Towards rigorous uncertainty quantification in nuclear data evaluation

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University of Tennessee
Oak Ridge National Laboratory, Los Alamos National Laboratory

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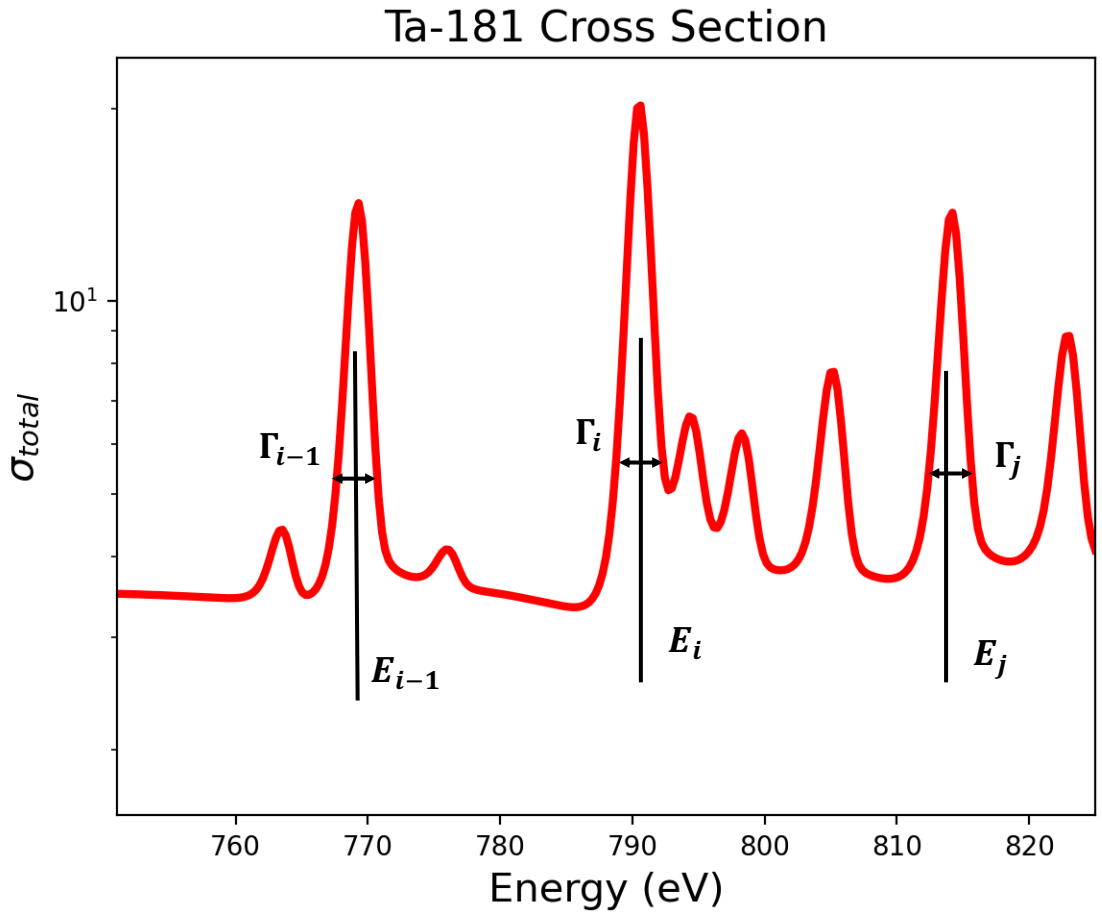
Introduction



Department and University: University of Tennessee Department of Nuclear Engineering
Academic Advisor: Vladimir Sobes
NSSC Research Focus Area(s): Nuclear Data
Academic Standing: Plan to graduate with PhD 12/2024

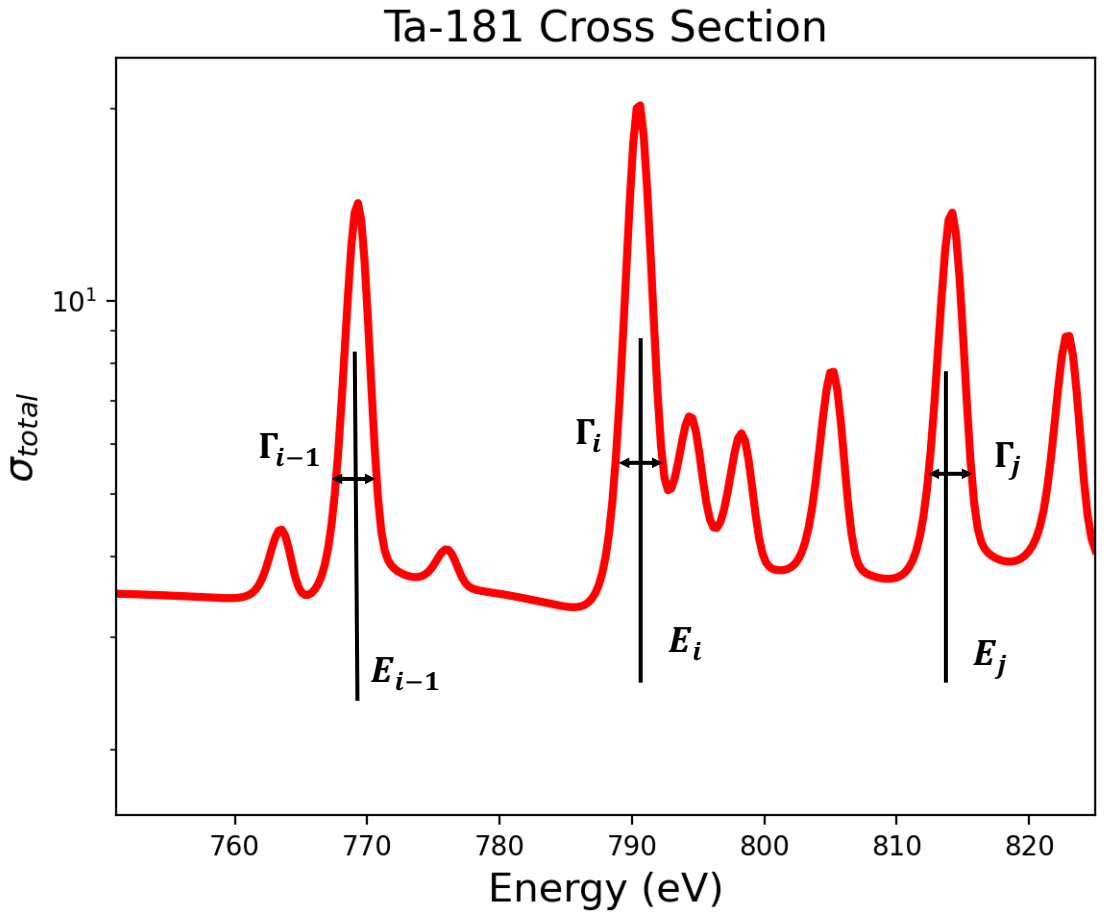
Lab Mentor and Partner National Laboratory:

- Jesse Brown, Oak Ridge National Laboratory
- Denise Neudecker, Los Alamos National Laboratory
- Mike Grosskopf, Los Alamos National Laboratory

Mission Relevance of Research:

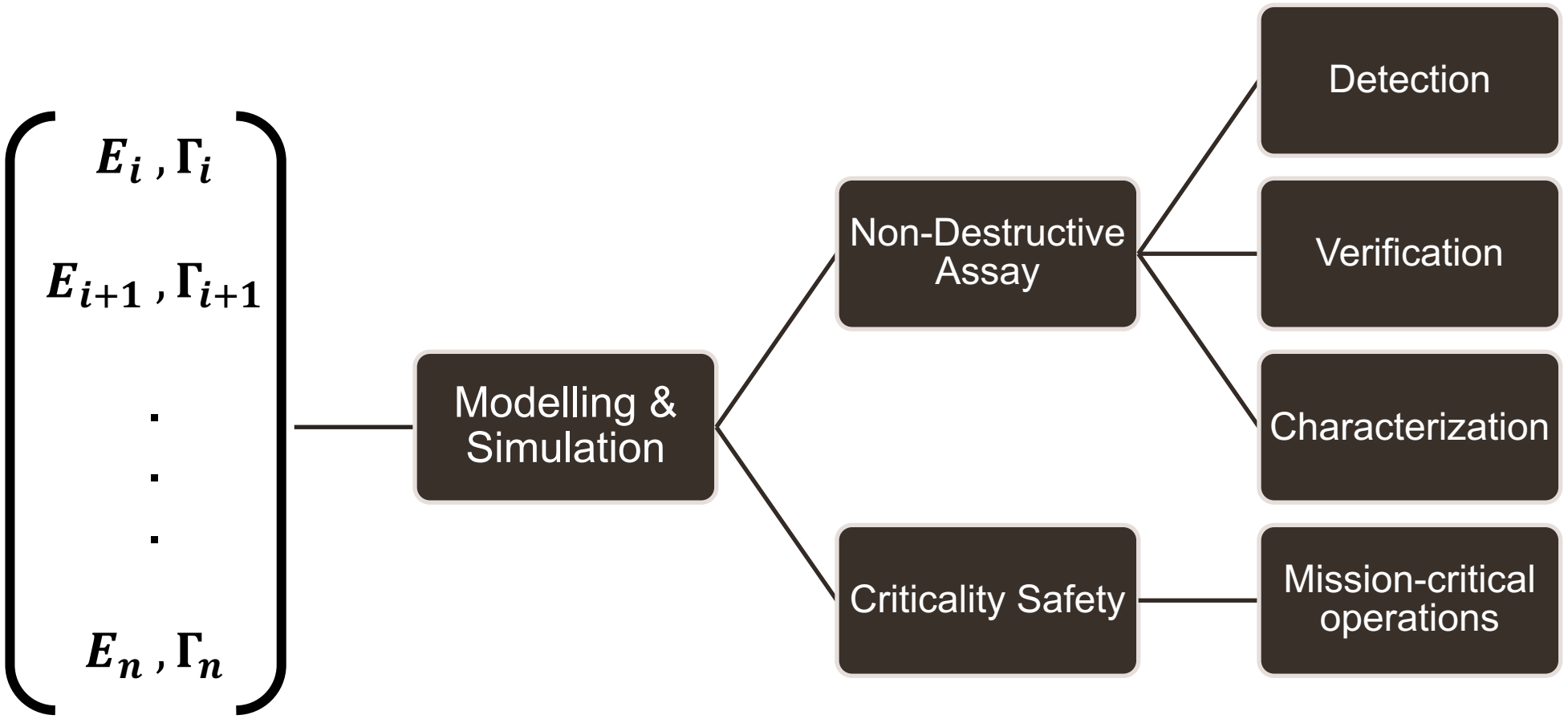
- Nuclear data underpins modelling & simulation (M&S)
- M&S plays a vital role in the nuclear security mission
- This research broadly improves accuracy and UQ on key nuclear data
- Specific demonstration focuses on Ta-181, a pertinent isotope for mission-critical operations and a focus of the nuclear data group at Los Alamos National Laboratory

Resonance parameters describe reaction cross sections

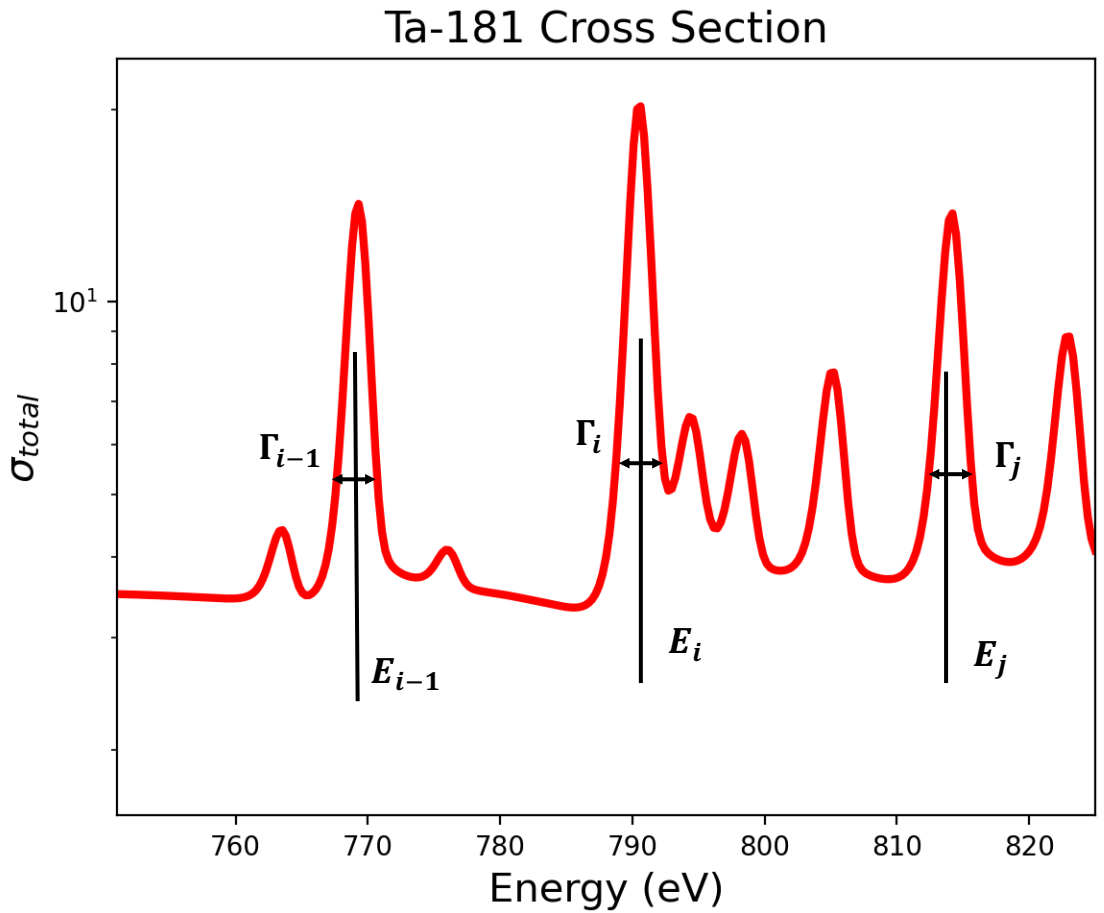


$$\begin{pmatrix} E_i, \Gamma_i \\ E_{i+1}, \Gamma_{i+1} \\ \vdots \\ E_n, \Gamma_n \end{pmatrix}$$

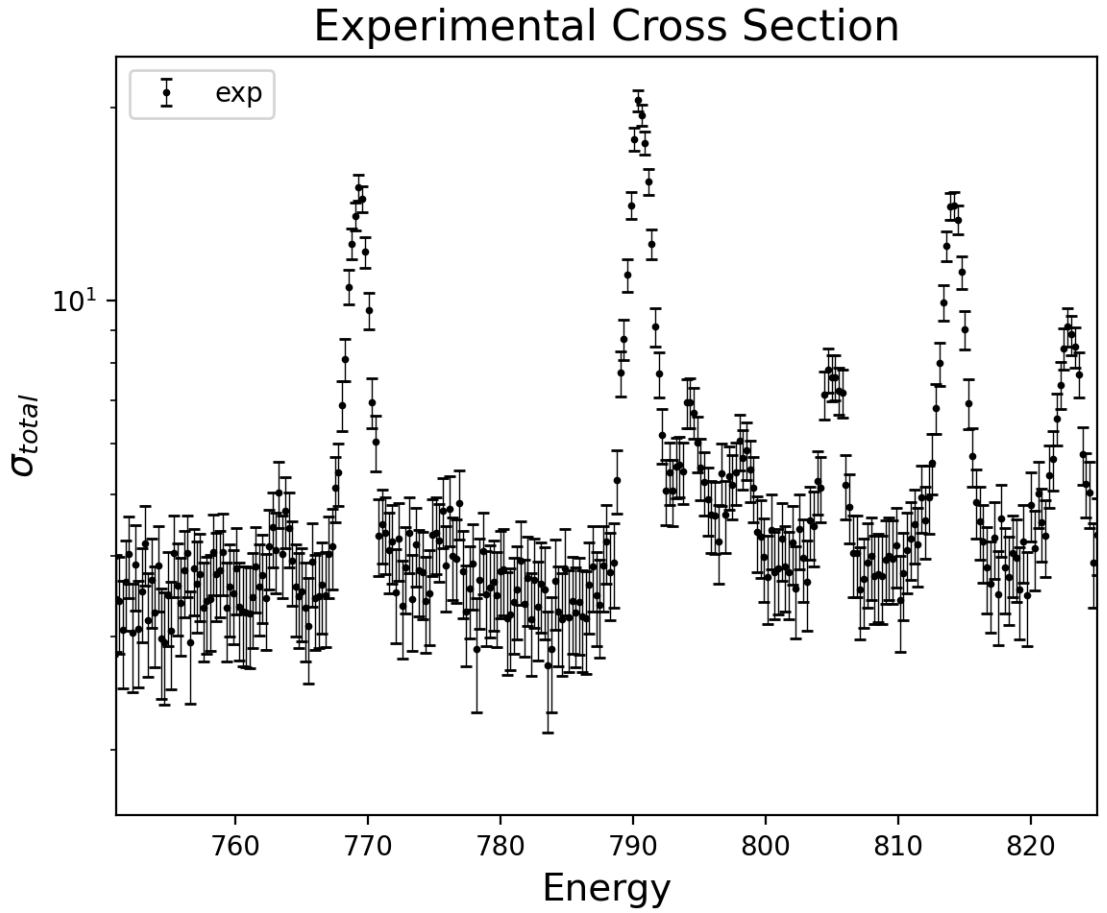
These parameters are an important piece of nuclear data



