A Case for Using Robust, Synthetic Data to Improve Nuclear Data Uncertainty Quantification

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Nuclear Data UQ Need

The nuclear data community needs reproducible methods for. . .

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1. Measuring the impact of select assumption violations on the accuracy of uncertainty quantifications.

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2. Augmenting existing uncertainty quantification methods to mitigate these impacts.

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The nuclear data community should support the use of robust, synthetic data to develop methods for improving uncertainty quantification.

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Syndat: Reproducible Synthetic Data

Walton, Brown, Fritsch, *et al.* [1] provide

> *"a generative model for the experimental observables produced by a determined total cross section in a neutron time-of-flight (TOF) transmission experiment,"*

and accompanying open source code [2].
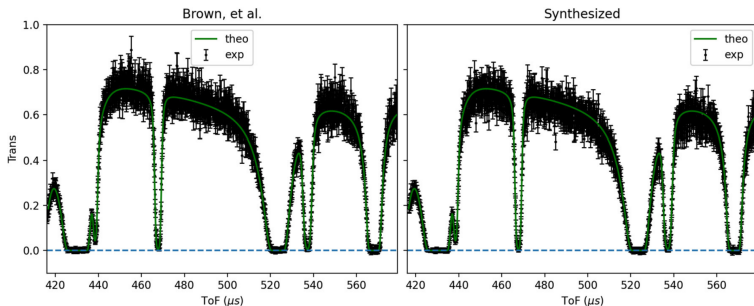
[1] N. Walton, J. Brown, W. Fritsch, D. Brown, G. Nobre, and V. Sobes, "Methodology for physics-informed generation of synthetic neutron time-of-flight measurement data," *Computer Physics Communications*, vol. 294, p. 108 927, 2024.

SAMMY UQ Limitations

Updated Users' Guide to SAMMY, Section IV.E.6:

"The posterior resonance parameter covariance matrix (RPCM) produced by SAMMY is a accurate representation of the uncertainties in the R-matrix evaluation. Nevertheless, uncertainties for evaluated cross sections reproduced by propagating the RPCM have historically been regarded as 'too small.'" [3]
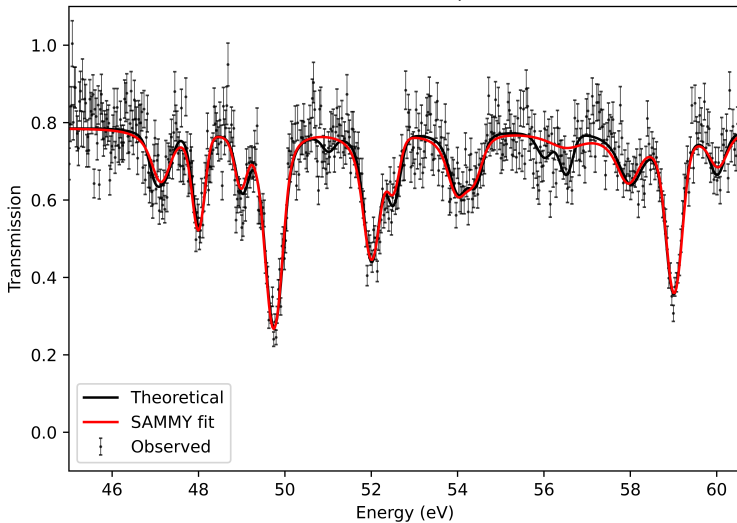
[3] N. M. Larson, "Updated users' guide for sammy: Multilevel r-matrix fits to neutron data using bayes' equations," ORNL, ORNL, Oak Ridge, TN, Tech. Rep. ORNL/TM-9179/R8, 2008, Section IV.E.6.

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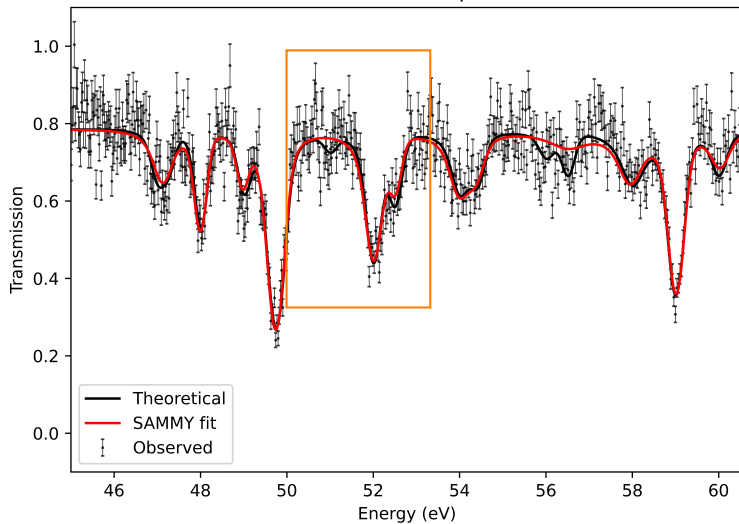# Ta-181 Example

