Applying Methodology for Evaluating and Validating TSLs to Materials of Interest to NCSP

Chris W. Chapman[1], Kemal Ramić[1], Goran Arbanas[1], Jesse Brown[1], Alexander I. Kolesnikov[1], Matthew B. Stone[1], Luke Daemen[1], Yongqiang Cheng[1], Anibal Ramirez Cuesta[1], Yaron Danon[2], Dominik Fritz[2]

[1]Oak Ridge National Laboratory
[2]Rensselaer Polytechnic Institute

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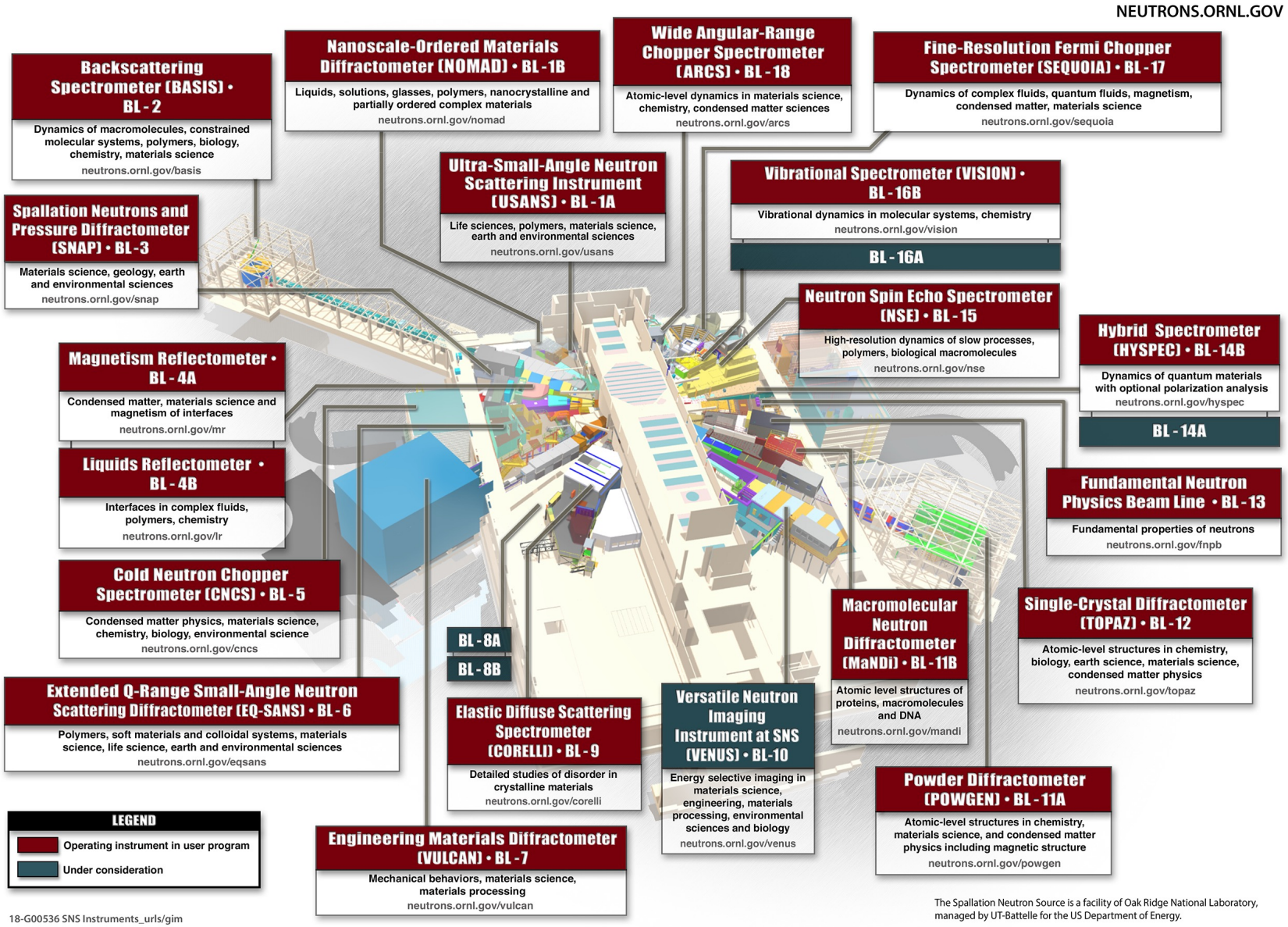
Overview

- Recent efforts in validating thermal neutron scattering cross sections:
  - Differential cross section measurements at ORNL for:
    - Evaluation [1]
    - Validation [2,3,4,5]
  - Total cross section measurements at RPI [6,7]
  - Pulsed-neutron die-away experiments at LLNL [8]
  - Integral criticality experiments by LLNL [9]
- Here, we propose a methodology for not only validating thermal scattering files that utilizes all available experimental data, but also for evaluating new libraries as demonstrated on Polystyrene and Lucite

Evaluation – Procedure

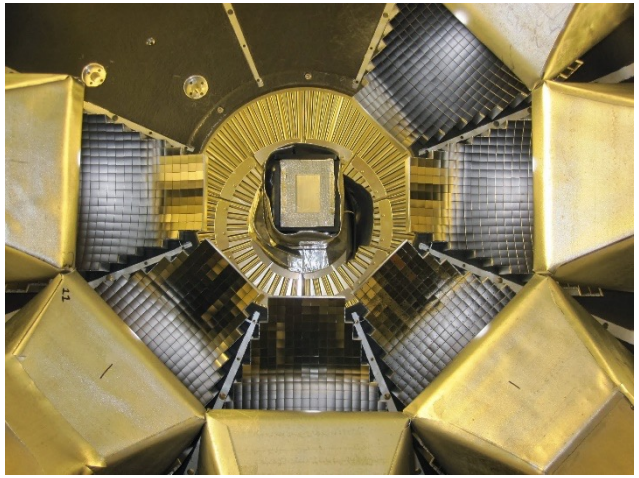
- Material (polystyrene or Lucite) simulated using DFT program VASP, then post-processed using Phonopy and OClimax to obtain Phonon density of states (PDOS)
- PDOS then optimized using NCrystal [11] and Dakota [12] using the following:
  - Process PDOS using NCrystal to calculate both the total cross section and VISION spectra
  - Calculate χ^2 of these datasets compared to experimentally measured total cross section and VISION spectra
  - Use Dakota to vary the PDOS based on the calculated χ^2 metric until convergence is achieved

