Thermal Energy Scattering Evaluation Framework

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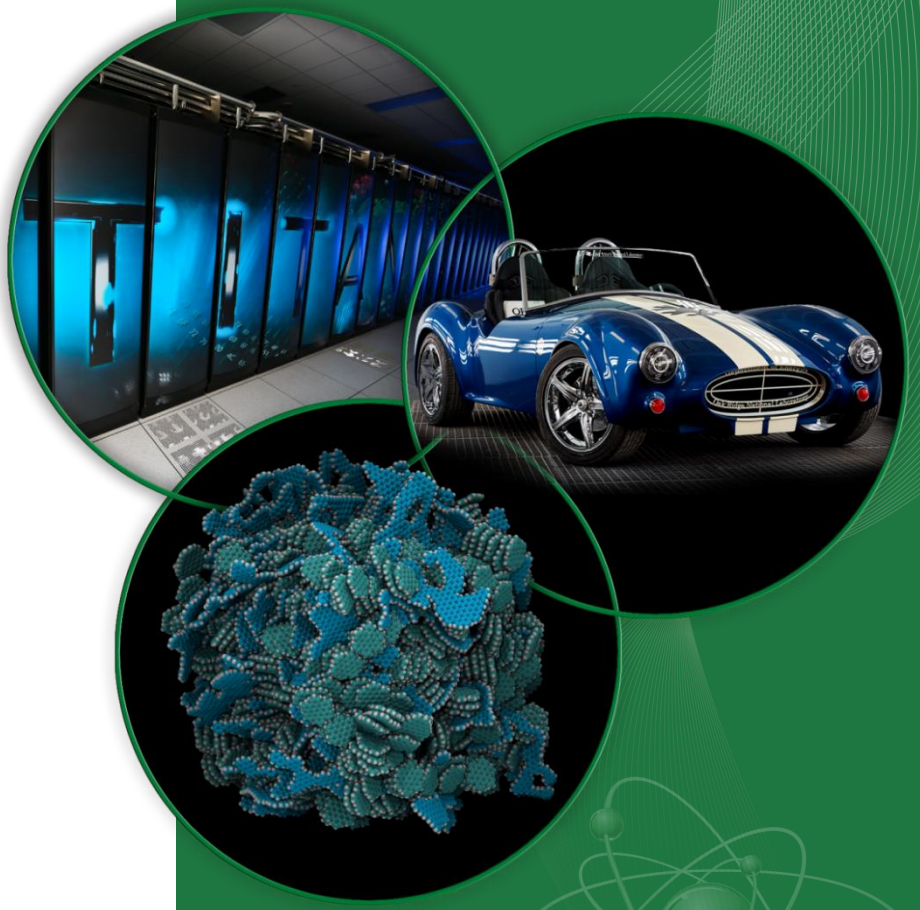

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Framework Motivation

- Thermal reactor systems sensitive to thermal scattering
- Several sets of new experimental double differential cross section data becoming available
- No uncertainty or covariance data
- Should accommodate any method for generating double differential scattering data

Framework Overview

- Combine experimental double differential scattering data and model parameters to yield best estimate of double differential cross section and uncertainties
- Data and simulation fit using Unified Monte Carlo (UMC) [1] method
- Framework will be tested on light water
  - Data collected from ORNL Spallation Neutron Source (SNS)
  - RPI collaboration
- Validate using benchmarks from the ICSBEP handbook

Framework Specifics – Simulation

- Run simulations of TIP4P/2005f [2] water in a box in classical molecular dynamics (MD) code GROMACS [3]
- Compute density of states using trajectories calculated in GROMACS
- Calculate intermediate structure factor using Gaussian approximation
  - Intermediate structure factor → dynamic structure factor → scattering law
- Run simplified MCNP code to simulate multiple scattering effects
- Double differential cross section convoluted with SNS detector resolution function

Framework Specifics – Unified Monte Carlo

- Capable of handling non-linearities which may exist in analyses
  - Ratio data
  - Data with large uncertainties
- Based on Bayes Theorem & Principle of Maximum Entropy
- Prior and likelihood functions assumed to be multivariate Gaussian functions
- Generates an ensemble of quantities used to calculate cross section and covariance values
- Two ‘flavors’ of UMC: UMC-G and UMC-B

