OAK RIDGE National Laboratory

Thermal Neutron Scattering Research at ORNL – ENDF File Validation

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NCSP Technical Program Review
15-17 February 2022- Online

Outline

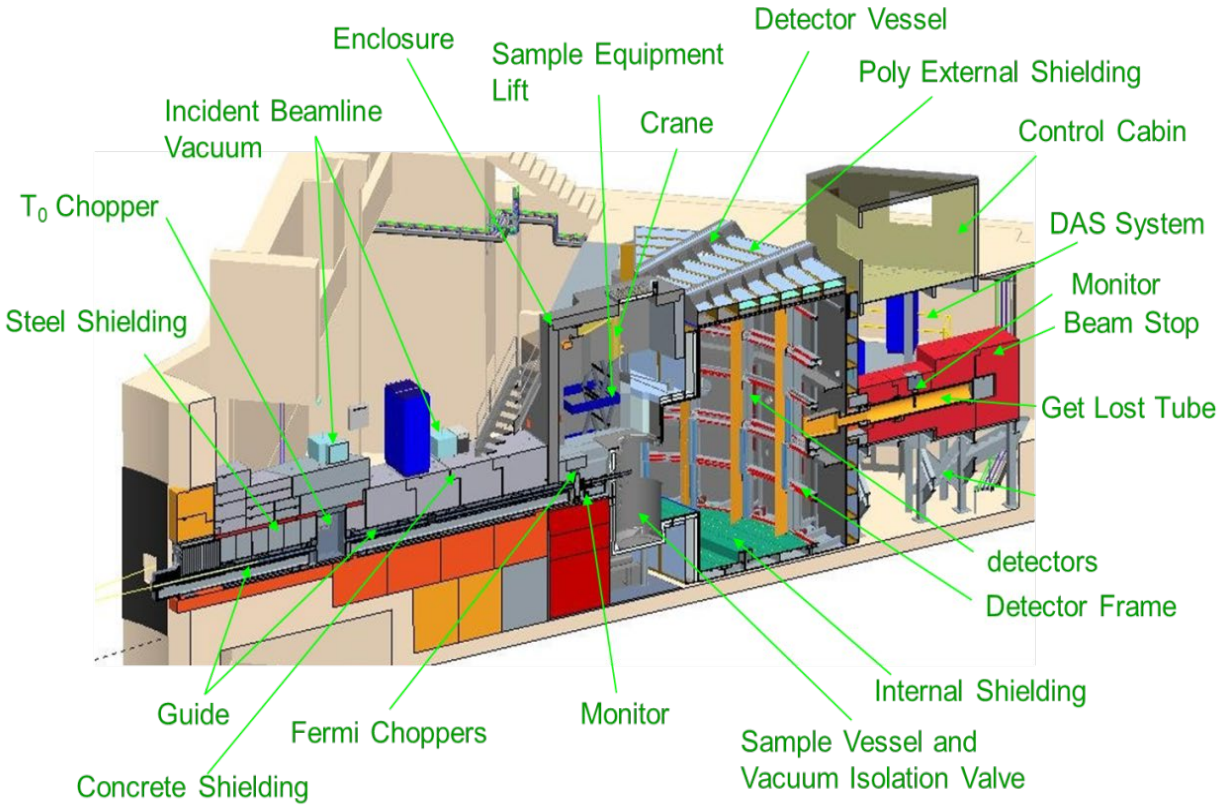
- ENDF File Validation
  - Processing code
  - Example comparisons
- Polyethylene Discrepancy
  - Underlying cause
  - Correction made

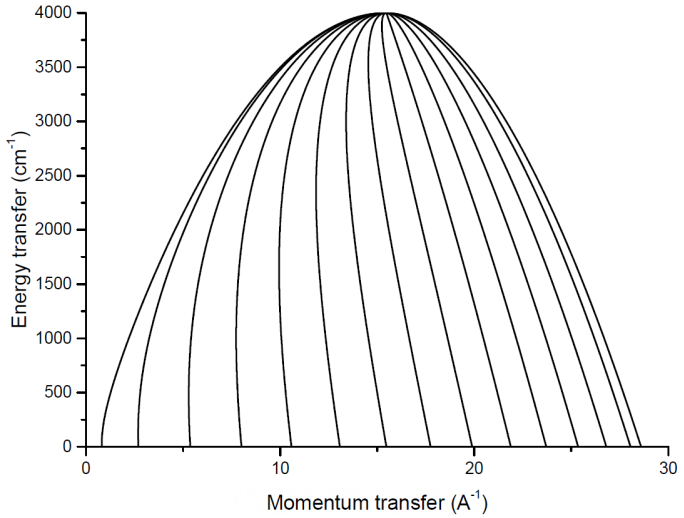
ENDF File Validation - Overview

- Recent efforts in validating total thermal neutron cross sections [1]; important to extend to double differential cross sections
  - Especially important in cases where high-quality differential data were unavailable when ENDF file was produced
- Previous experience validating files against SNS data
  - ARCS/SEQUOIA [2-3]
- VISION presents challenges
  - Direct vs. Indirect geometry
  - Difficult to model