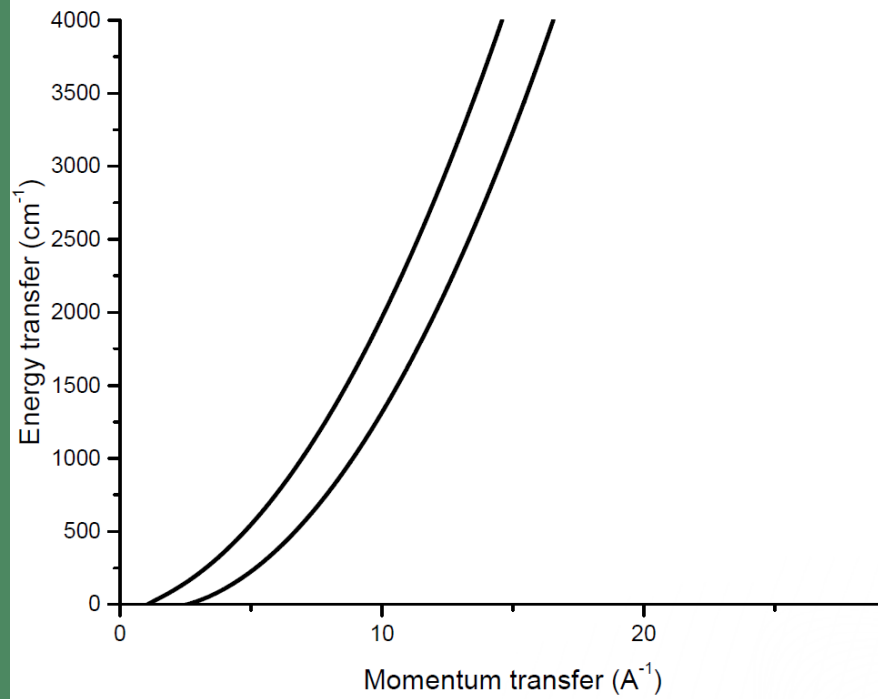
Evaluation – SNS Facility

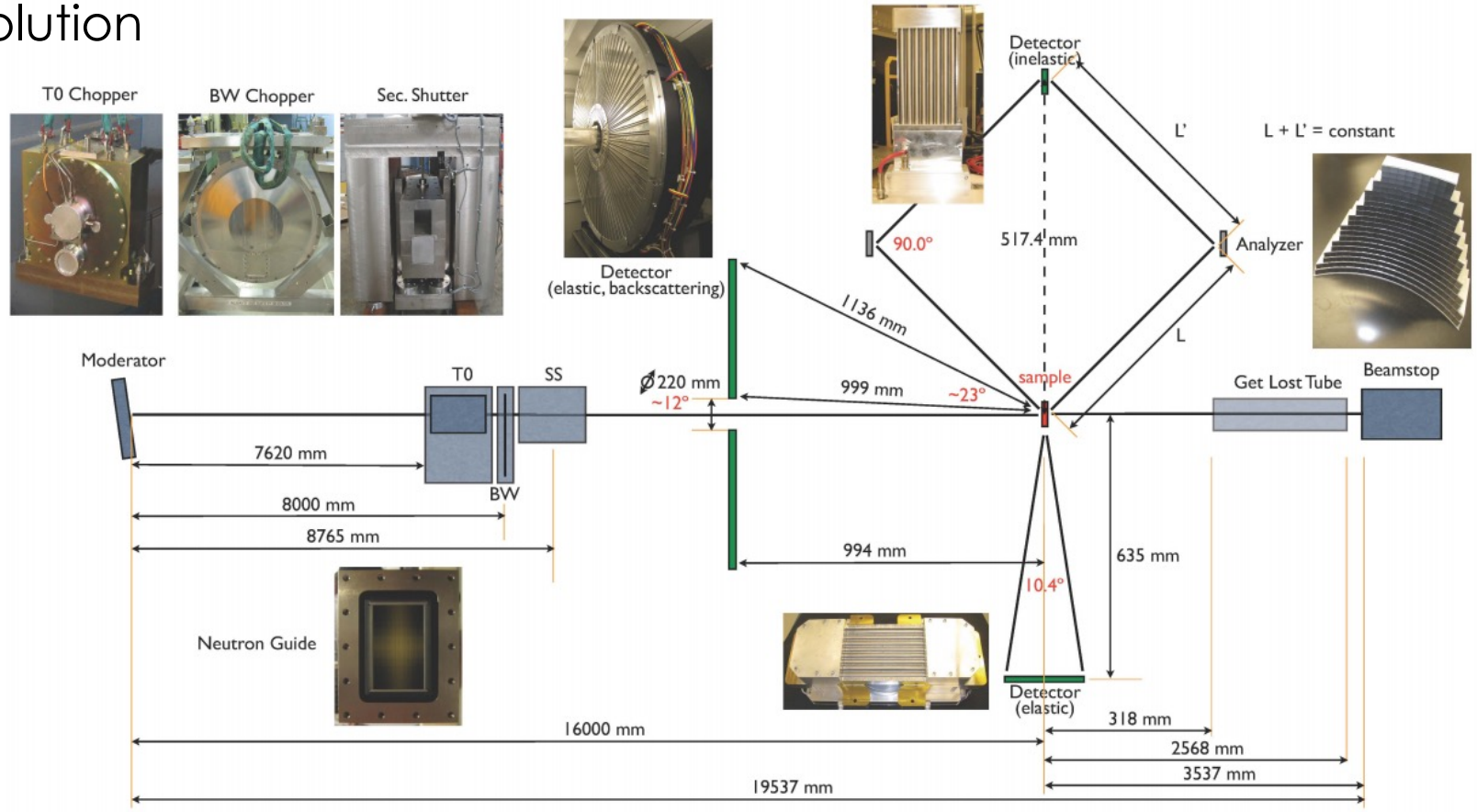


Evaluation – VISION beamline

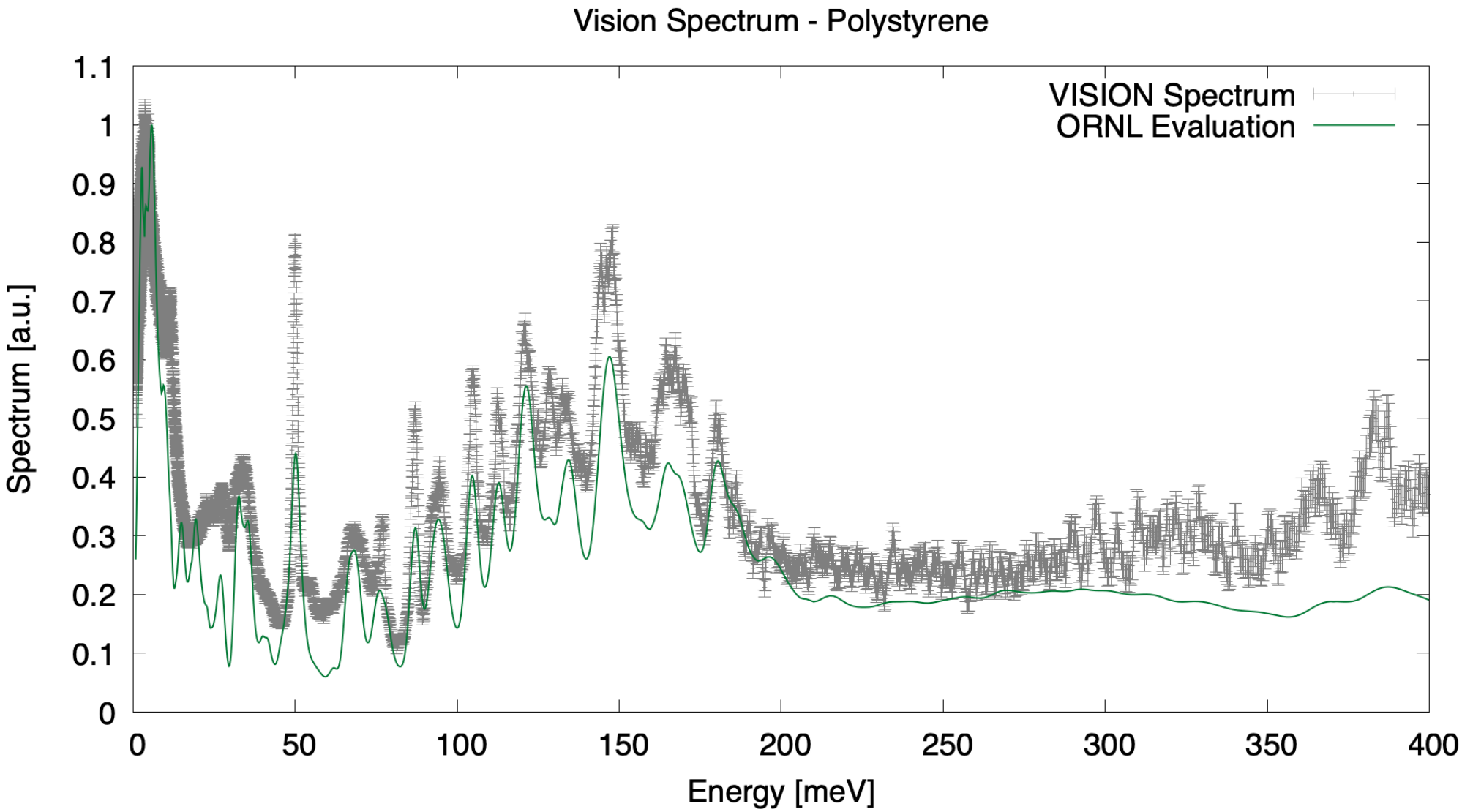
- Indirect geometry vibrational spectrometer
- White beam of neutrons hits sample
- Scattered neutrons reflected off graphite blocks to two detectors for forward- and backward-scattering angles
- Graphite blocks configured to scatter neutrons at 4 meV
- Constant relative energy resolution