Ta-181 Sample
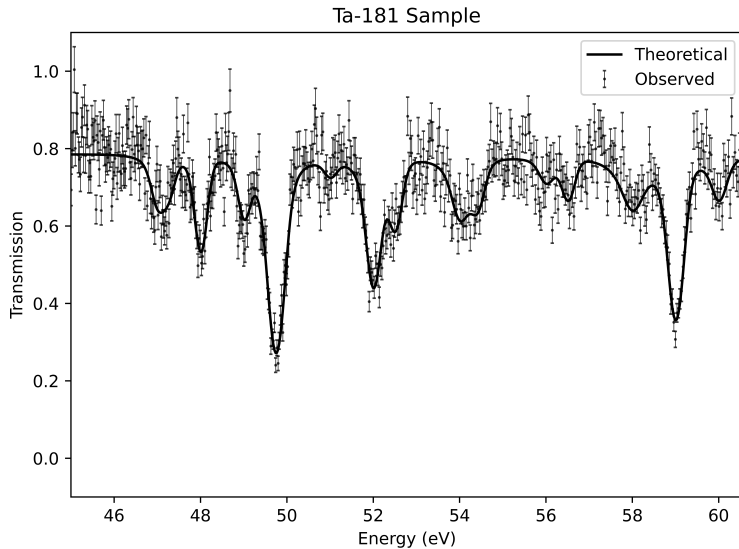
Ta-181 Example

A SAMMY Fit with Underspecified Model
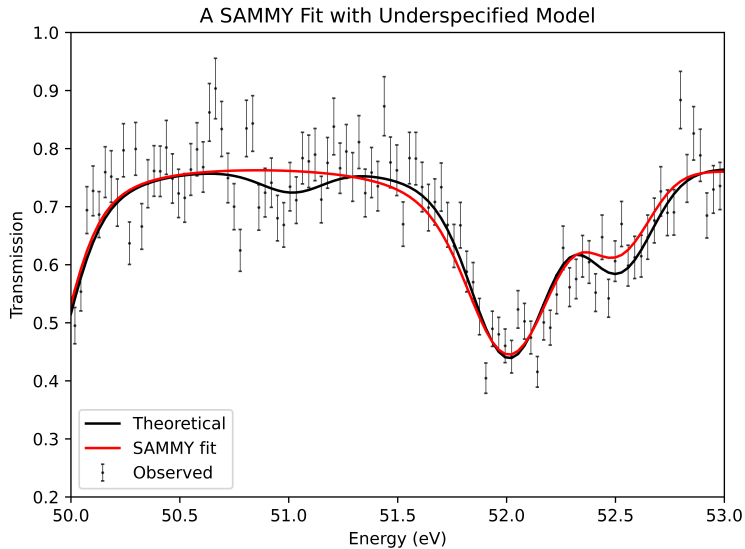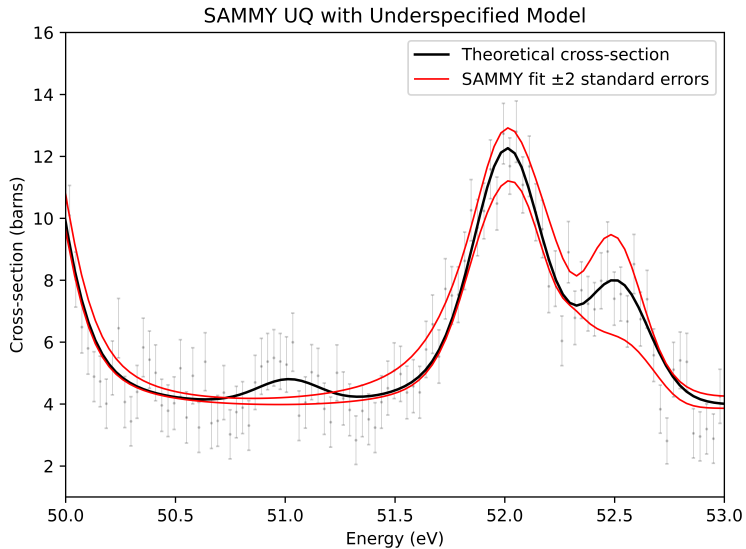
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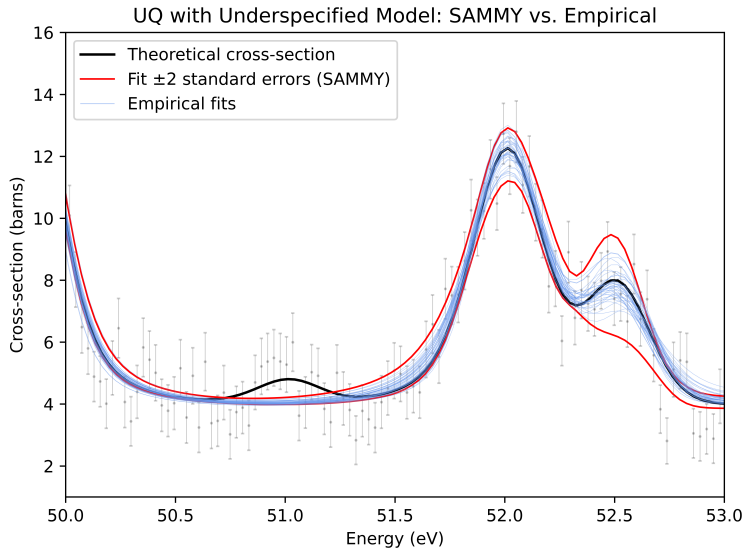
UQ with Underspecified Model: SAMMY vs. Empirical