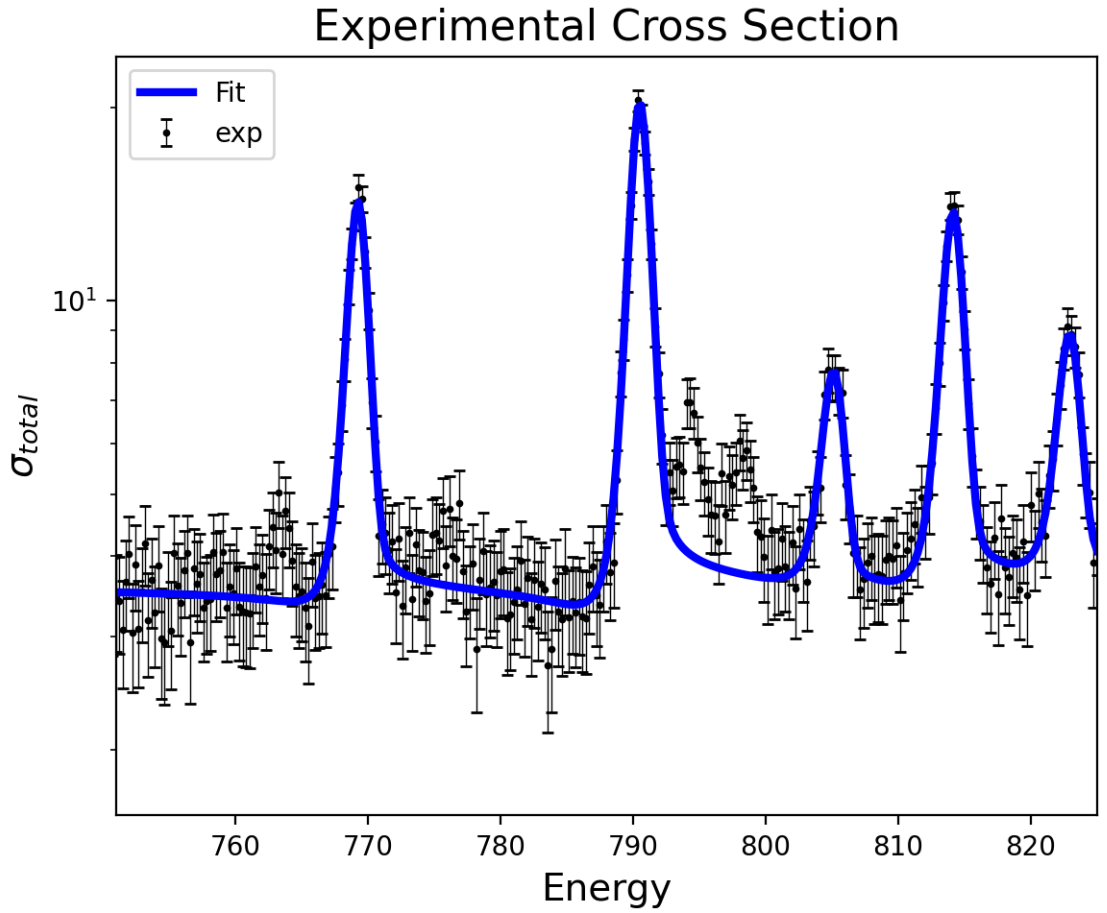
Resonance parameters are not known from first principles



The values are estimated through measurement & theory



Evaluators infer a theoretical model from experimental data



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Challenges for nuclear data evaluators

The big picture

- Nuclear data evaluation is a manual, laborious process
- Lacking reliability & reproducibility
- RRR evaluation method is known to underpredict uncertainty
  - Solution has been to conservatively inflate uncertainties

Application

- Improved knowledge and reduction in uncertainty on cross section data propagates to a broad range of NNSA applications
- Mission-critical operations at Los Alamos National Lab (LANL) are highly sensitive to Ta-181
- Demonstration on Ta-181 cross section directly supports the NNSA mission at LANL