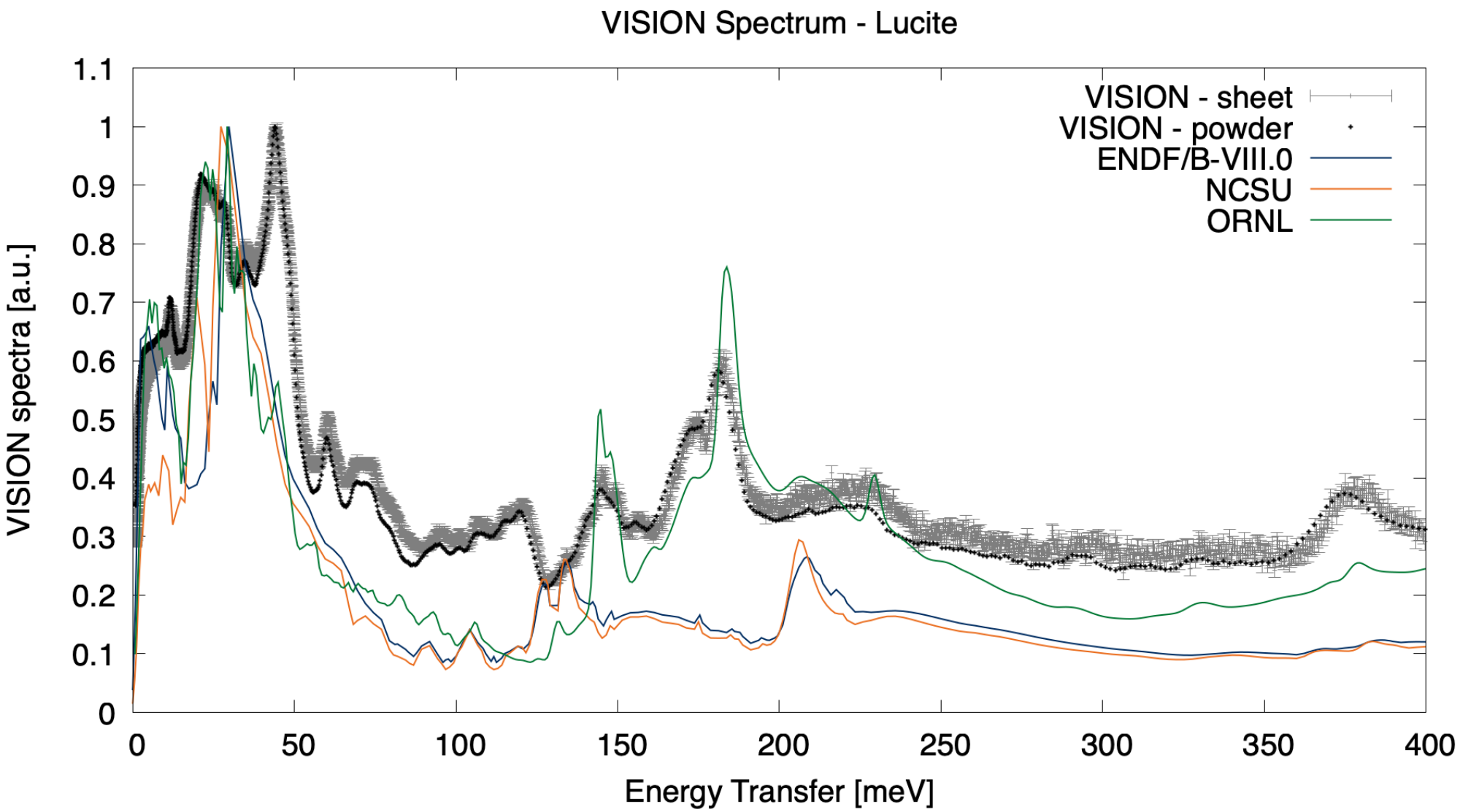




Evaluation – Differential Scattering – Polystyrene



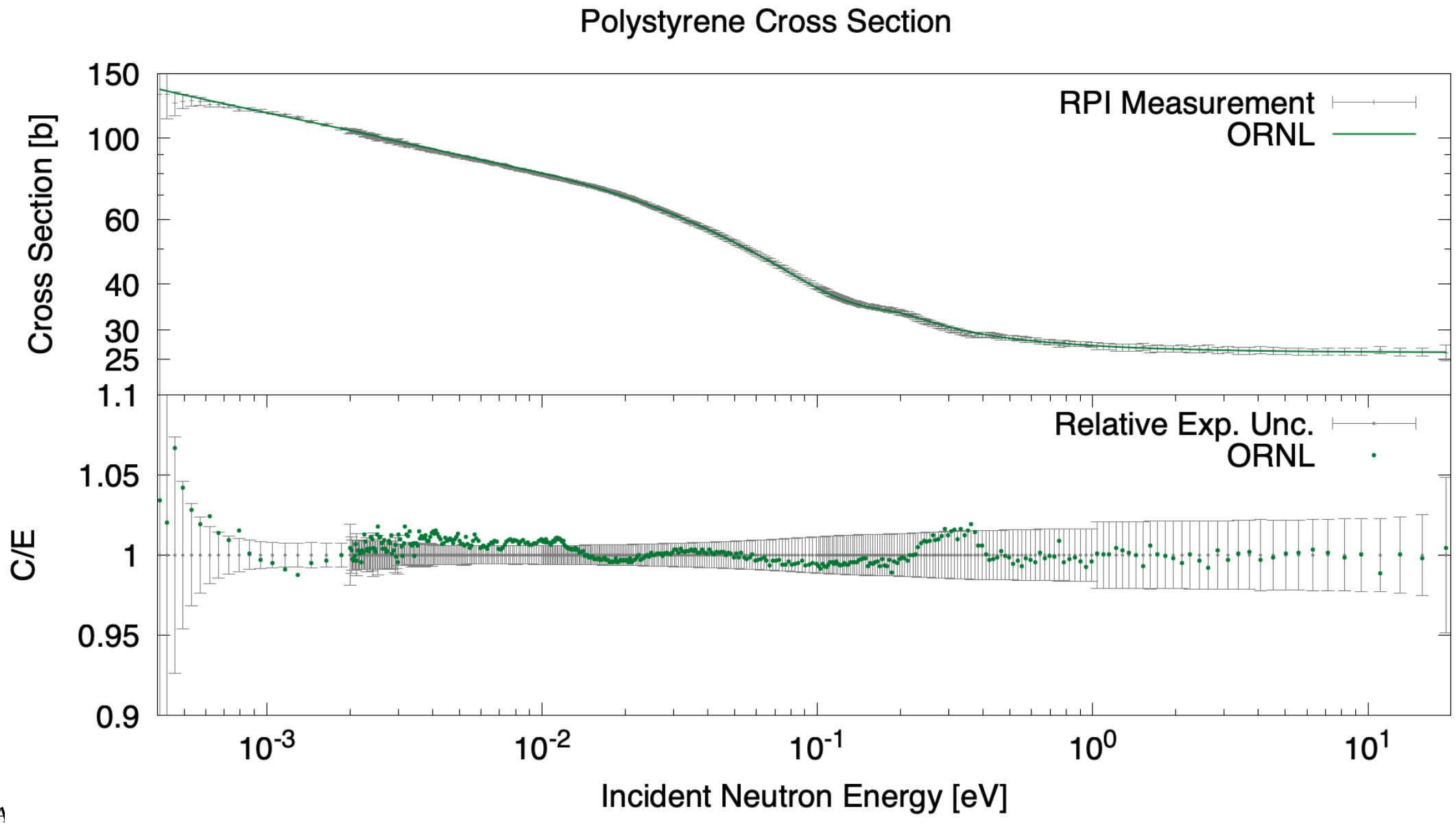
Evaluation – Differential Scattering – Lucite