Framework Specifics – UMC-B

- UMC-B chosen for this framework
  - Information from the prior distribution is perfectly preserved, as opposed to UMC-G, where it is approximated
  - Don’t need simulation covariance matrix
- Calculates scalar weighting functions
- More applicable for Total Monte Carlo approach

Framework Specifics – Validation

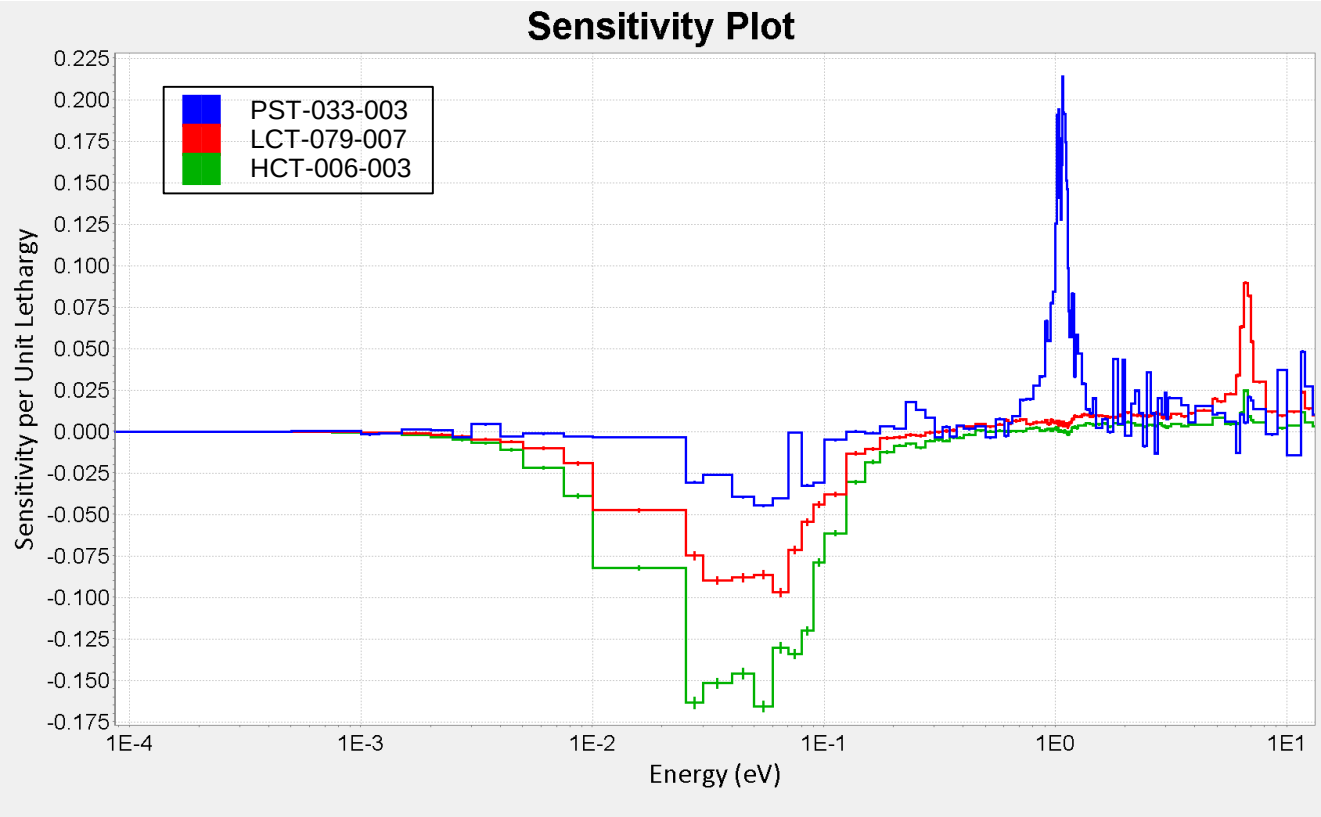
- Cross sections validated two ways
  - Against independent cross sections
    - Double differential in scattering energy and angle
    - Single differential in scattering angle
    - Total scattering
  - Against experimental benchmark problems sensitive to hydrogen
    - From ICSBEP handbook
    - Compare against benchmarks run with ENDF/B-VII.1 and ENDF/B-VIII.beta3 data