SNS Beamlines: ARCS & SEQUOIA

- Time-of-flight direct geometry spectrometer
- User chooses incident energy; Fermi choppers rotate to select energy from white beam
- Detector & data acquisition system (DAS) setup measures final energy and scattering angle
  - SEQUOIA: better energy resolution
  - ARCS: larger angular range
- Selection of furnaces and refrigerators for temperatures range 5 – 1800 K





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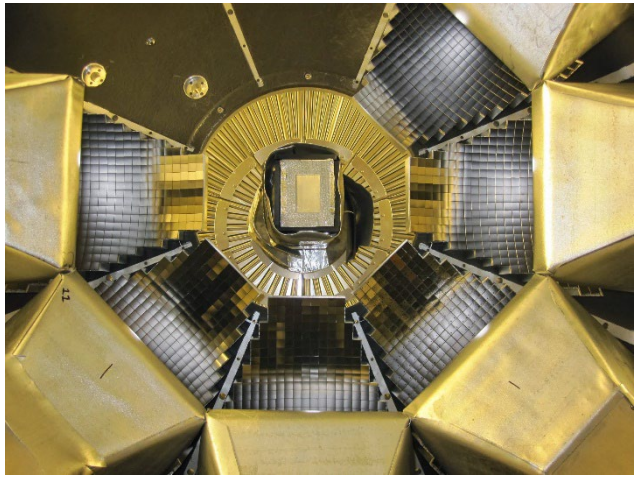
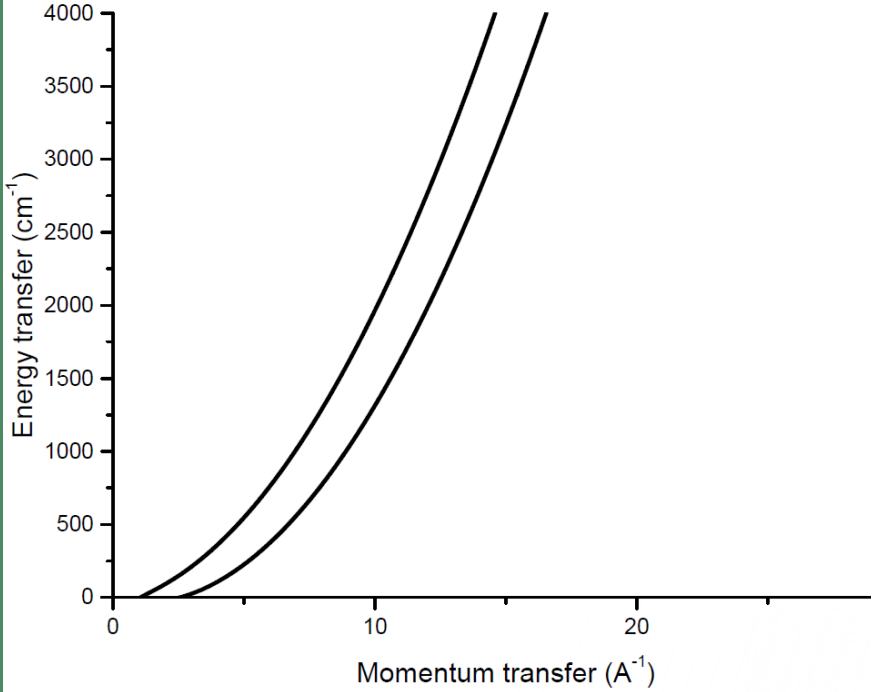
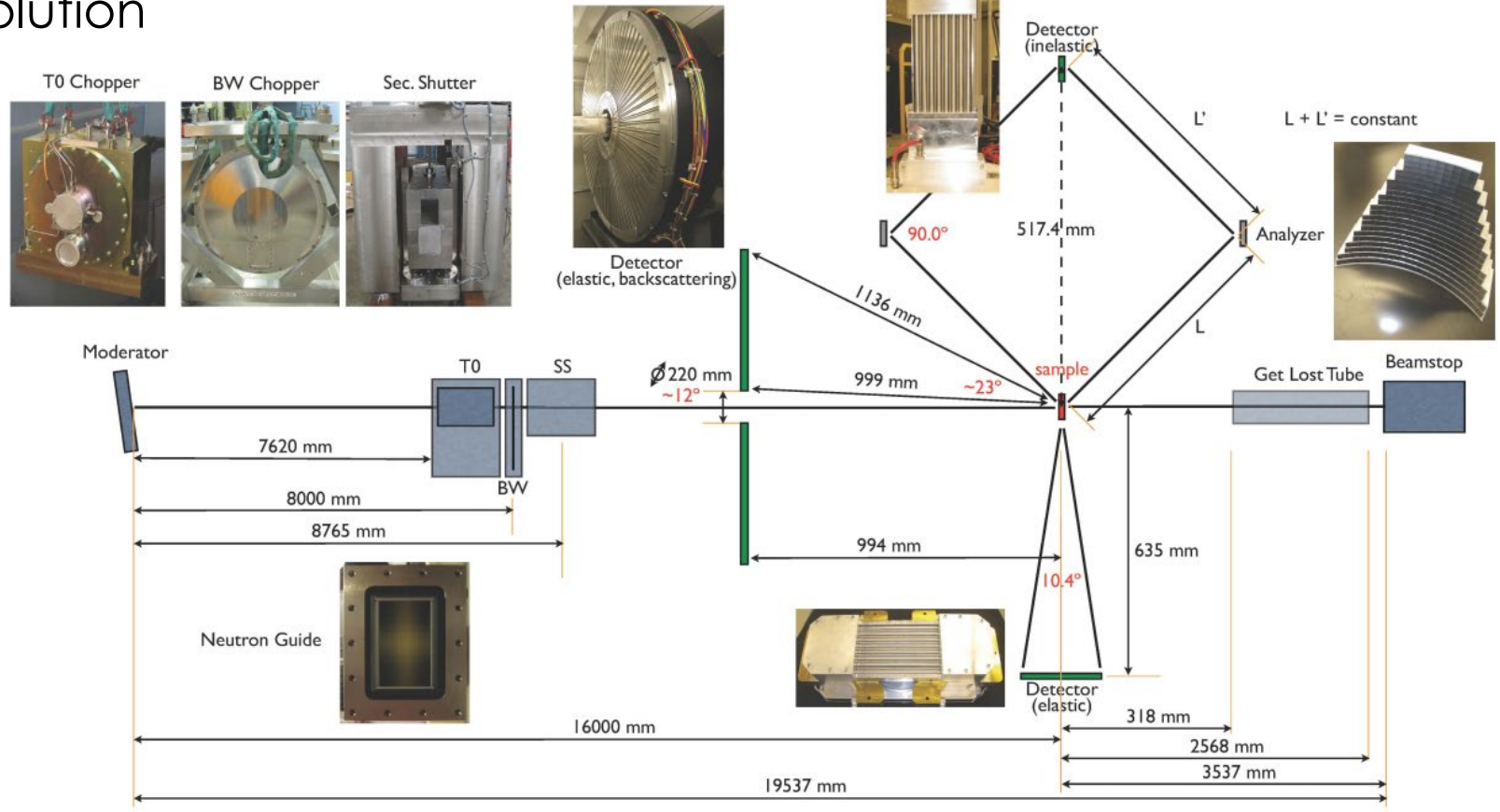
SNS Beamlines: VISION