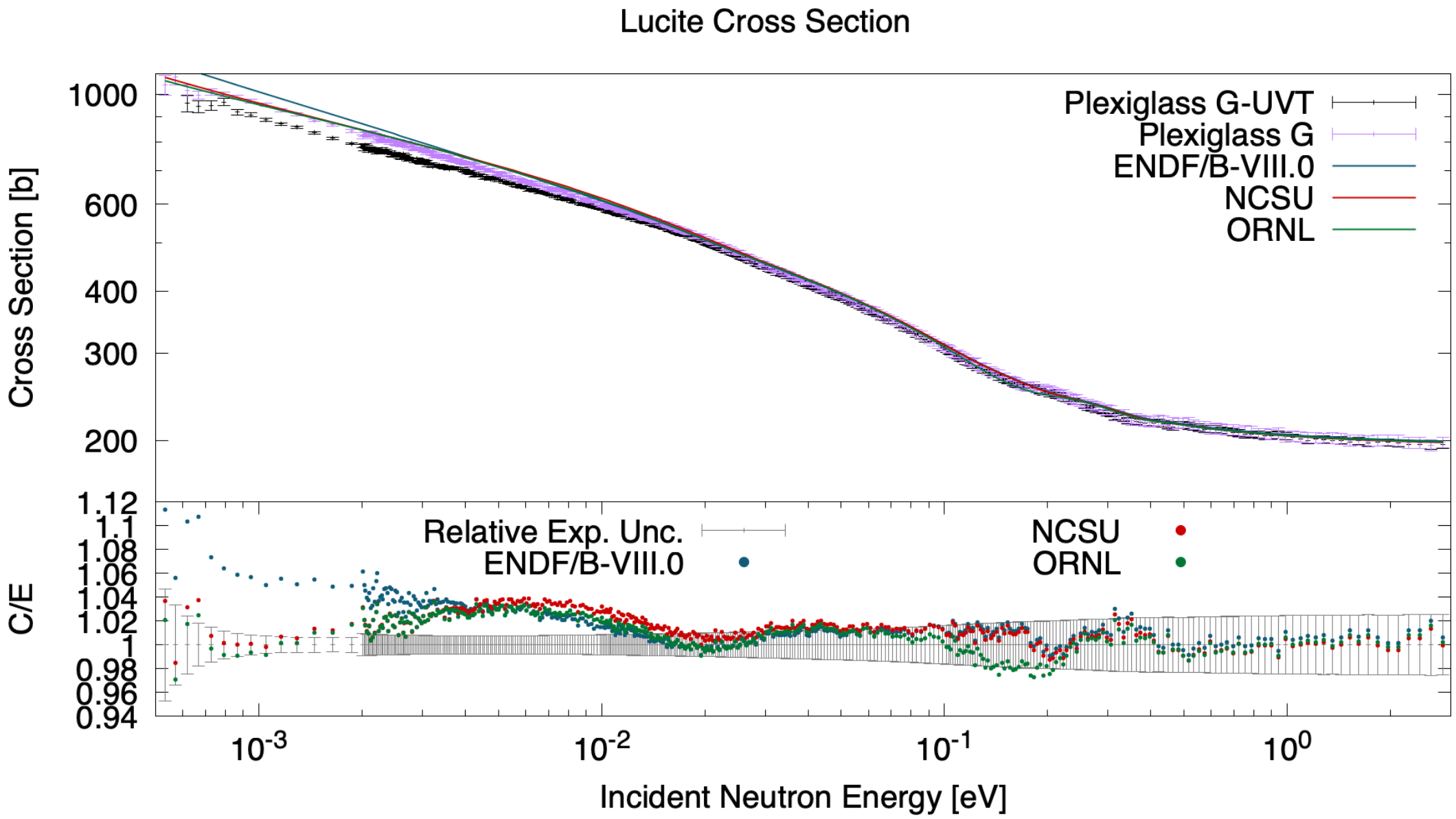
Evaluation – Total Cross Section

- Comparison of evaluation to experiment straightforward
- Transmission measurements carried out at RPI
  - Utilized NCSP-funded enhanced thermal target + cold moderator addition to LINAC
  - Used for evaluation; cannot be used for validation
- Ideally, multiple samples/experiments would be used
  - Some for validation, some for evaluation
  - See Kemal's talk

Evaluation – Total Cross Section – Polystyrene



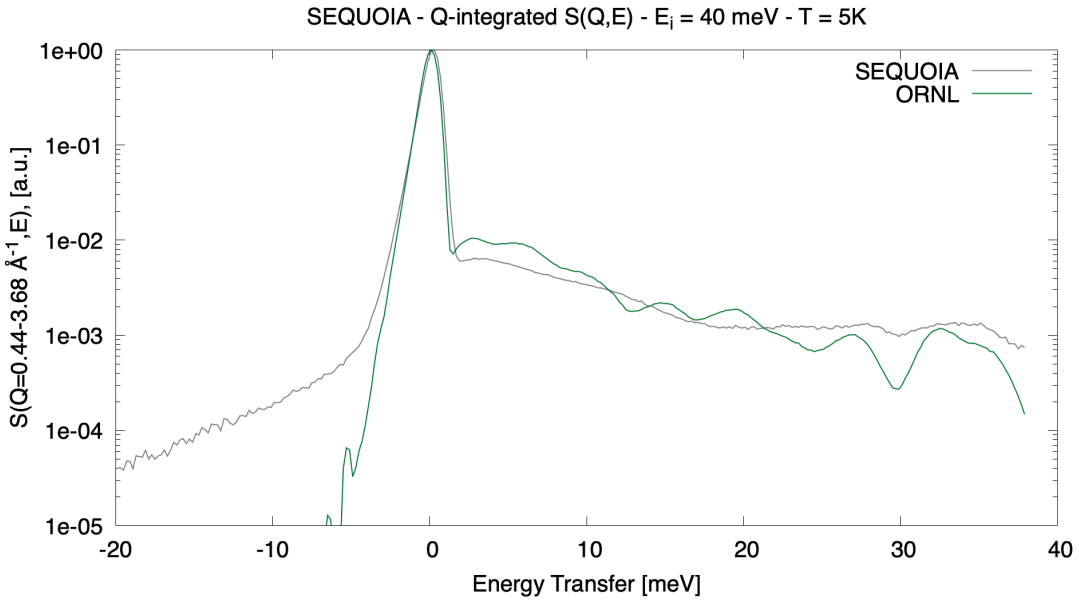
Evaluation – Total Cross Section – Lucite

