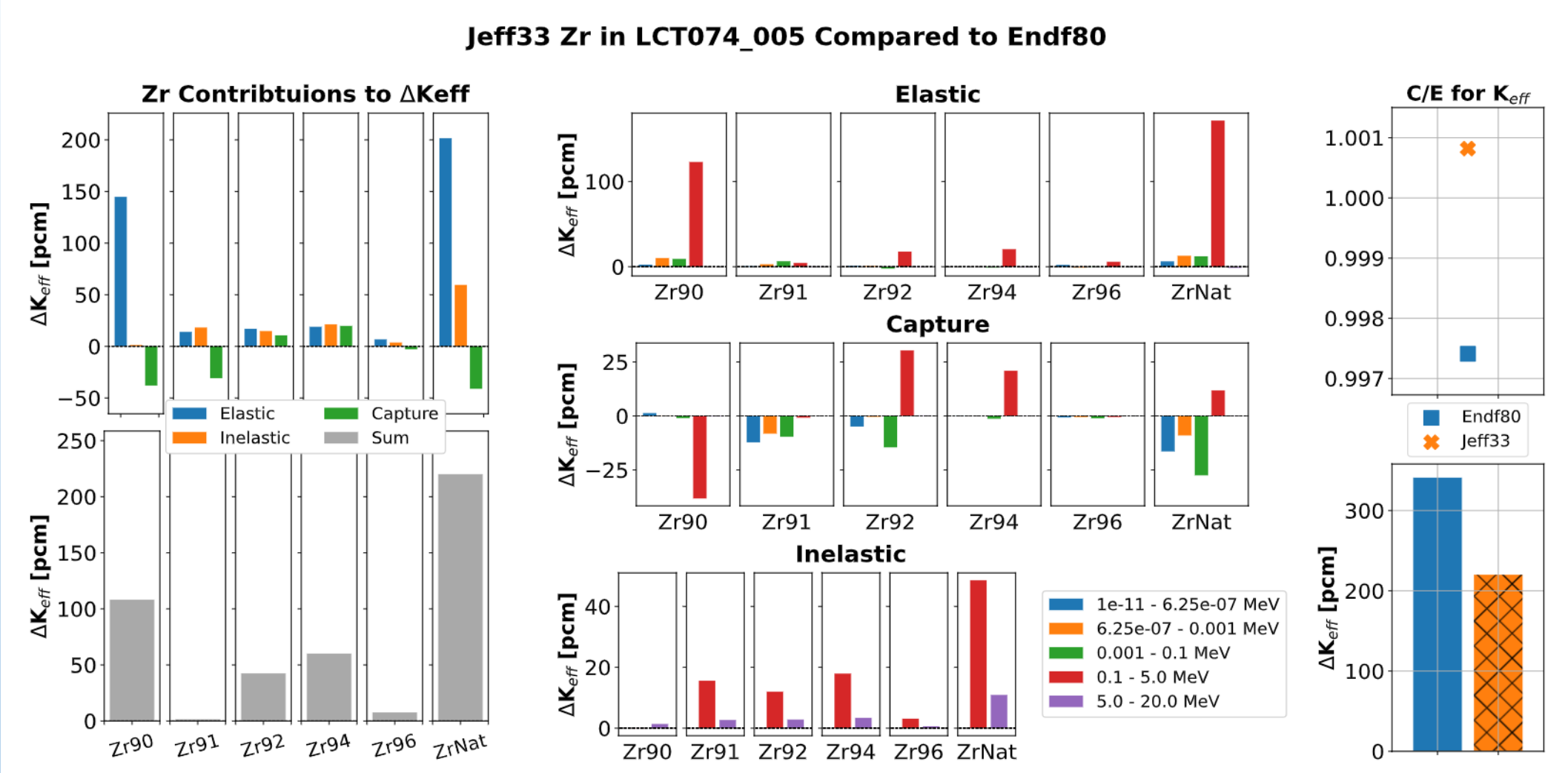


Cross Section Contribution to Eigenvalue Difference



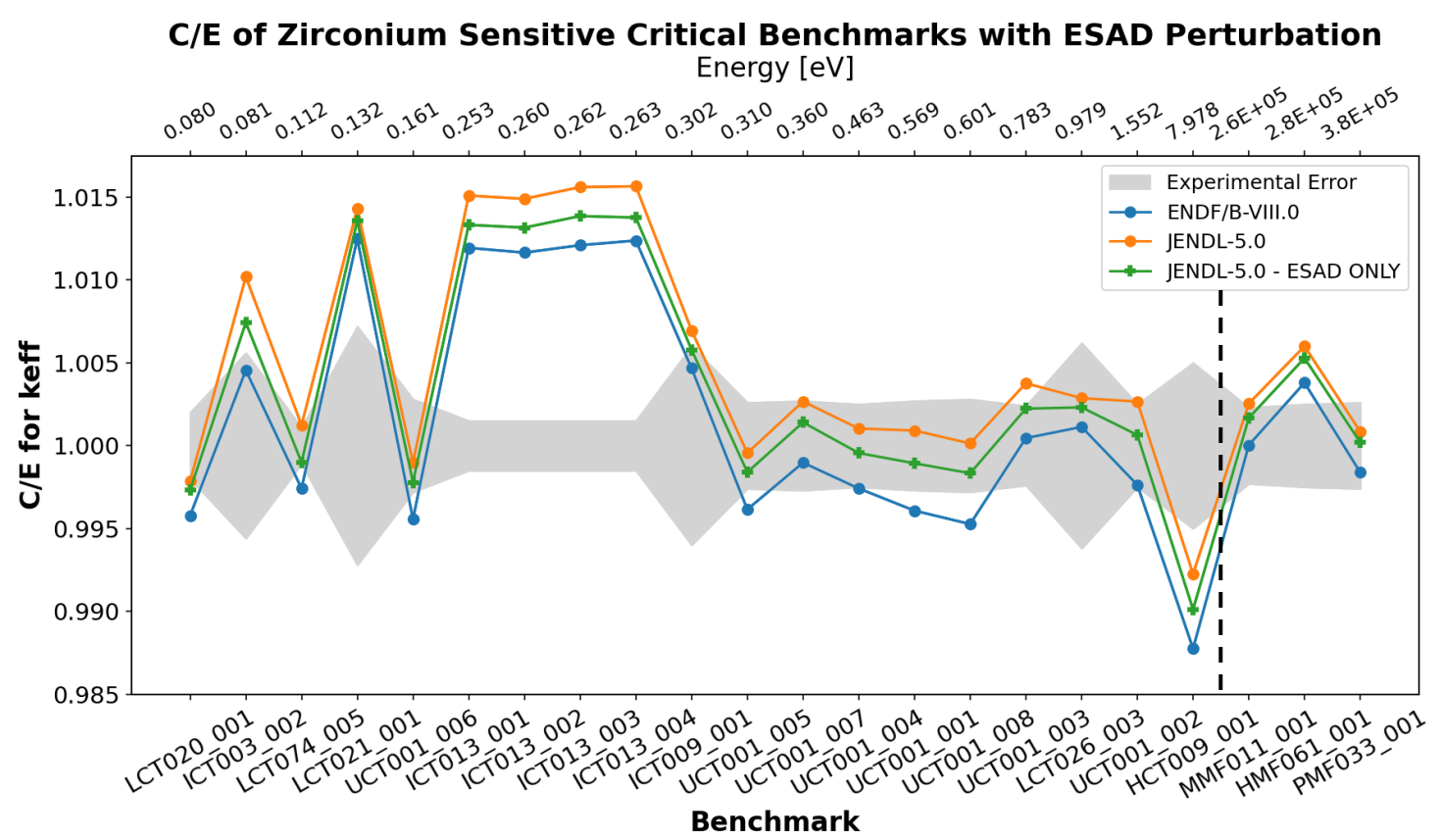
***K_{eff}* Driven Primarily by ^{91,92}Zr Thermal Capture + All Isotopes Elastic and Inelastic Scattering in Fission Spectra**