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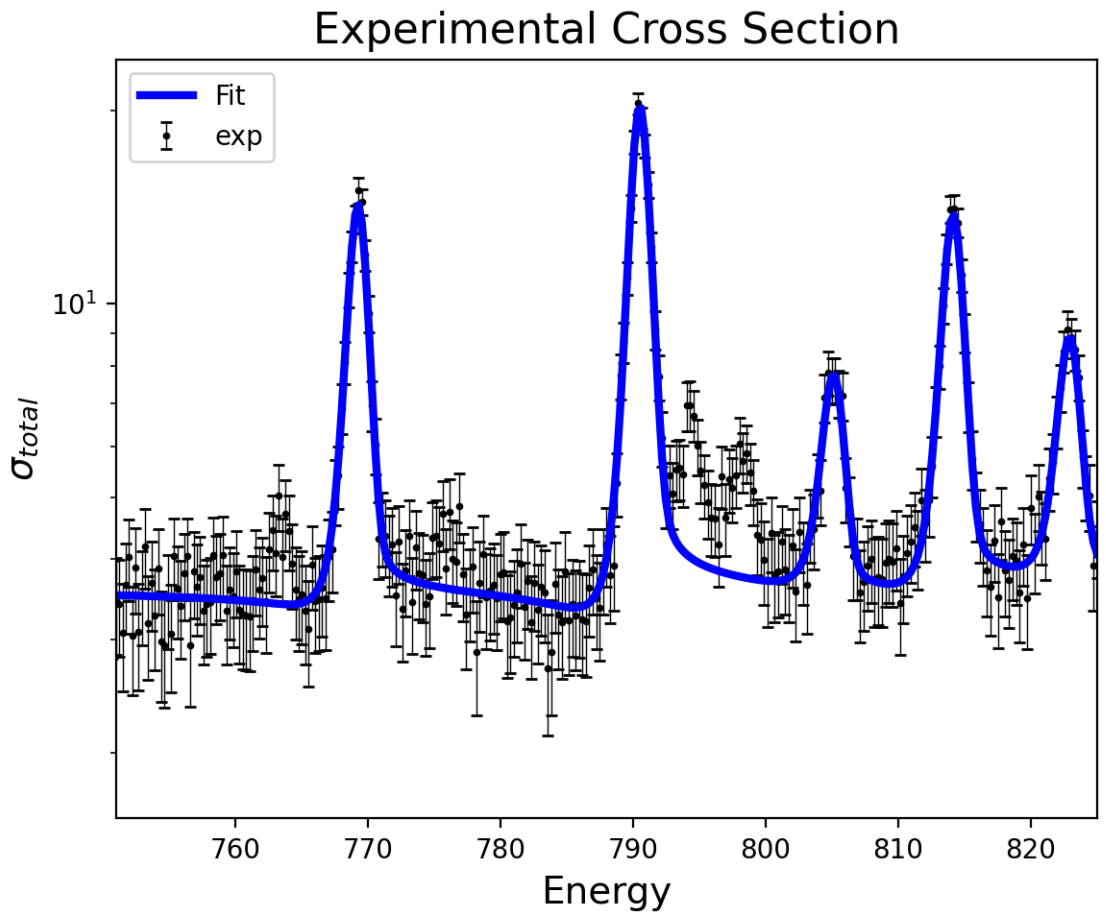
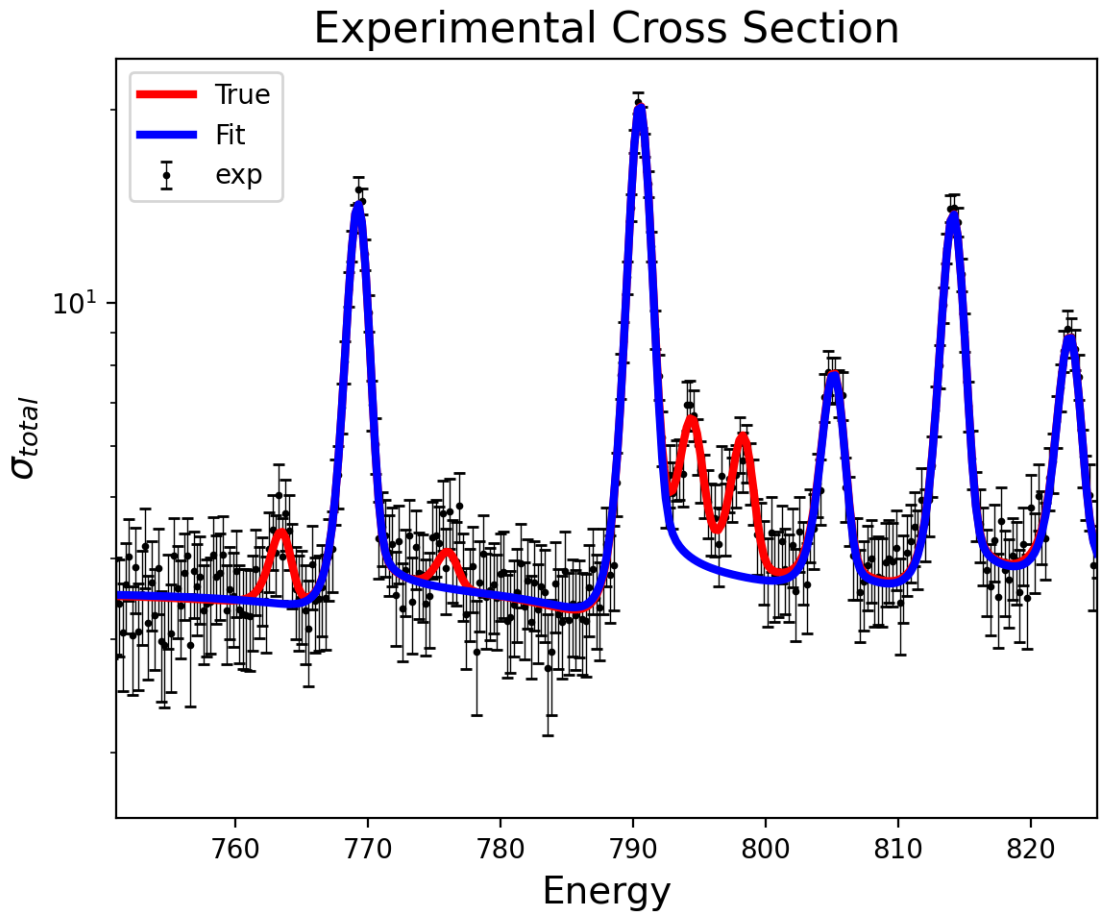
How can we improve this process?



Reproducibility and **manual effort** can be improved by automating a systematic, computational approach to inferential regression

How can we improve the result?



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Without access to the solution (labelled data) an assessment of **accuracy** and **precision** is impossible

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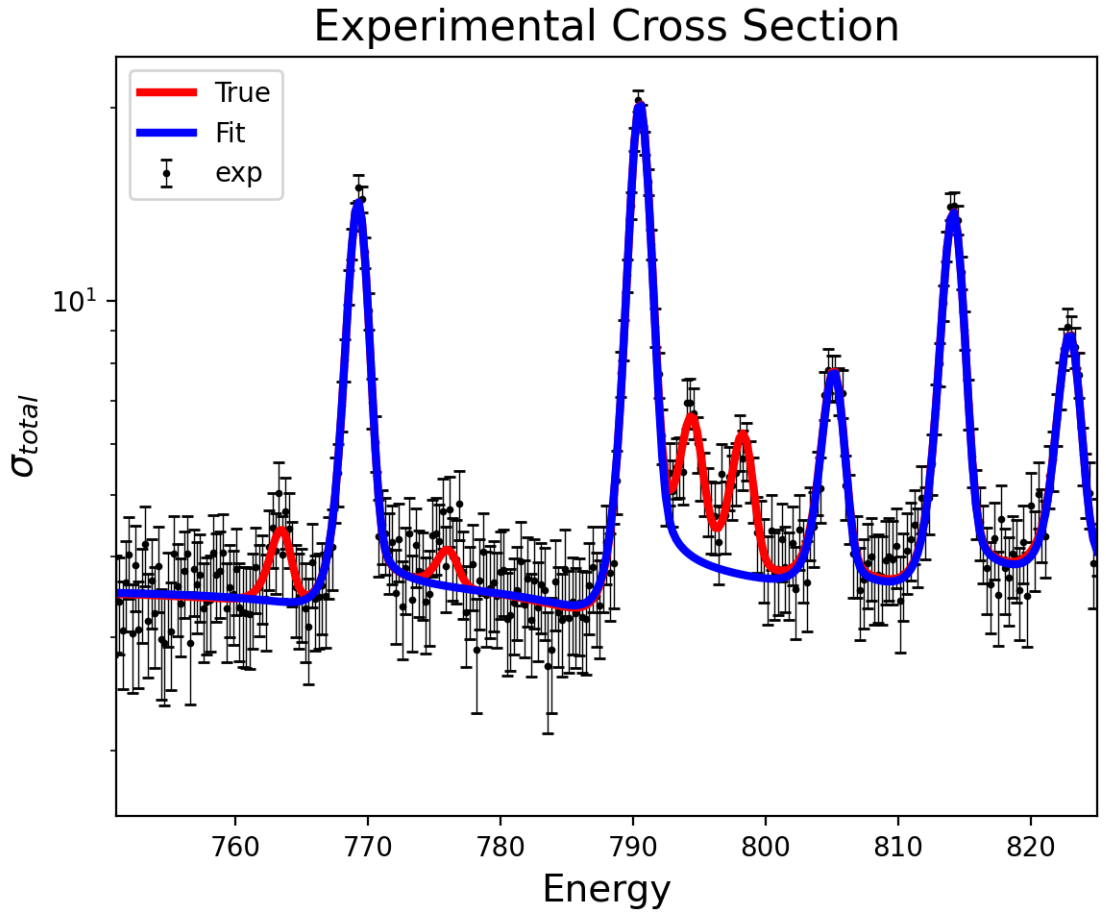


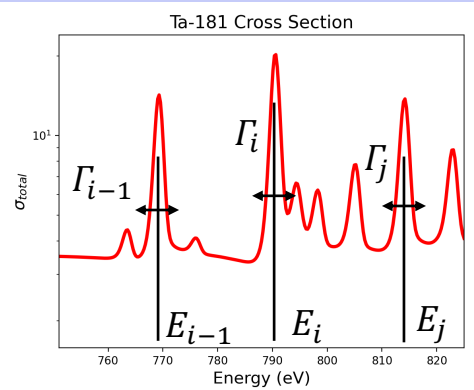
Reproducibility and **manual effort** can be improved by automating a systematic, computational approach to inferential regression

Without access to the solution (labelled data) an assessment of **accuracy** and **precision** is impossible

High-utility synthetic data enables **learning**/improvement and **benchmarking**