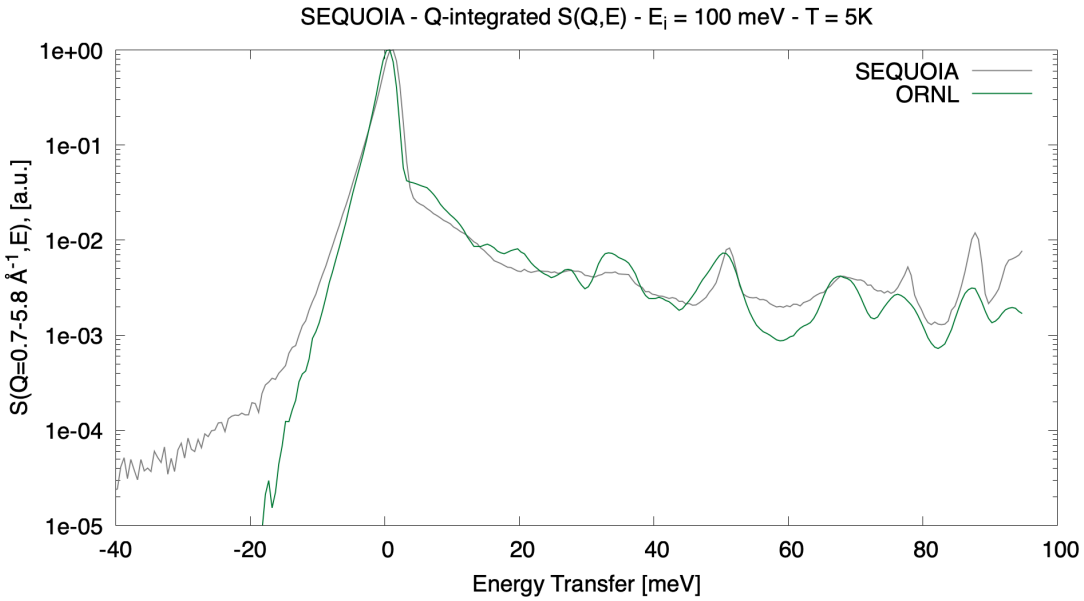


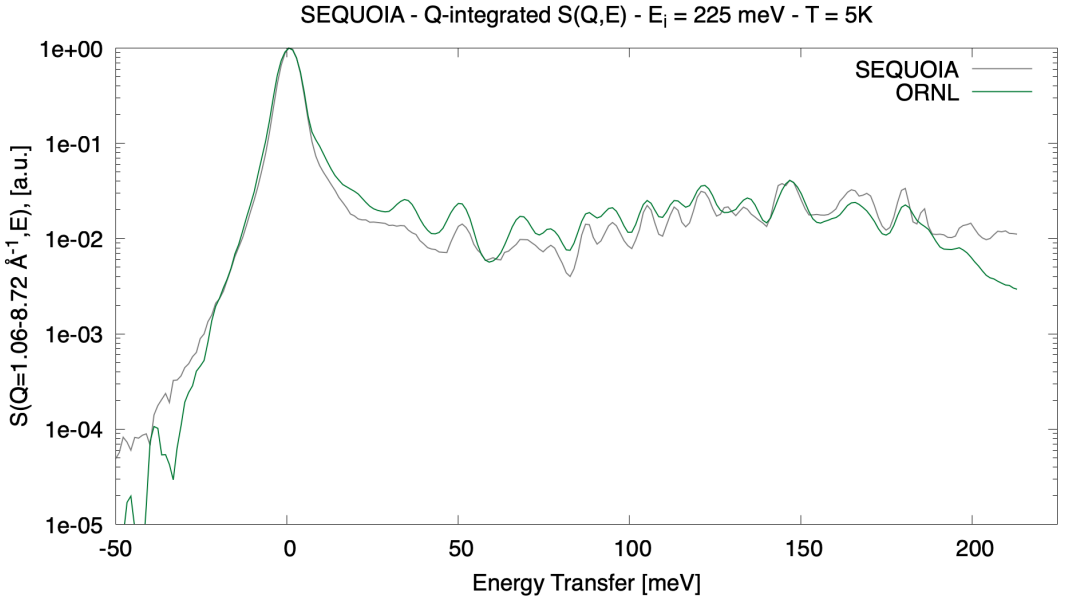
Validation – Differential Scattering

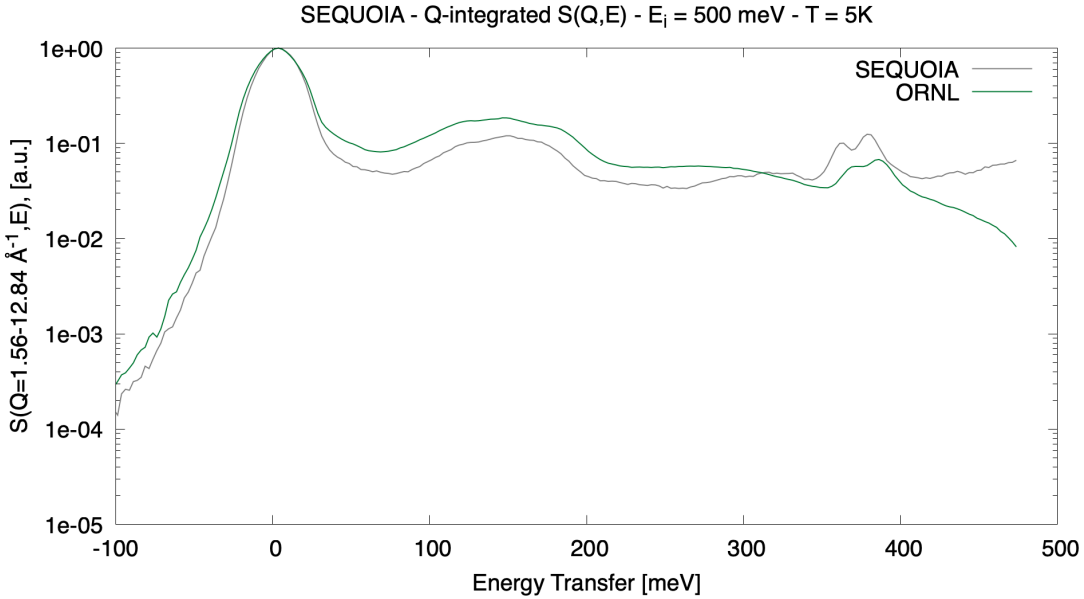
- Direct comparison to double differential measurements is difficult for several reasons:
  - Large number of datapoints (~1e5-1e6 points per incident energy)
  - Experimental uncertainties are normally very small, leading to unrealistic chi-squared values
- Several ways to combat these issues
  - Slice data into several 2-D sets (e.g., DDXS at specific scattering angles)
  - Integrate data over angle/energy