- Indirect geometry vibrational spectrometer
- White beam of neutrons hits sample
- Scattered neutrons reflected off graphite blocks to two detectors for forward- and backward-scattering angles
- Graphite blocks configured to scatter neutrons at 4 meV
- Constant relative energy resolution





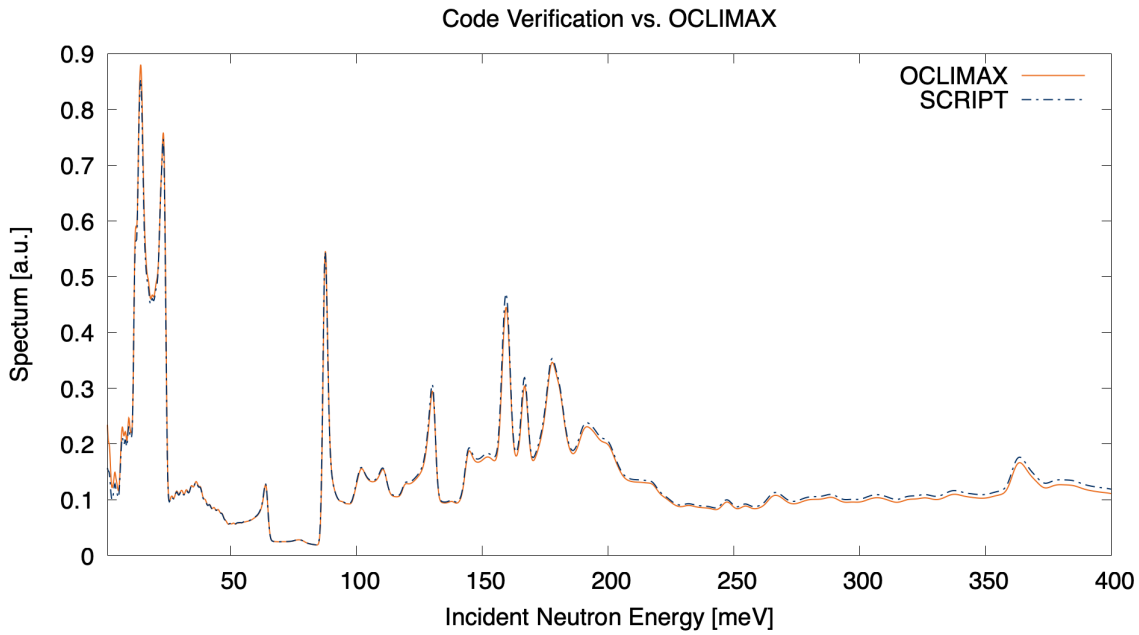


ENDF File Validation – VISION

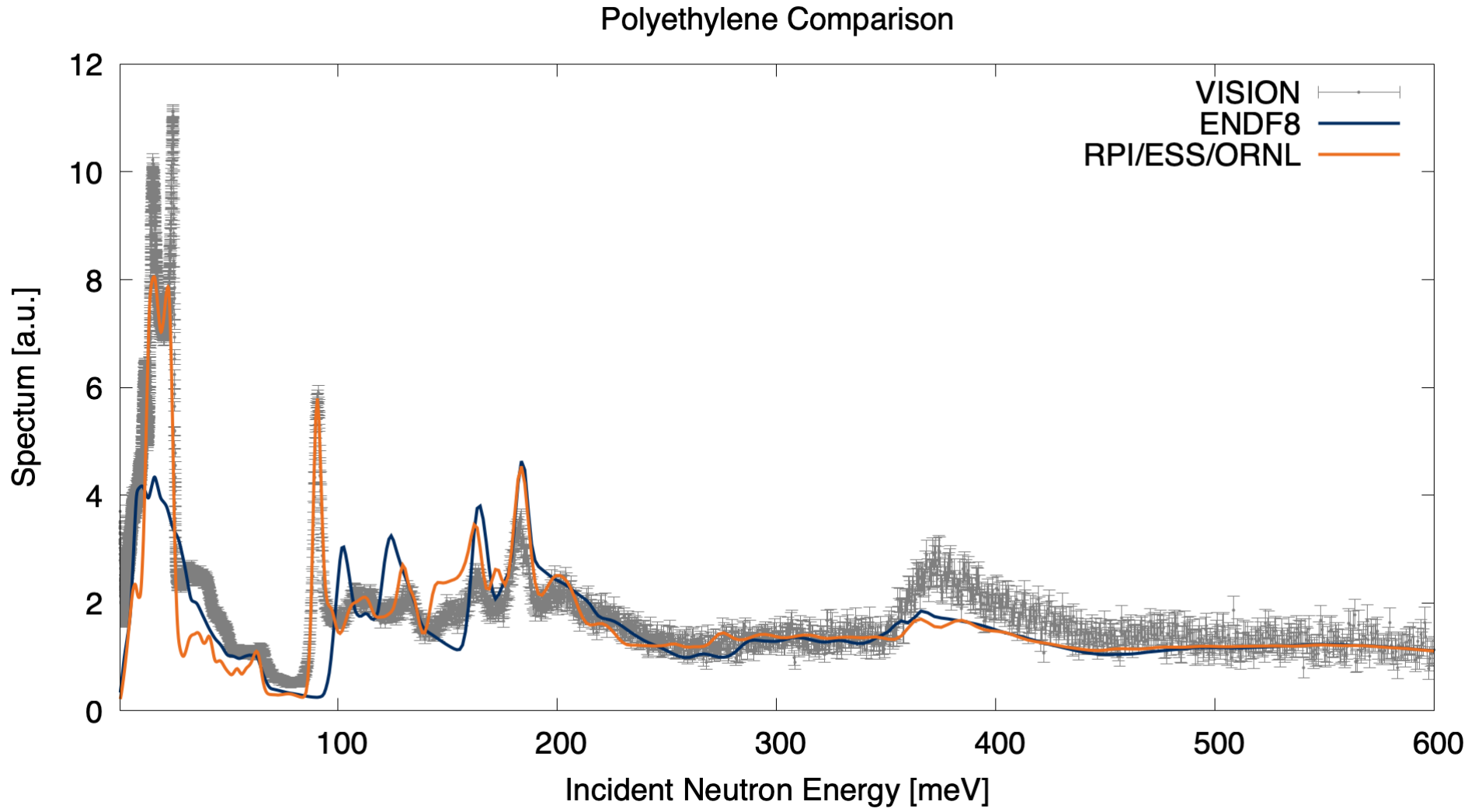
- Solution: develop method to model VISION spectra from ENDF file and apply necessary experimental corrections
  - Calculate (Q,E) grid for VISION spectra
  - Convert ENDF TSL file $S(\alpha, \beta)$ to S(Q,E)
  - Extract input S(Q,E) data along precalculated (Q,E) grid
  - Apply energy-dependent instrument resolution function