Experimental design isolates phenomena driven by the cross-section

True cross section in nature



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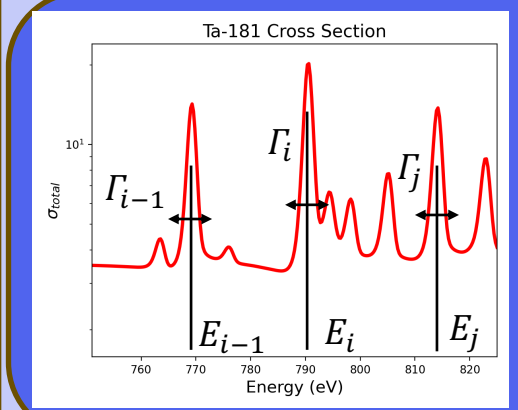
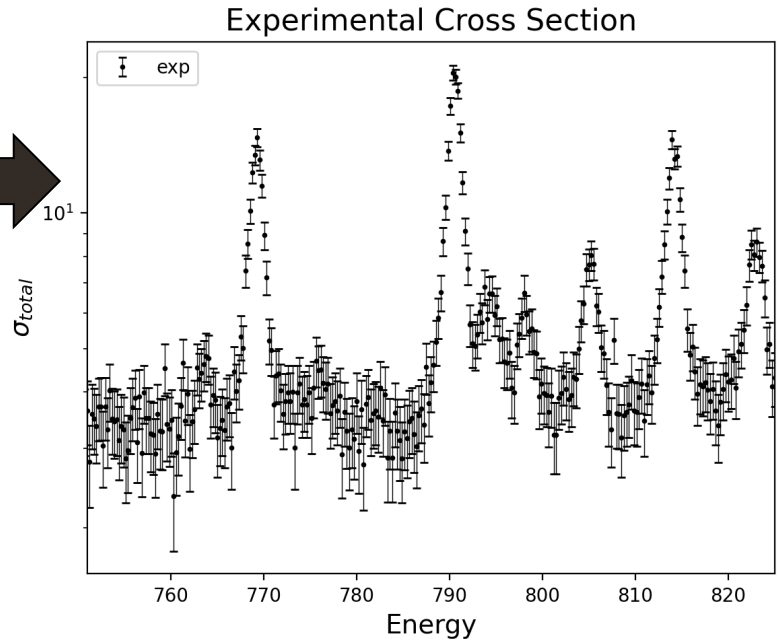
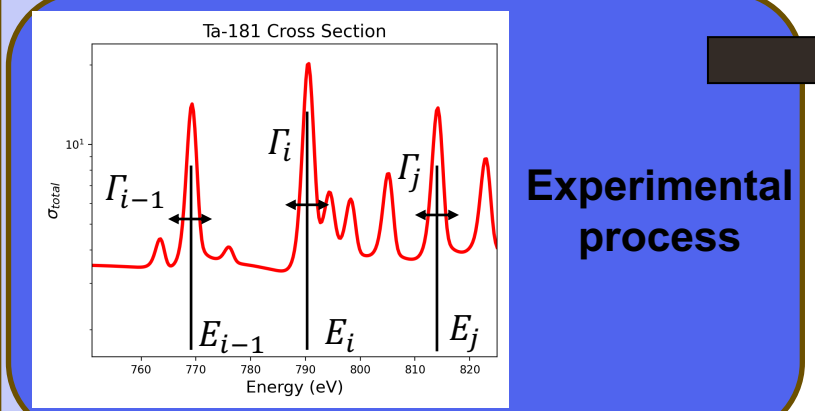


Experimental process



Experimental data is evaluated giving estimate & uncertainty

True cross section in nature



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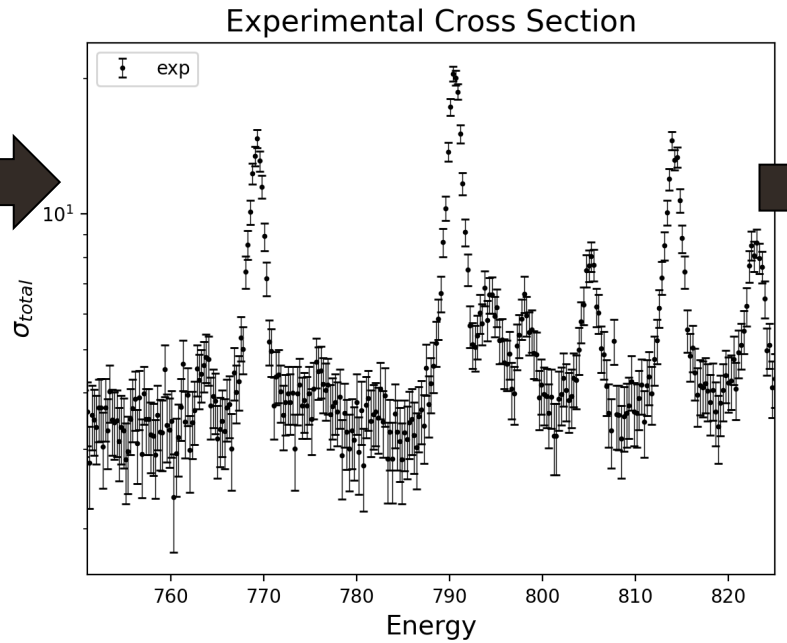
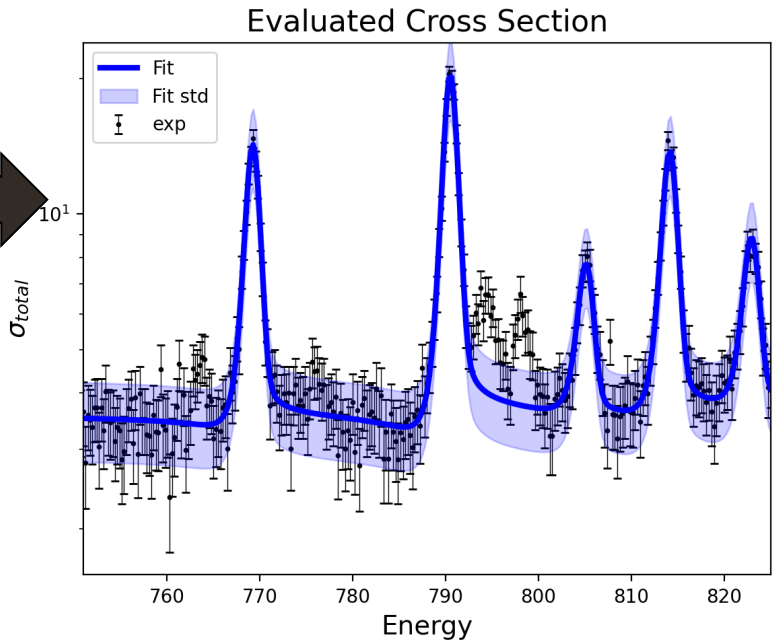
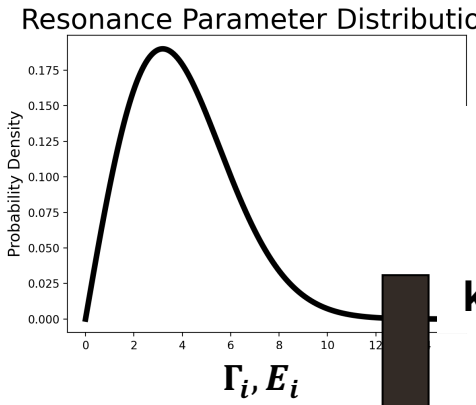


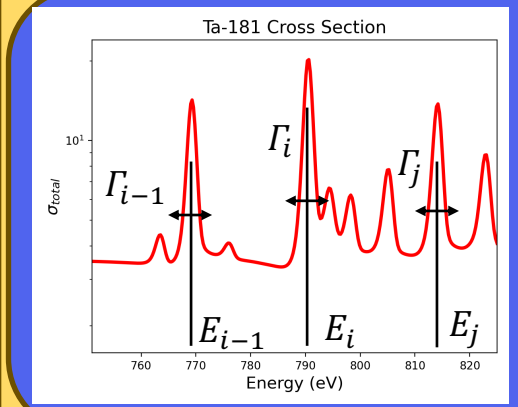


Generative model for resonance parameters



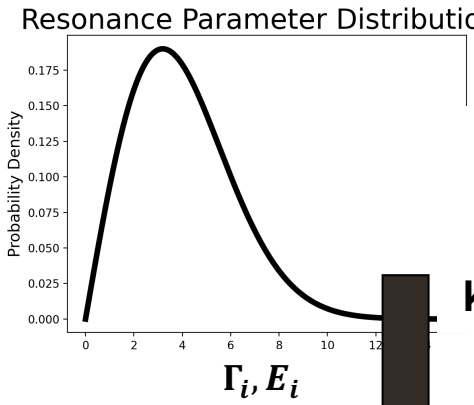
PDFs for resonance parameters known a-priori