Validation – Differential Scattering – Polystyrene



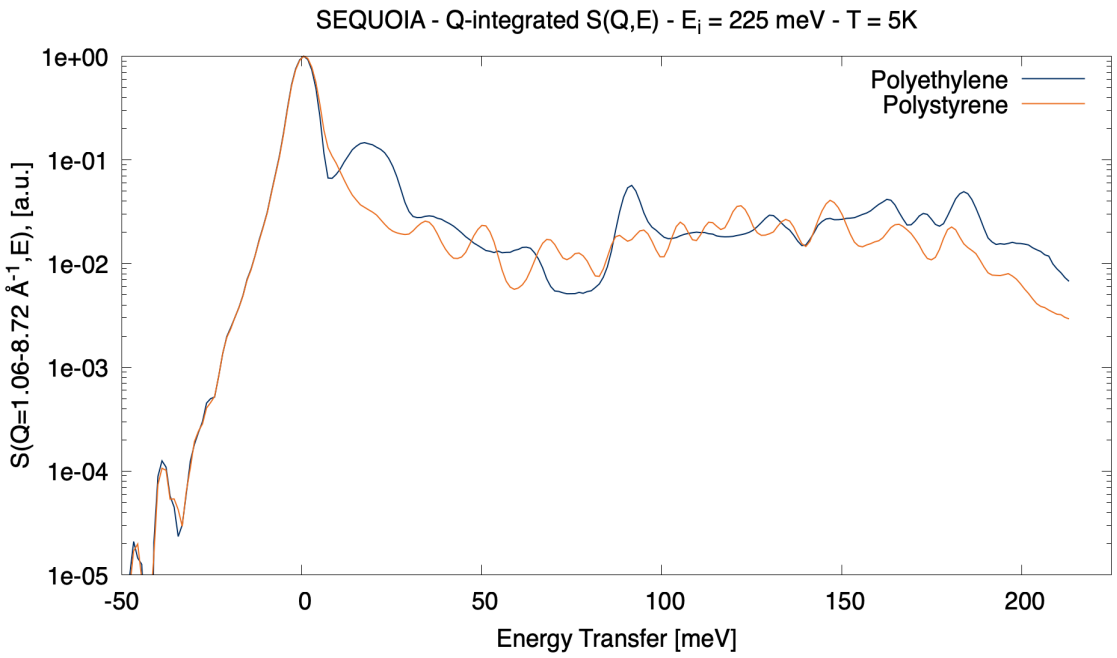


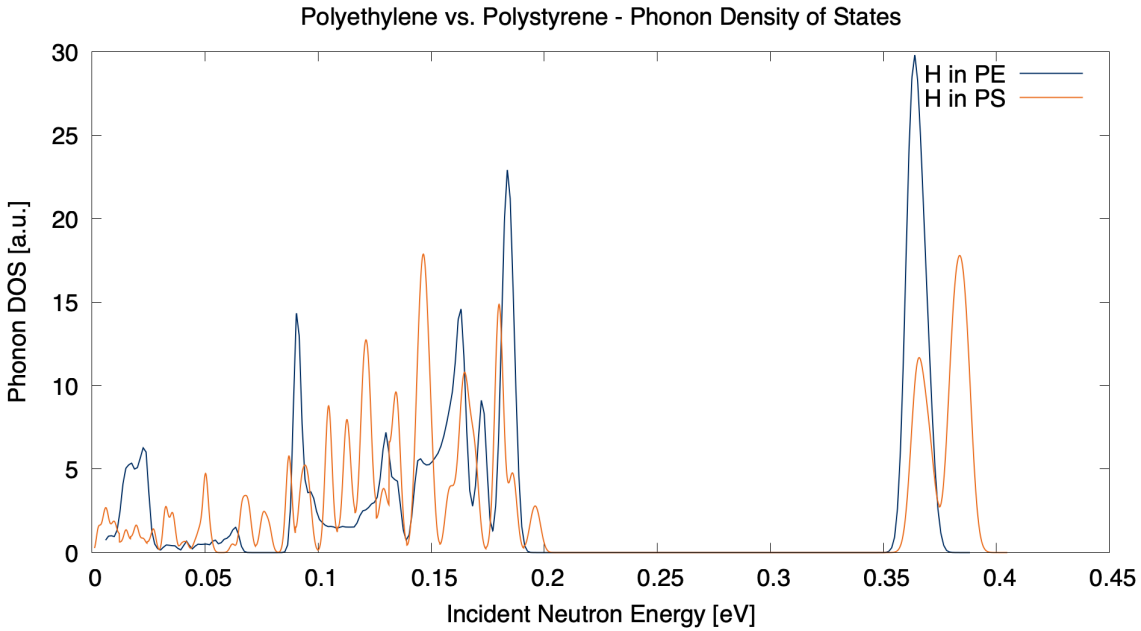


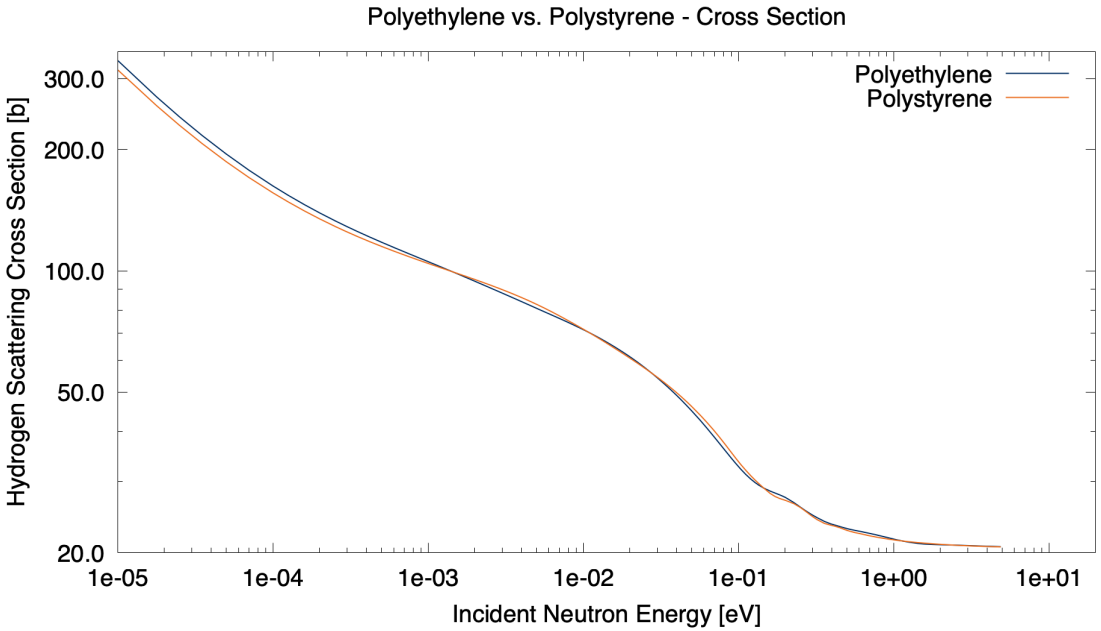


Validation – Polystyrene

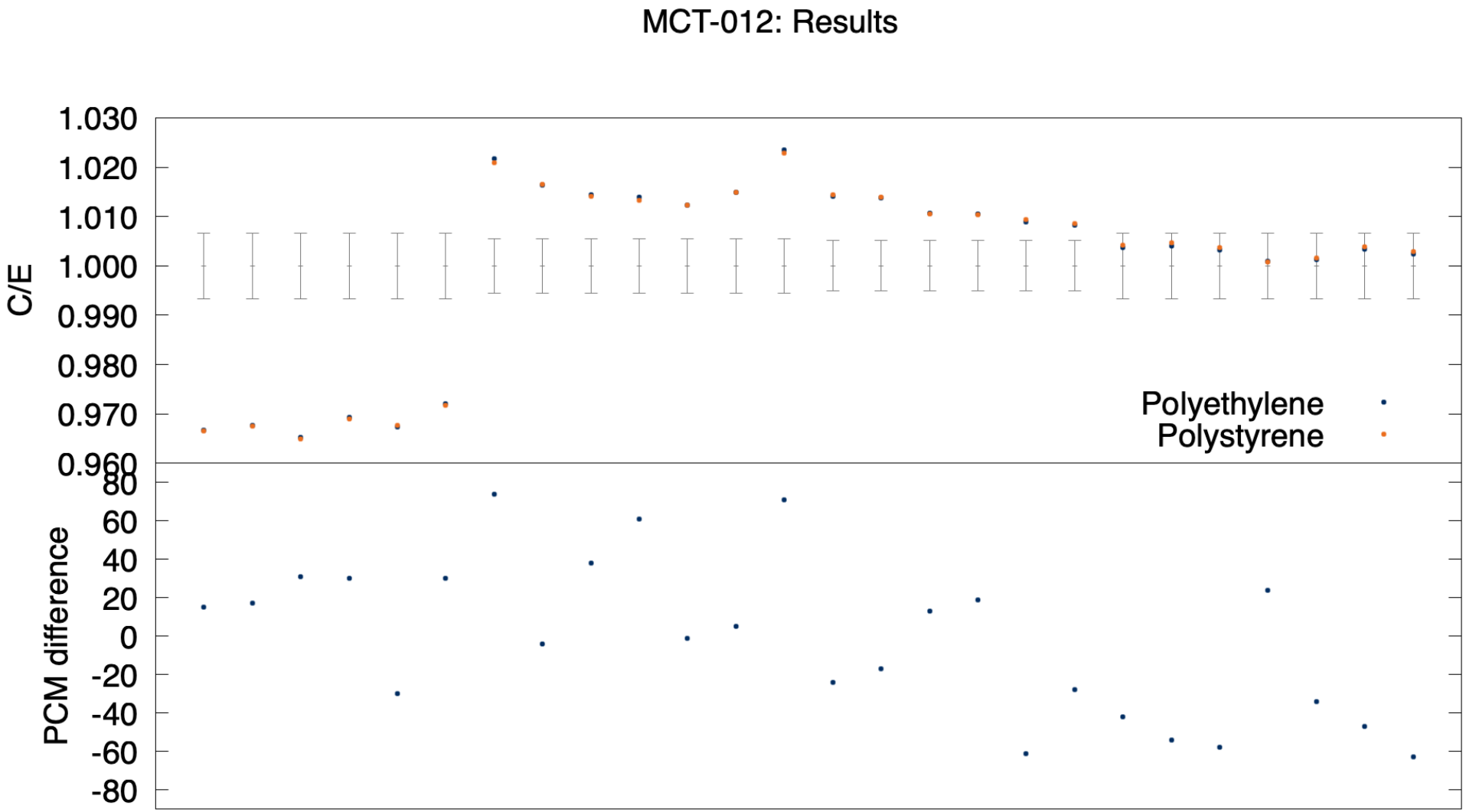
- Several ICSBEP benchmarks contain polystyrene
- Previously used polyethylene TSL library as a surrogate for polystyrene
  - Is this a good approximation?