ENDF File Validation – VISION

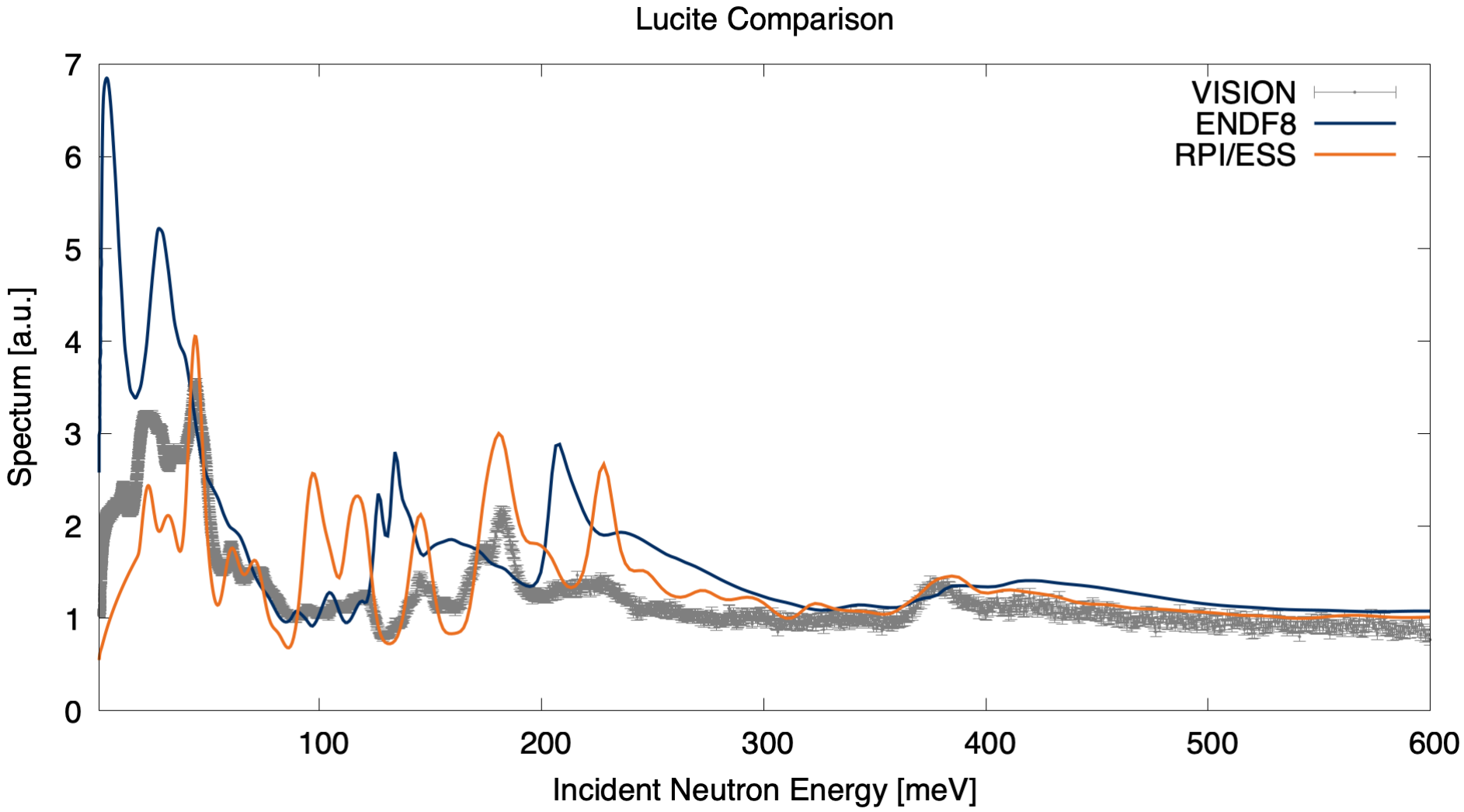
- Code verification
  - Run DFT simulation of material (in this case, polyethylene)
  - Generate both the VISION spectra & S(Q,E) files using OCLIMAX [4]
    - OCLIMAX takes DFT/MD files as inputs, not ENDF files
  - Run S(Q,E) file through code to generate VISION spectra
- Various materials used for validation [5-8]
  - Polyethylene, Yttrium Hydride, Lucite, Ice
  - All measurements & libraries at 5K