Synthetic cross section realizations



Experimental process

Generative model for experimental measurement data



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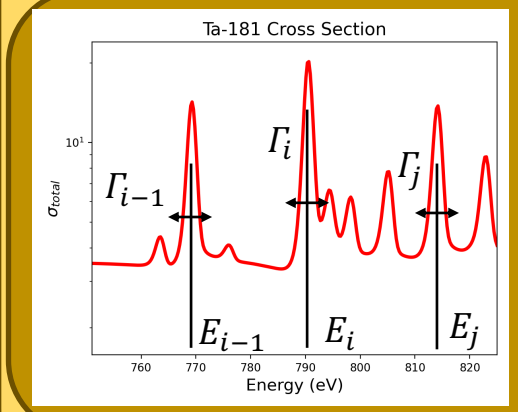
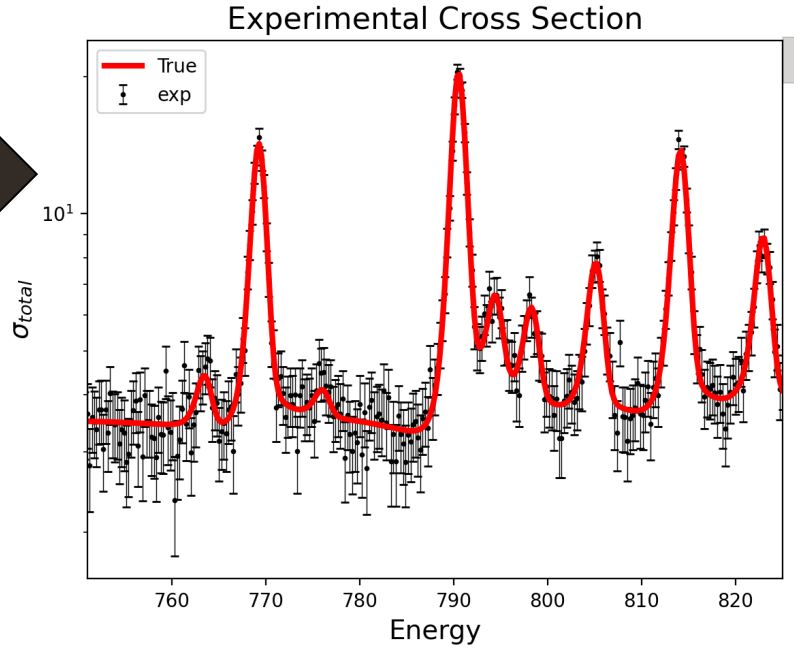
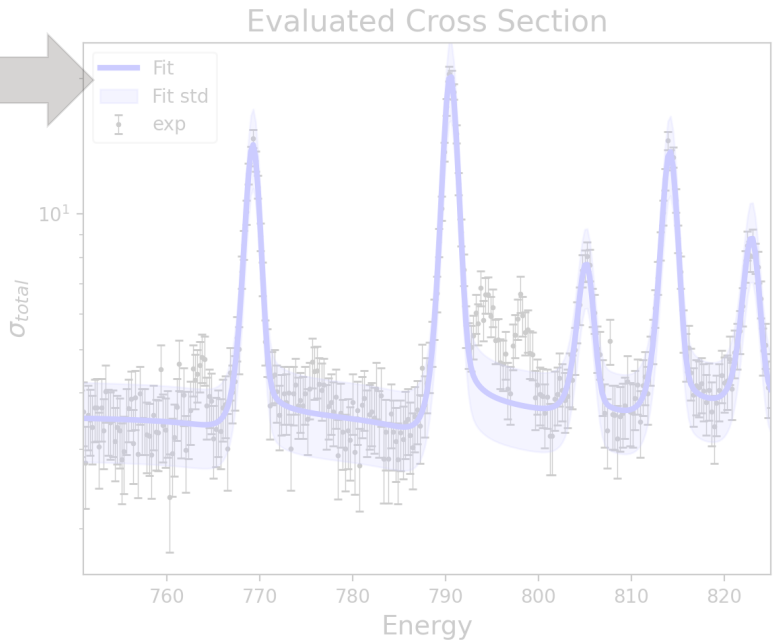


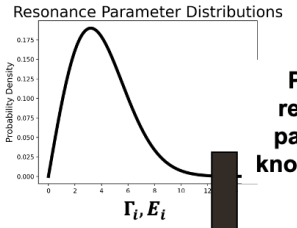
Probabilistic Generative Model



Evaluation



Hide solution, produce evaluated estimates & uncertainty



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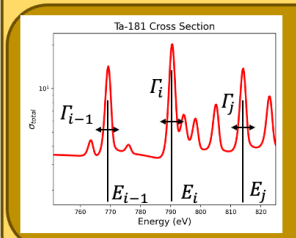

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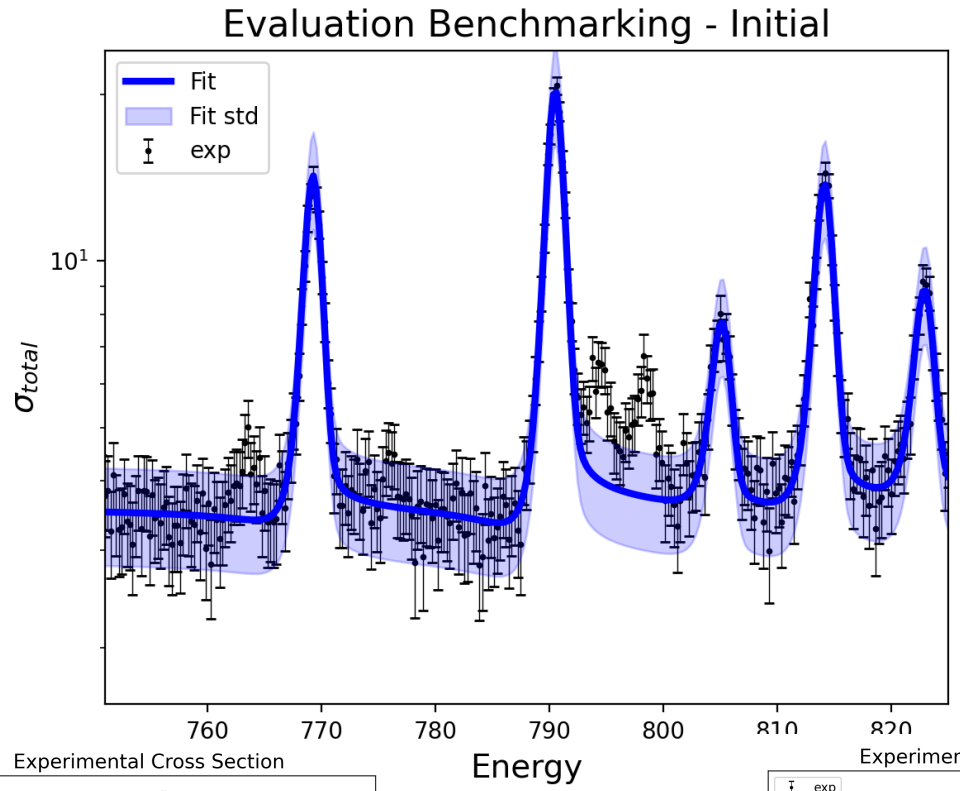
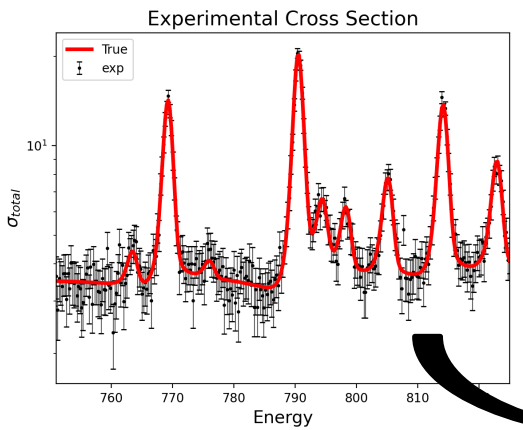
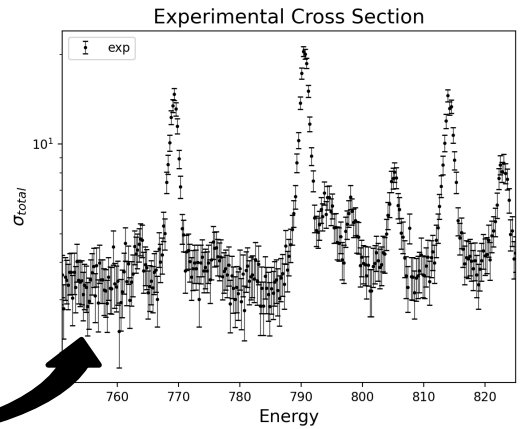