Legend:
- Theoretical cross-section
- Fit ±2 standard errors (SAMMY)
- Empirical fits

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Ta-181 Example

UQ with Underspecified Model: SAMMY vs. Empirical

Legend:
- Theoretical cross-section
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- Fit ±2 standard errors (Empirical)
- Empirical fits

Y-axis: Cross-section (barns)
X-axis: Energy (eV)

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Ta-181 Example

UQ with Underspecified Model: SAMMY vs. Empirical
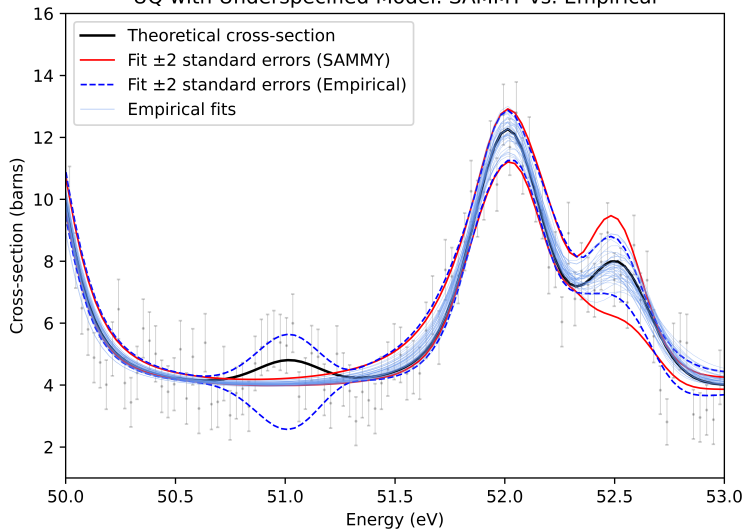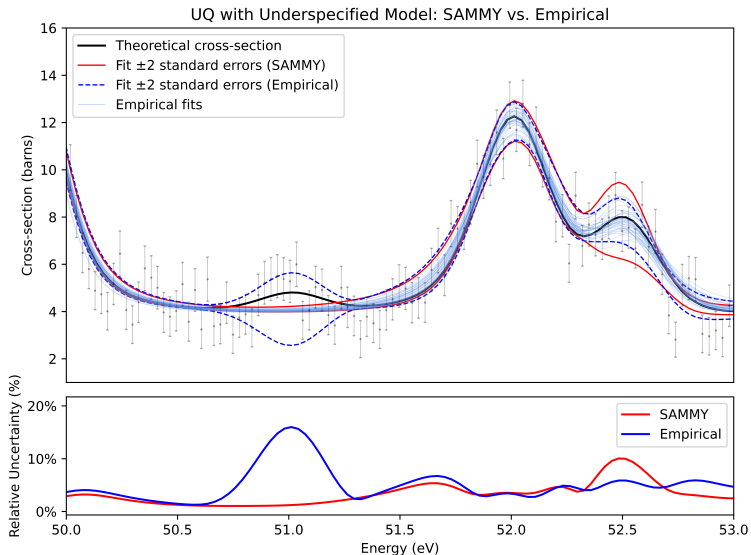
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What Synthetic Data Can do for UQ

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Recommendation

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[1] N. Walton, J. Brown, W. Fritsch, D. Brown, G. Nobre, and V. Sobes, "Methodology for physics-informed generation of synthetic neutron time-of-flight measurement data," *Computer Physics Communications*, vol. 294, p. 108 927, 2024.

[2] N. Walton, *Syndat: Synthetic Data Generation*, https://github.com/Naww137/Syndat, 2024.

[3] N. M. Larson, "Updated users' guide for sammy: Multilevel r-matrix fits to neutron data using bayes' equations," ORNL, ORNL, Oak Ridge, TN, Tech. Rep. ORNL/TM-9179/R8, 2008, Section IV.E.6.

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