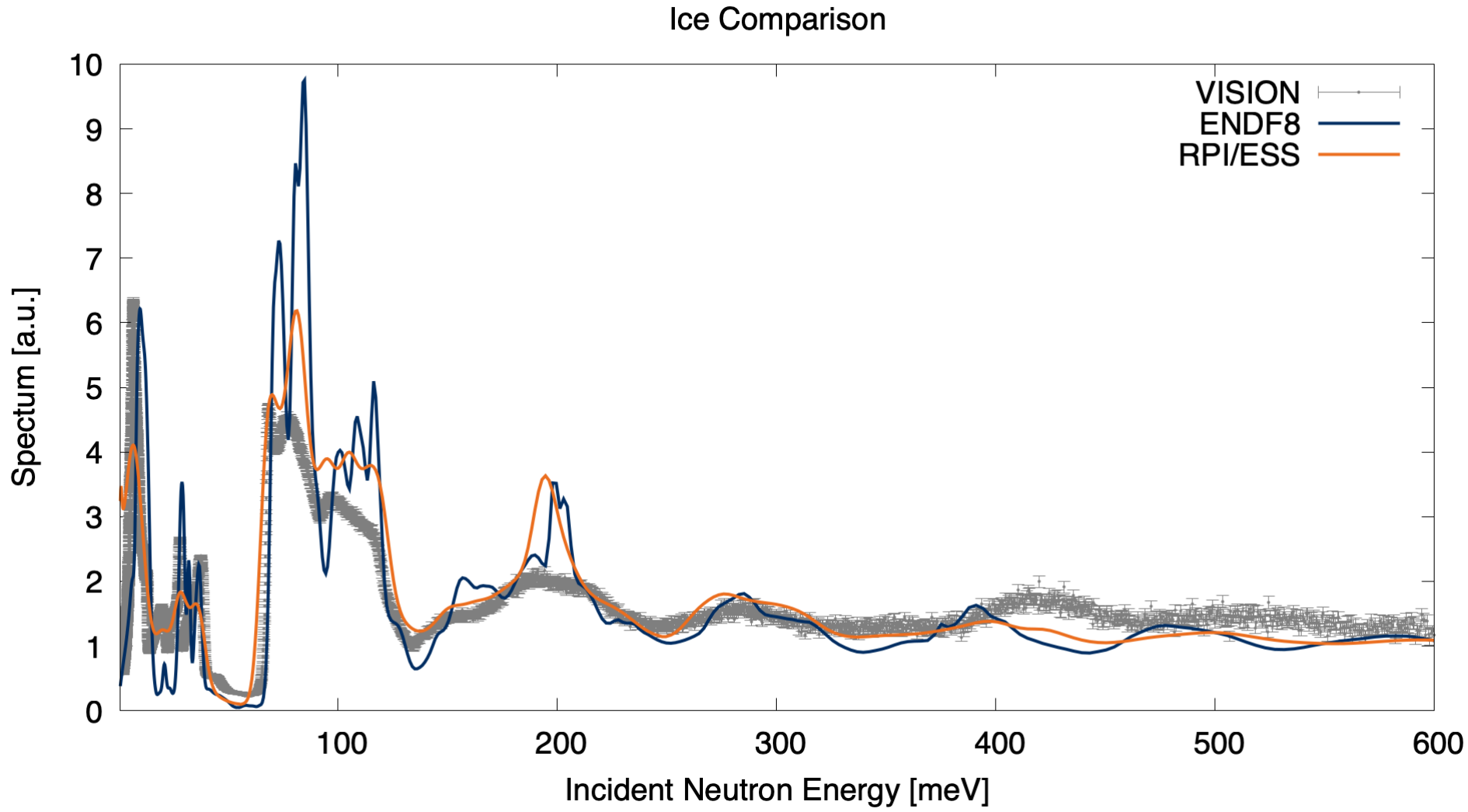
ENDF File Validation – Polyethylene



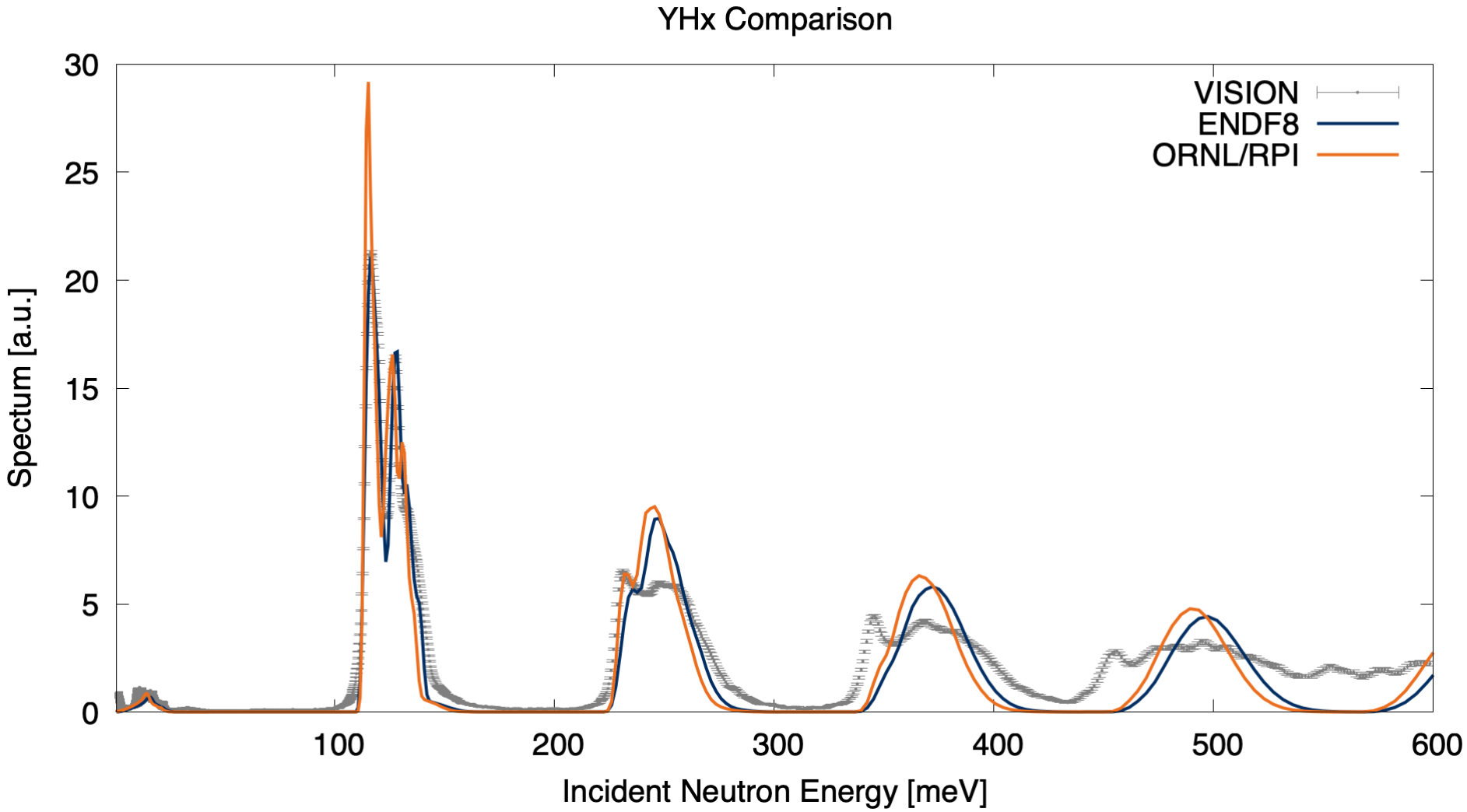
ENDF File Validation – Lucite



ENDF File Validation – Ice



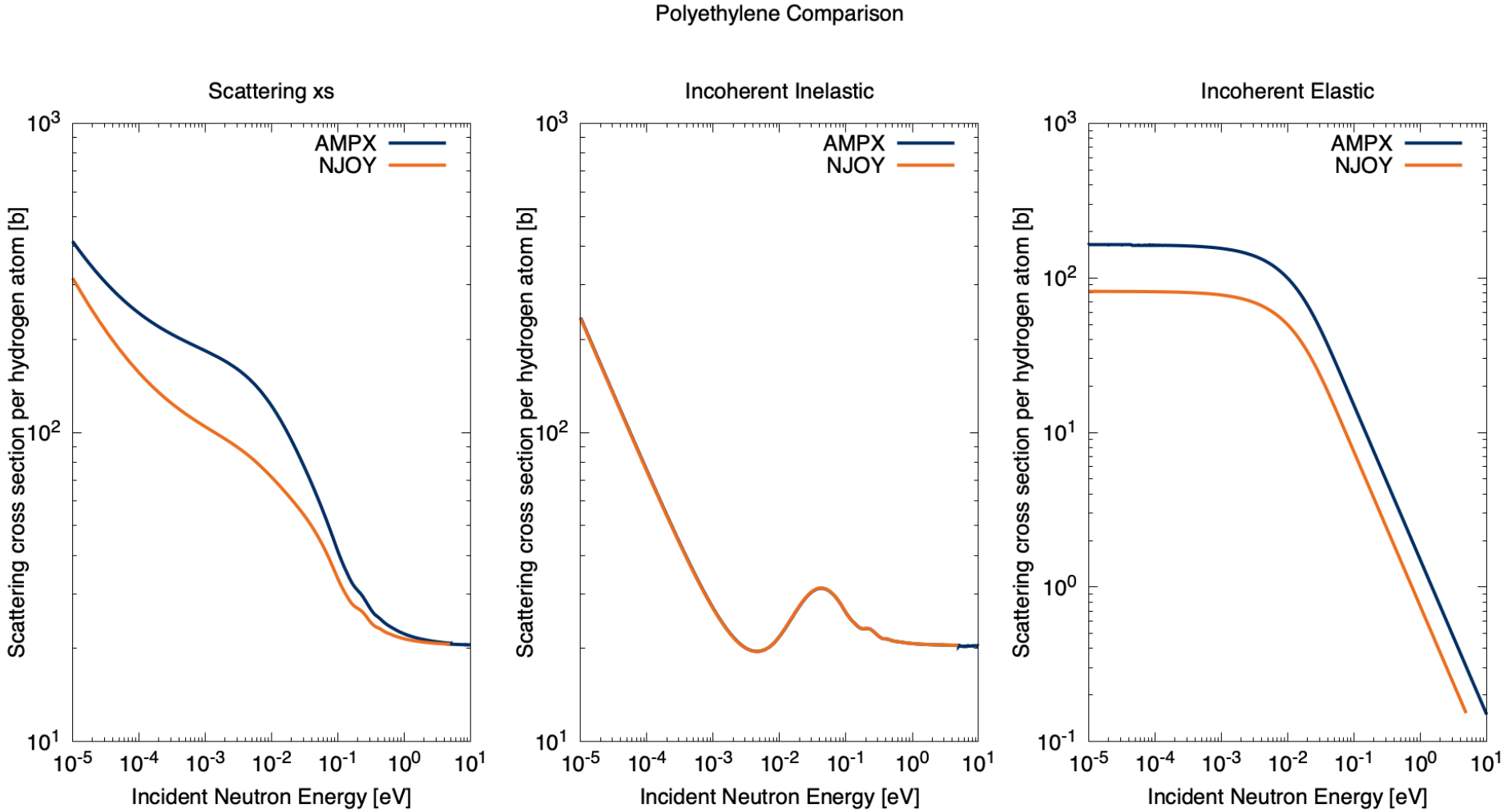
ENDF File Validation – YHx



Polyethylene Discrepancy – Underlying Cause

- Discrepancy noticed between how AMPX and NJOY processed hydrogen in polyethylene
- Investigation showed it was due to ambiguous wording in ENDF manual regarding incoherent elastic scattering
  - Manual: Characteristic bound cross section (barns)
  - Implementation: bound cross section * number of constituent atoms in molecule
- This led to a 2x over-prediction of incoherent elastic scattering contribution