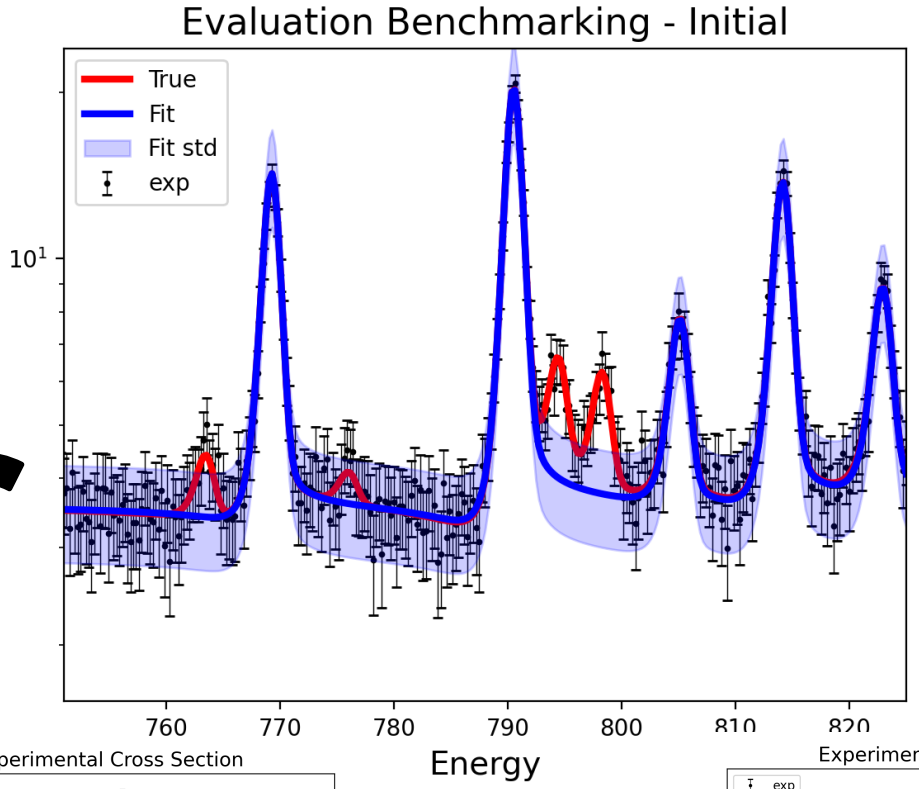
Automated evaluation





Compare evaluation to solution, learn, & repeat

Learn hyperparameters optimize & benchmark accuracy



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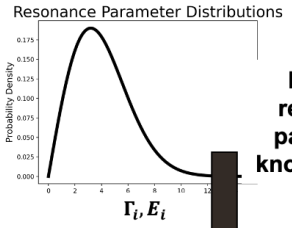

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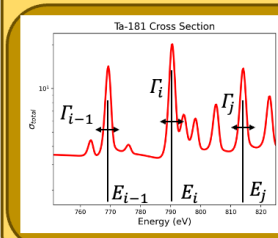

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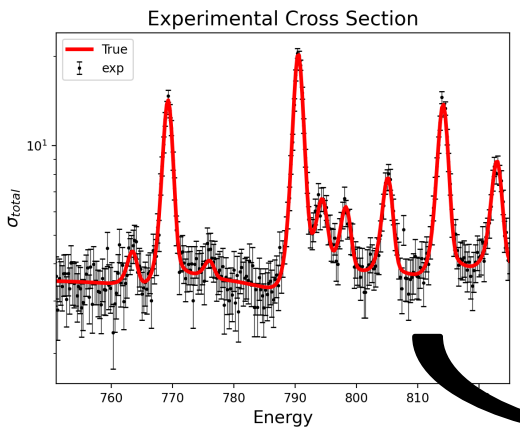
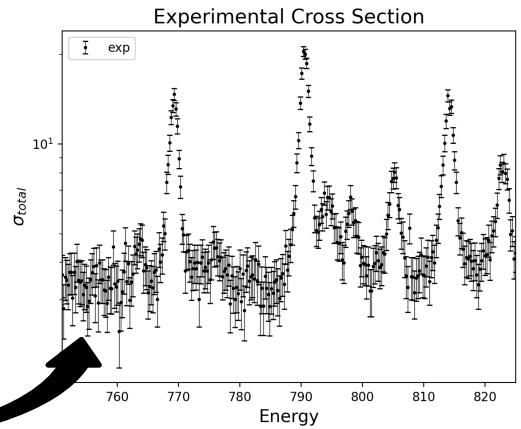
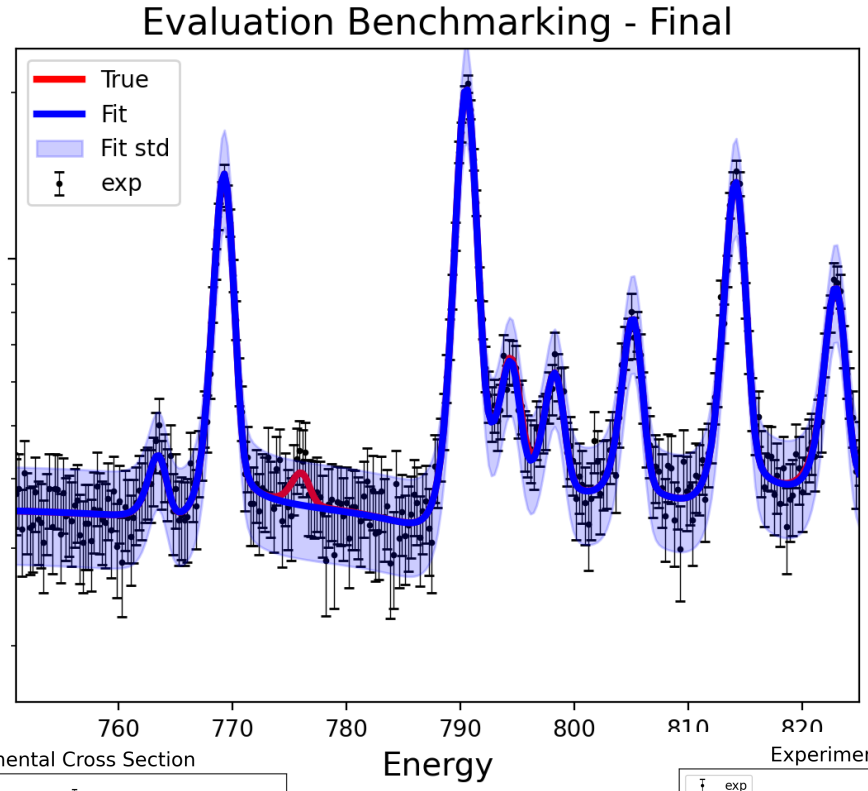




Improve automated evaluation algorithm & benchmark results

Learn hyperparameters optimize & benchmark accuracy



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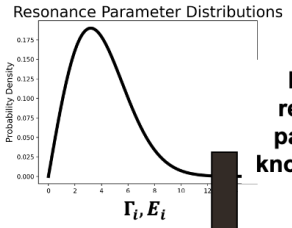

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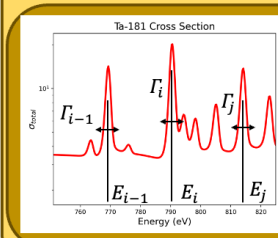