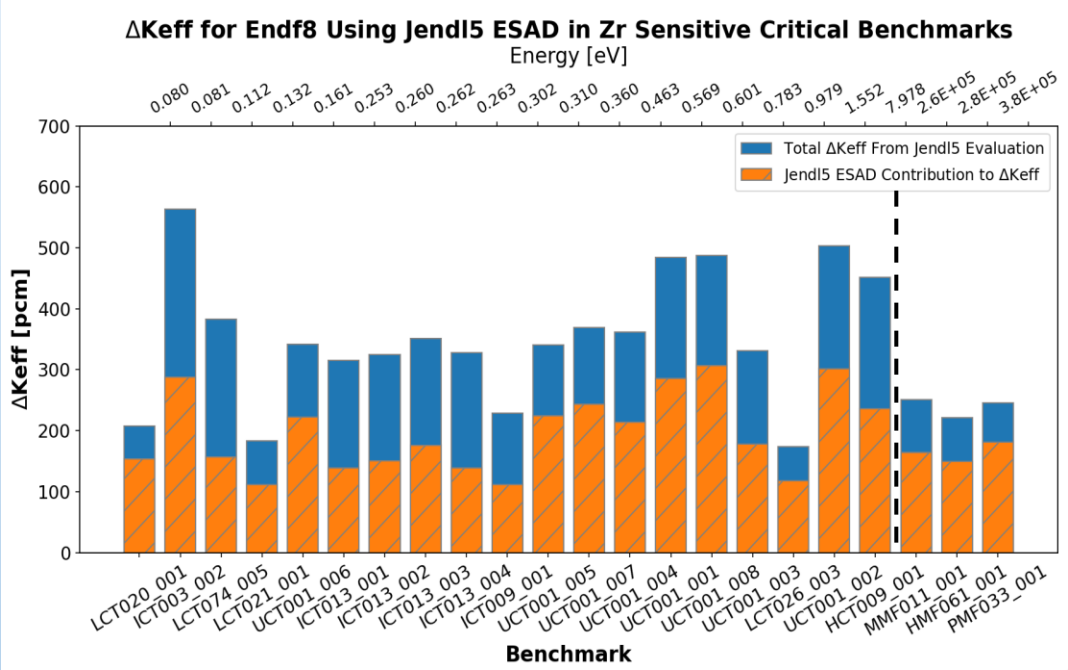
Cross Section Contribution to Eigenvalue Difference



***K_{eff}* Driven Primarily by ^{90}Zr Elastic and Inelastic Scattering in Fission Neutron Energy Emission Spectra**

Elastic Scattering Angular Distribution Contribution to Eigenvalue Difference





* Energy in top x-axis corresponds to the energy corresponding to the average lethargy of a neutron causing fission

Project Takeaways and Goals For 2023

Accomplishments from 2022

1. Preliminary resonance parameters determined for RPI ^{90}Zr evaluation
2. Development and employment of eigenvalue sensitivity analysis on critical experiments
   - **~50%** of eigenvalue differences between evaluations attributable to elastic scattering angular distributions
   - **Major disagreements** observed in all Zr isotope cross section evaluations
     - Fission neutron emission energy spectrum/neutron slowing down region (~100 keV – 5 MeV) **most influential region of evaluation** for NCSP applications

Goals for 2023

1. Obtain final set of resonance parameters for RPI ^{90}Zr evaluation using new ORNL/Geel 2021 capture experiment
2. Complete eigenvalue sensitivity study
   - Validate current cross section findings with manual perturbations
   - Further quantify angular distribution contributions
3. Assess current nuclear data in most discrepant evaluation regions
   - Conclude if new experiments are needed for resolution
4. Determine level of RPI involvement in URR and fast region ^{90}Zr evaluation

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