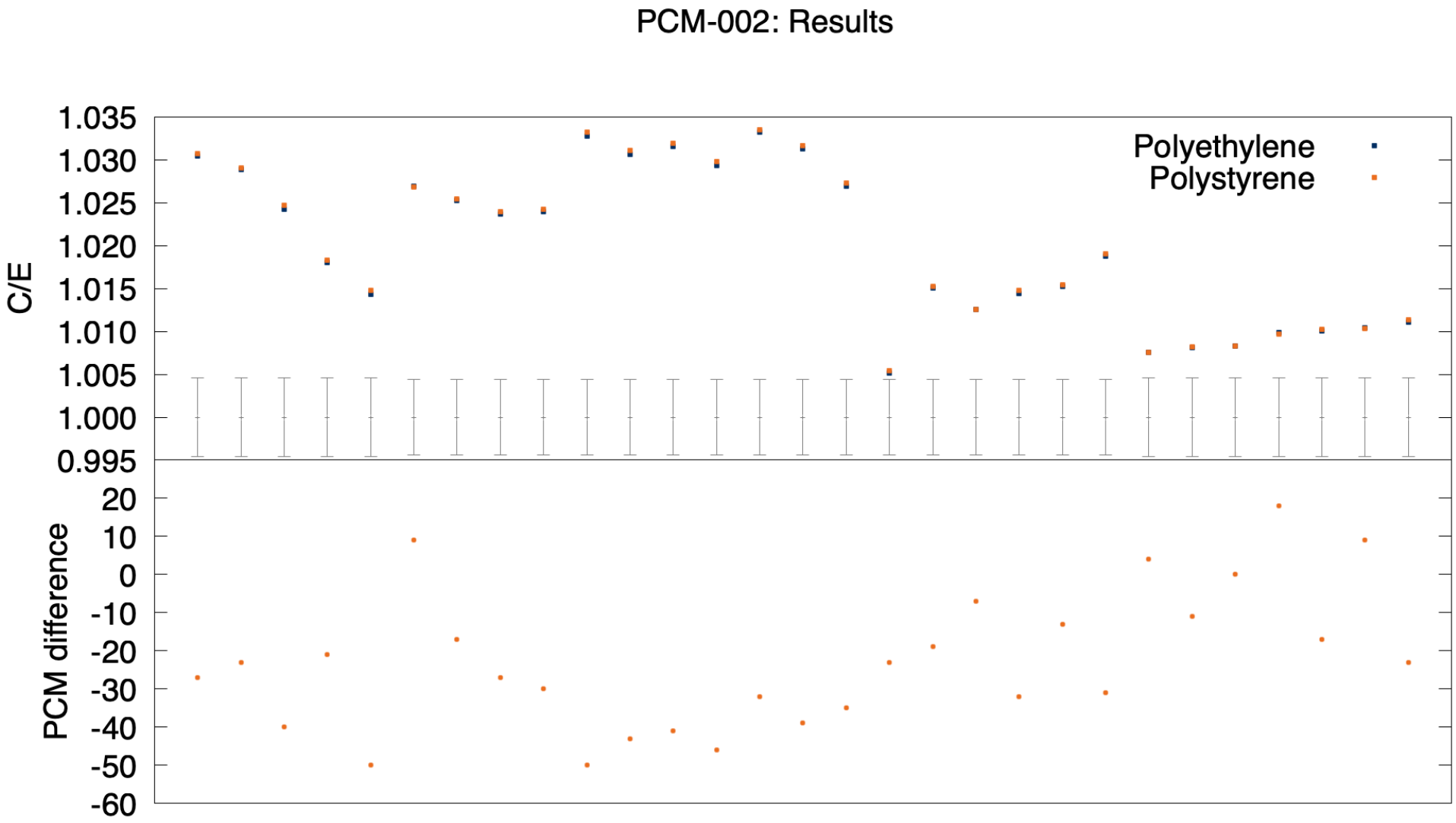


Validation – Polystyrene – MCT-012



Material	χ^2/dof
Polyethylene	9.12
Polystyrene	9.13

Validation – Polystyrene – PCM-002

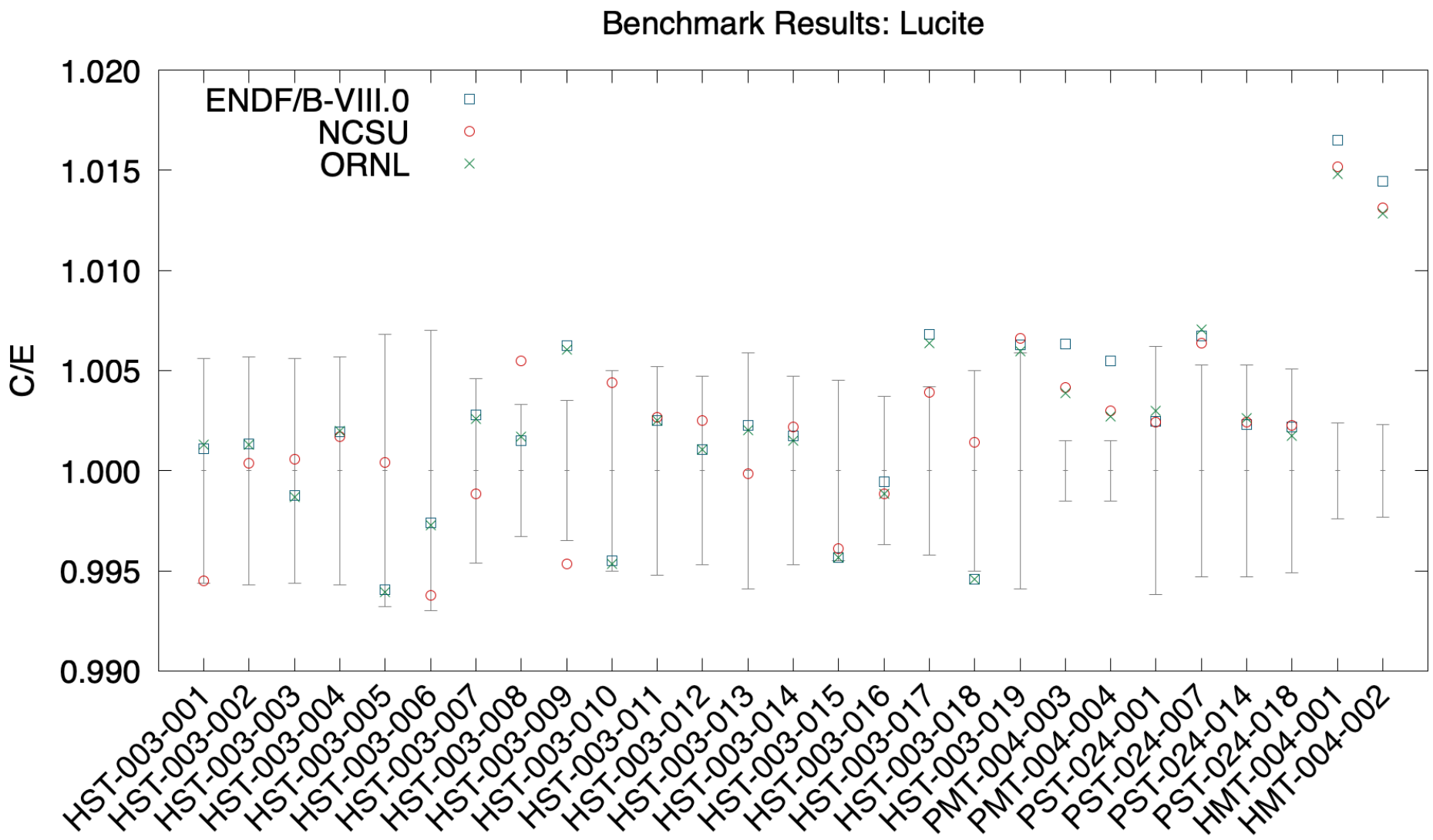


Material	χ^2/dof
Polyethylene	24.2
Polystyrene	24.7

Validation – Lucite

- Several different evaluations for Lucite exist:
  - ENDF/B-VIII.0
  - NCSU
  - ORNL
- Validate using two independent integral techniques
  - ICSBEP benchmarks
  - Pulsed neutron die-away (PNDA) experiments

Validation – Lucite – ICSBEP Benchmarks



Library	χ^2/dof
ENDF/B-VIII.0	0.899
NCSU	0.784
ORNL	0.750

Validation – Lucite – PNDA

Experiment			ENDF/B-VIII.0		NCSU		ORNL	
Diameter [cm]	α [1/ms]	std (1/ms)	α [1/ms]	St.dev away	α [1/ms]	St.dev away	α [1/ms]	St.dev away
25.4632	5.896	0.006	6.011	19.118	5.955	9.803	5.960	10.628
22.9171	6.365	0.008	6.422	7.155	6.352	1.587	6.355	1.308
20.3707	6.884	0.009	6.981	10.759	6.896	1.372	6.903	2.154
17.8373	7.653	0.008	7.795	17.700	7.674	2.635	7.675	2.740
15.2441	8.821	0.01	9.006	18.450	8.870	4.920	8.861	4.047
12.7057	10.611	0.009	10.993	42.459	10.773	18.004	10.776	18.318
10.1765	13.804	0.01	14.320	51.574	13.965	16.125	13.997	19.327
7.6267	20.051	0.05	21.317	25.323	20.682	12.612	20.583	10.637
5.08	33.911	0.18	38.599	26.043	36.852	16.340	35.357	8.032

Conclusions

- Polystyrene & Lucite evaluations conducted using multiple experiments (differential and integral)
- Proposed methodology shown to improve neutron transport