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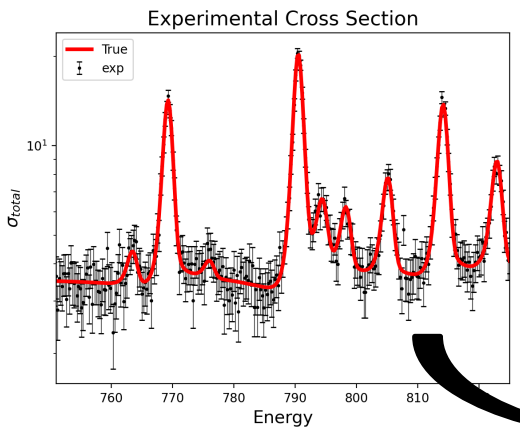
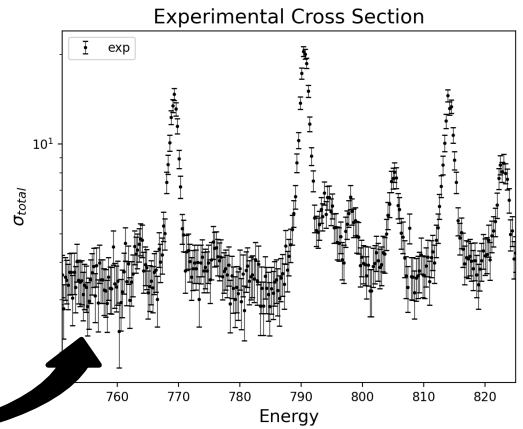
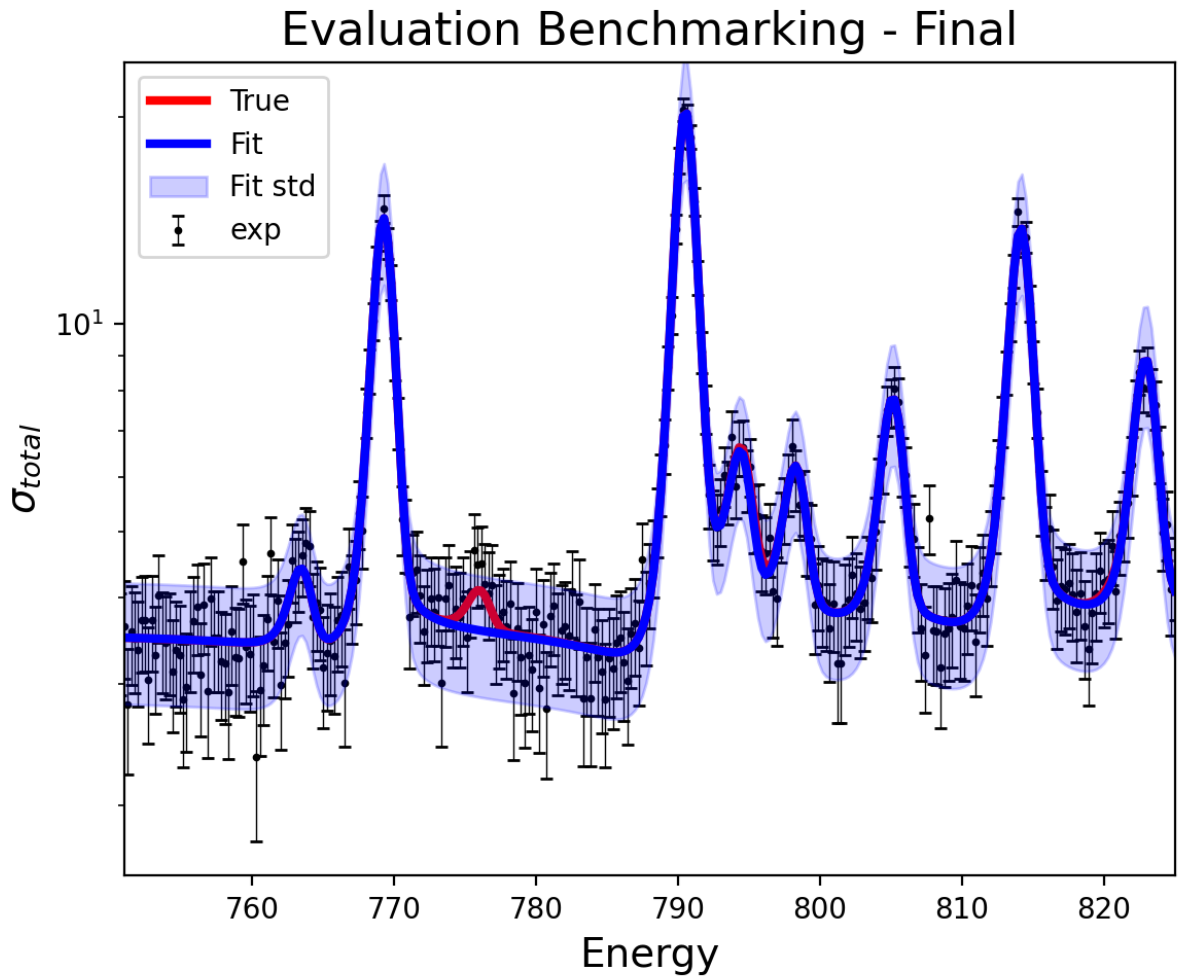




ATARI – AI/ML Tool for Automated Resonance Identification

- Lower-fidelity demonstration of automated regression
- Synthetic, labelled data allows:
  - Learning hyperparameters
  - Algorithmic training
  - Quantitative benchmarking
- Next steps:
  - Bring automated methodology to full fidelity
  - Extrapolate learned algorithm to real data
- **Impact:**
  - **Reproducible evaluations**
  - **Rigorously benchmarked uncertainty**
  - **Propagates to many NNSA applications**



Walton, N.A.W., Armstrong, J.L., Sobes, V., *Automated resonance evaluation tool; non-convex decomposition method for resonance regression and uncertainty quantification.* Proceedings of the 2022 International conference on Nuclear Data, (2022).

The NSSC Experience

- Invaluable relationship with laboratory mentors
- **2023 Keepin program at LANL**
  - **Experience working on different nuclear data**
  - **Valuable methods to bring to this research**
- 2022 NSSC nuclear data summer school
- Conferences
  - 2022 International Conference on Nuclear Data for Science and Technology
  - 2022 Cross Section Evaluation Working Group
  - 2023 Workshop for Applied Nuclear Data

Los Alamos NATIONAL LABORATORY

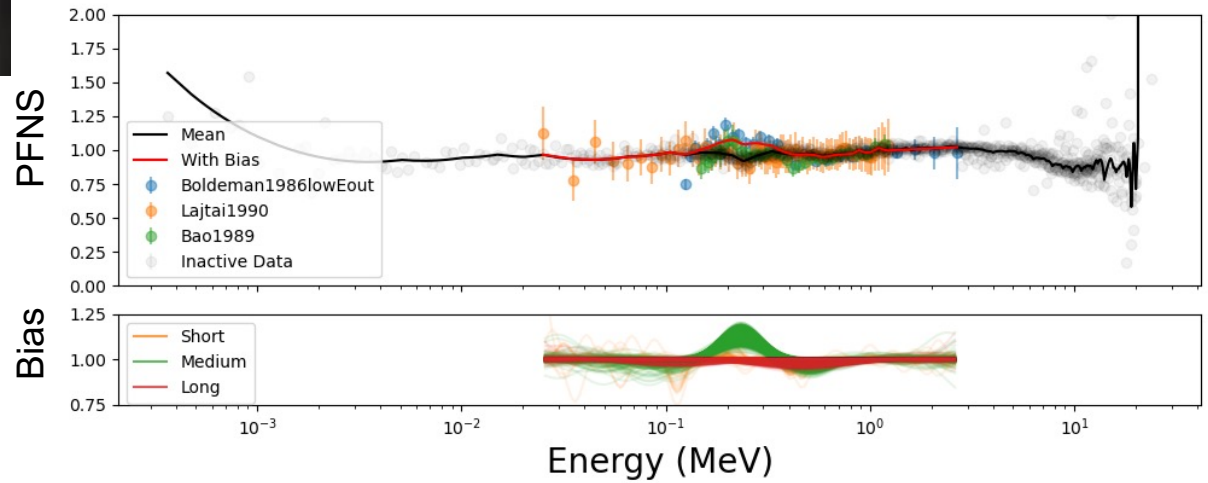
OAK RIDGE National Laboratory


Neudecker


Brown


Grosskopf

ML Identification of Experimental Bias



Acknowledgements

This material is based upon work supported by the Department of Energy National Nuclear Security Administration under Award Number **DE-NA0003996.**