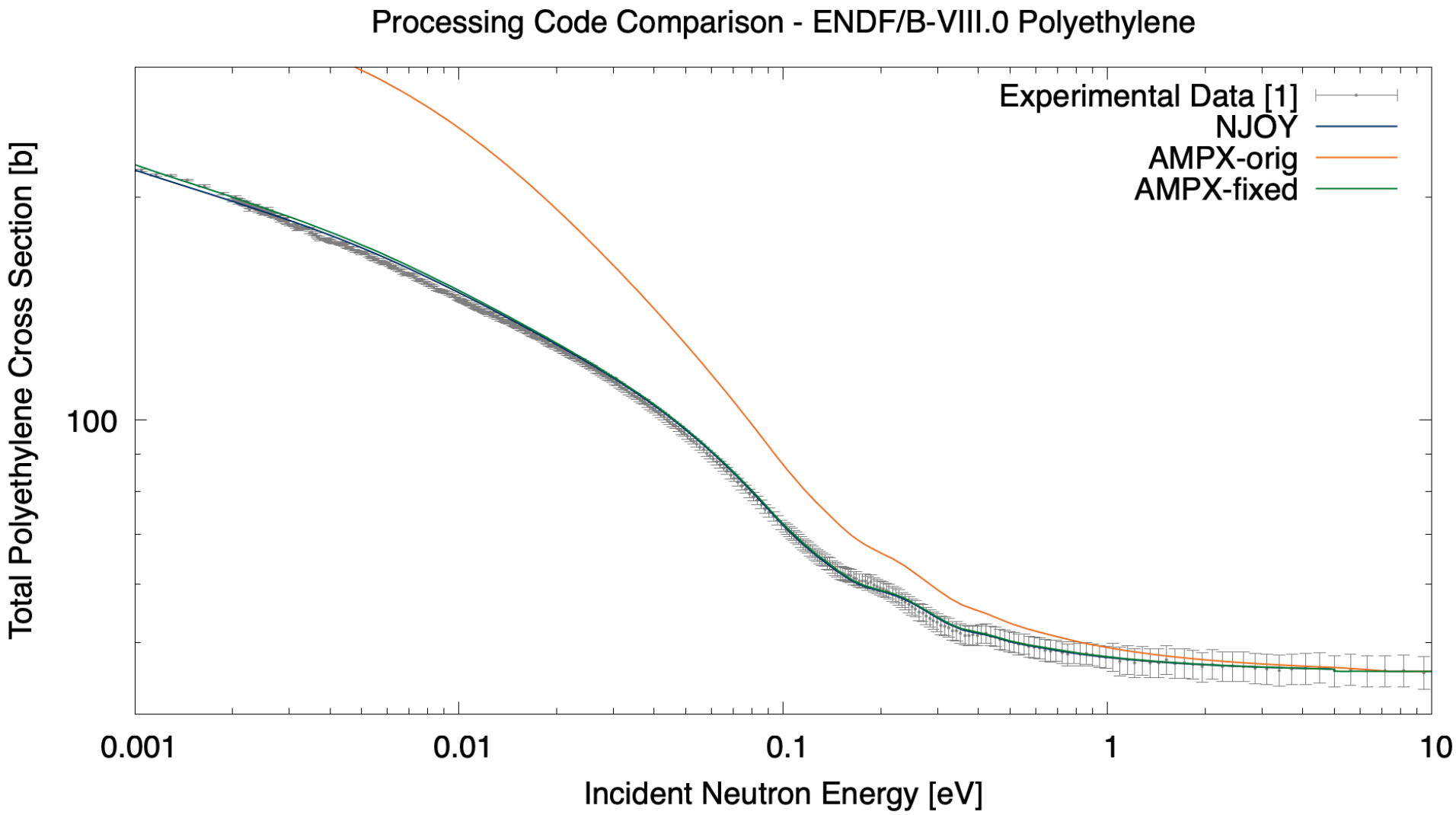
Polyethylene Discrepancy – Underlying Cause



Polyethylene Discrepancy – Solution

- Issue corrected by manually changing value in ENDF file to be the bound scattering cross section
  - Verified by plotting against experimental cross section – next slide
- Confirmed that issue only exists in materials with:
  - Incoherent elastic scattering contribution
  - Multiple scattering atoms per molecule
  - **Does not affect light water**
- Issue submitted to ENDF repository at NNDC

Polyethylene Discrepancy – Solution



Conclusions

- ENDF File Validation
  - Process developed to simulate VISION experiments
  - Method showed significant differences in inelastic spectra compared to experimental measurements
  - Differential data should be incorporated into thermal neutron scattering evaluation process to ensure accurate TSL files

- Polyethylene Discrepancy
  - Issue found and corrected
  - ENDF manual change submitted & currently under review

Acknowledgments

- This work was supported by the Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the Department of Energy
- This research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.
- This research used resources of the Compute and Data Environment for Science at ORNL, which is supported by DOE SC under Contract No. DE-AC05-00OR22725.
- Computational resources were also provided by the Rensselaer Polytechnic Institute Center for Computational Innovations, more specifically the Artificial Intelligence Multiprocessing Optimized System supercomputer.
- These measurements were carried out with the assistance of Luke Daemen & Timmy Ramirez Cuesta of the VISION beamline at the Spallation Neutron Source
- The analysis and fixing of the polyethylene discrepancy was done in collaboration with Doro Wiarda, Andrew Holcomb, and B.J. Marshall

Reference

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Questions?