Framework Specifics – ICSBEP Benchmarks

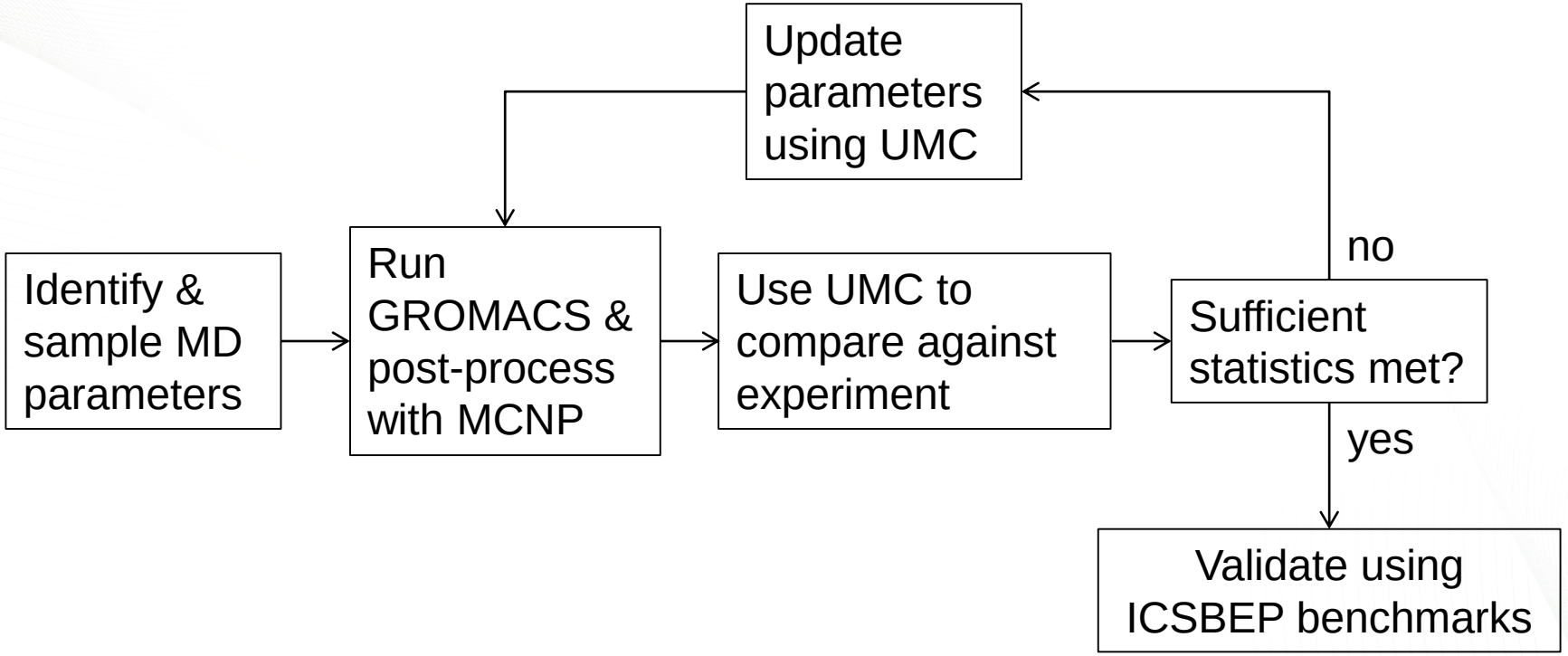
Benchmarks

- PST-033-003
  - Plutonium Nitrate solution surrounded by water
- LCT-079-007
  - Water moderated & reflected triangular pitched UO_2 fuel elements
- HCT-006-003
  - Water moderated hexagonally pitched high enriched (80% U^{235}) fuel rods