- Files submitted to NNDC for inclusion in ENDF/B-VIII.1 release
- Differences in differential results don't always propagate to differences in integral results
  - Hence why evaluation of differential data important

Acknowledgements

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Questions ?

Extra slides – Evaluation

- PDOS chosen to vary because it affects all forms of thermal neutron scattering:

$$\frac{d^2\sigma}{dE_f d\Omega} = \frac{\sigma_b}{4\pi k_B T}\sqrt{\frac{E'}{E}}\, e^{\frac{-\beta}{2}}\, S(\alpha,\beta) \qquad S(Q,E) = \frac{1}{k_B T} e^{\frac{-\beta}{2}}\, S(\alpha,\beta)$$

  - Inelastic

$$S(\alpha,\beta) = e^{-\alpha\lambda}\sum_{n=0}^{\infty}\frac{\alpha^n}{n!}\frac{1}{2\pi}\int_{-\infty}^{\infty} d\hat{t}\, e^{i\beta\hat{t}}\left[\int_{-\infty}^{\infty} d\beta'\, P(\beta') e^{i\beta'\hat{t}} e^{-\beta'/2}\right]$$

$$P(\beta) = \frac{\rho(\beta)}{2\beta\sinh(\beta/2)}$$

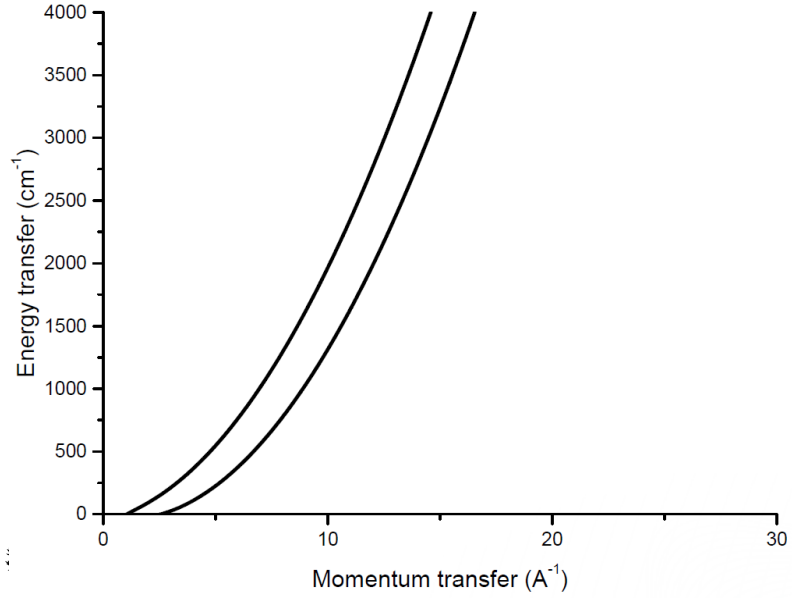
  - Elastic

$$\sigma_{el}^{inc}(E) = \frac{\sigma_b}{2}\left(\frac{1-e^{4WE}}{2WE}\right) \qquad \sigma_{el}^{coh}(E) = \frac{\sigma_c}{E}\sum_{E_i<E} f_i e^{4WE_i} \qquad W = \frac{\int_{-\infty}^{\infty} d\beta\, P(\beta) e^{-\beta/2}}{AkT}$$

Extra Slides – Validation

- Indirect Geometry
  - Currently used for evaluation
- 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

- Direct Geometry
  - Currently used for validation
- 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



Complimentary measurement techniques