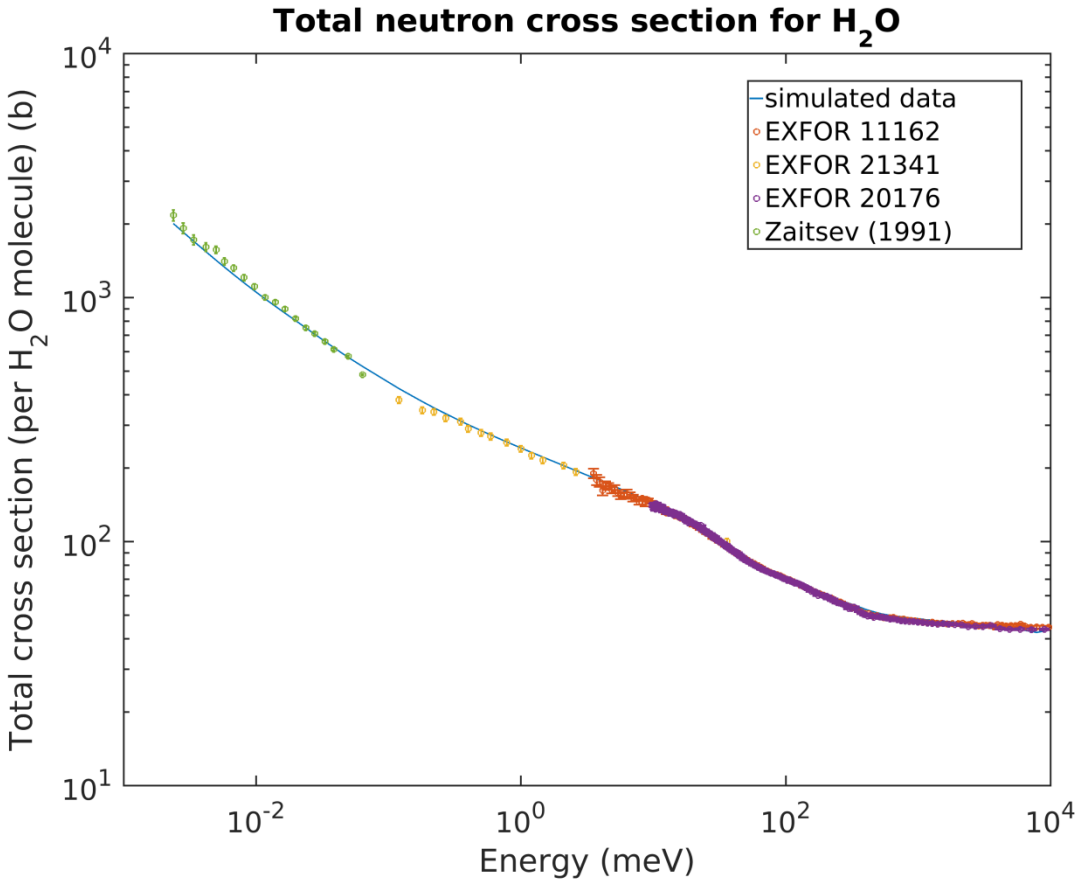
Sensitivity Plot

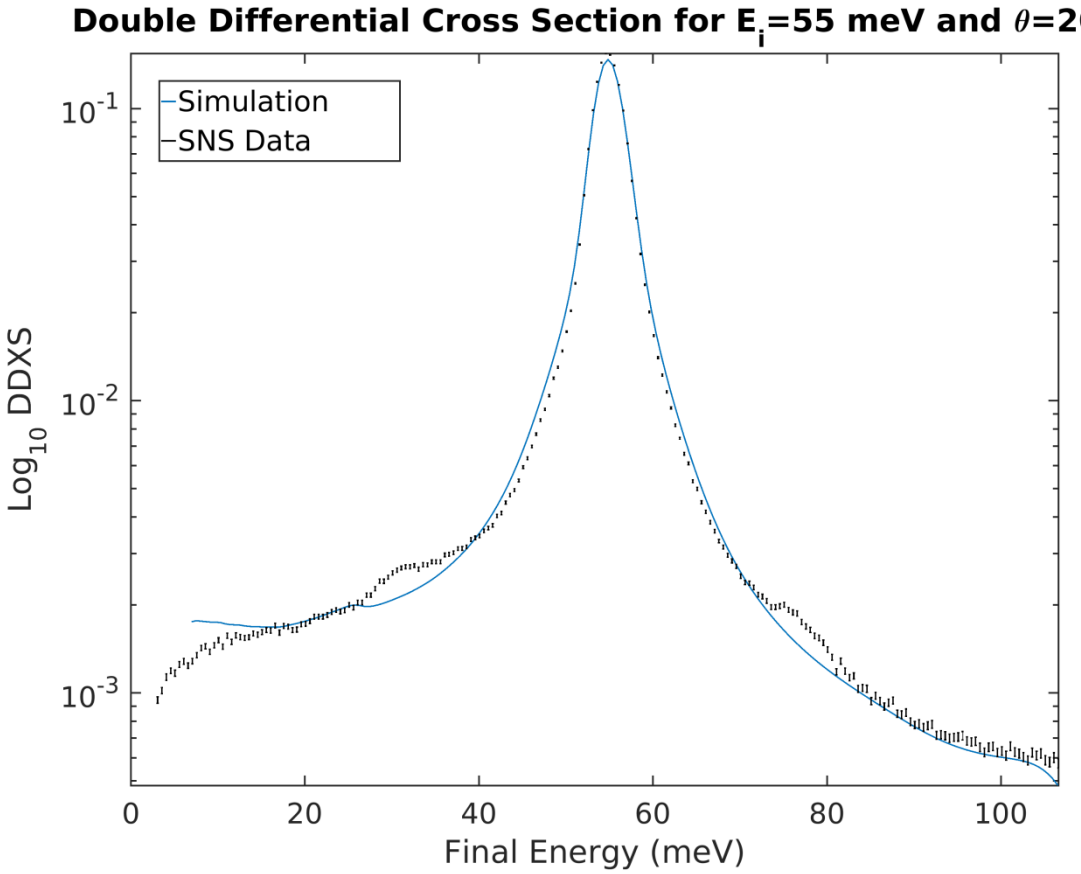


Framework Outline

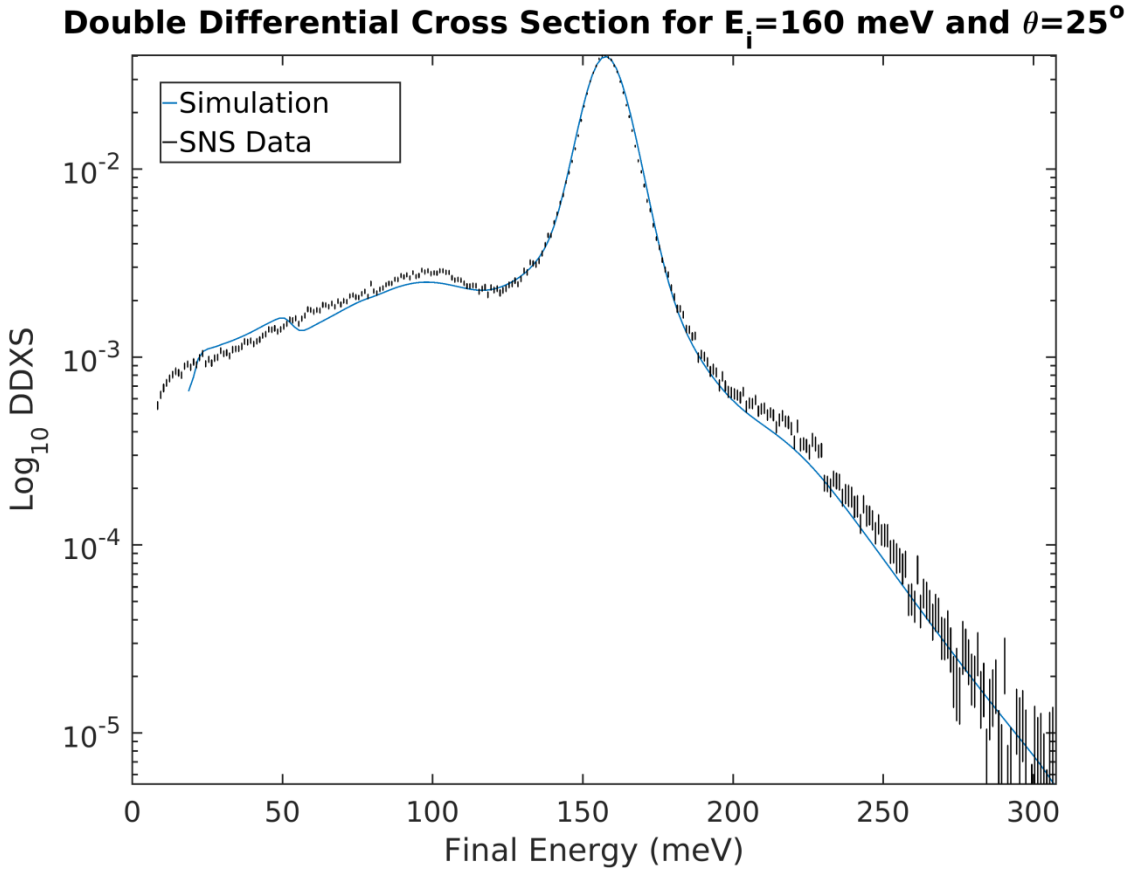


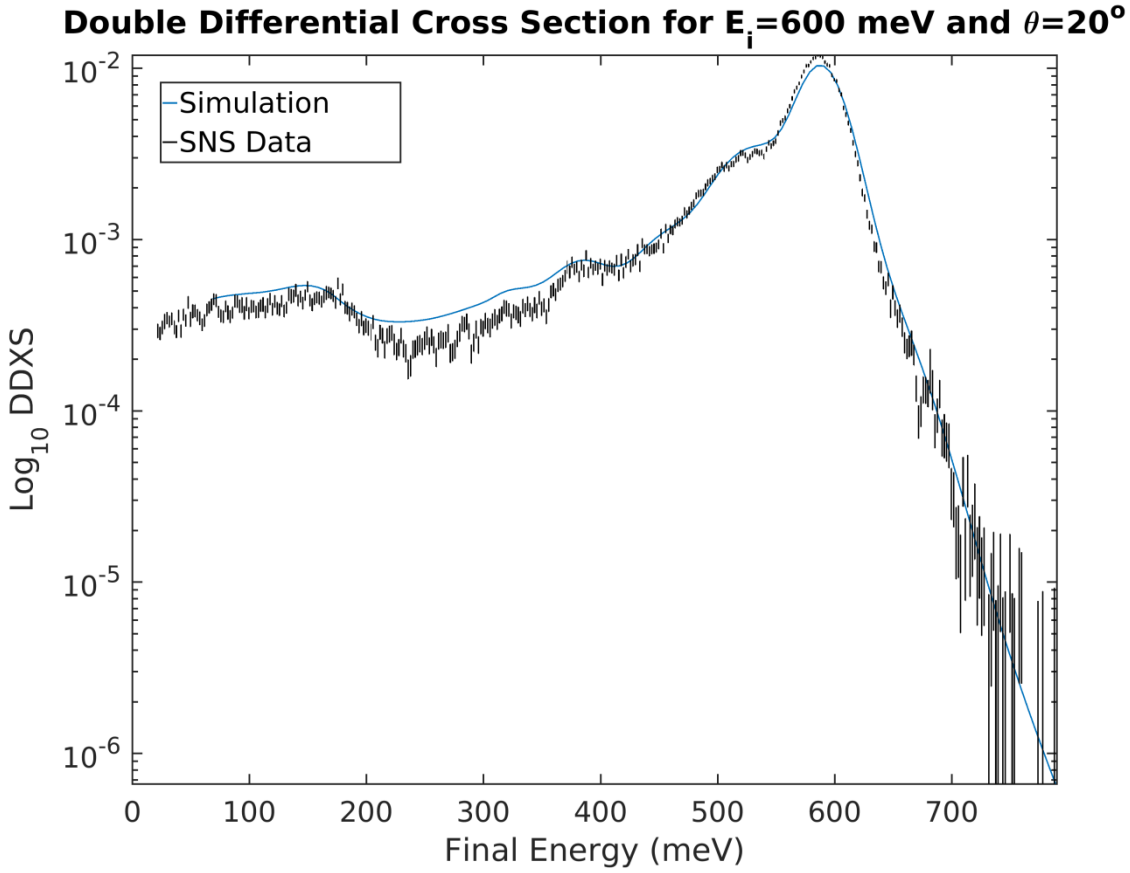
Preliminary Results





Preliminary Results (cont.)





Acknowledgements

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- SNS: Garrett Granroth & Alexander Kolesnikov

References

- [1] R. Capote and D. L. Smith, "An Investigation of the Performance of the Unified Monte Carlo Method of Neutron Cross Section Data Evaluation," *Nuclear Data Sheets,* vol. 109, pp. 2768-2773, 2008.
- [2] M. Gonzalez and J. Agascal, "A flexible model for water based on TIP4P/2005," *The Journal of Chemical Physics,* vol. 135, 2011.
- [3] D. Van Der Spoel, E. Lindahl, B. Hess, G. Groenhof, A. Mark and H. Berendsen, "GROMACS: Fast, flexible, and free," *Journal of Computational Chemistry,* vol. 26, no. 16, pp. 1701-1718, 2005.