Thermal Scattering Law Research and Development at North Carolina State University

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NUCLEAR CRITICALITY SAFETY PROGRAM (NCSP)
TECHNICAL PROGRAM REVIEW
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Acknowledgement

- NNSA Nuclear Criticality Safety Program (NCSP)
  - Collaboration with LLNL
- Naval Nuclear Propulsion Program
- The LEIP Team
  - Thermal scattering









FY 2023 Tasks

Task	Task Title
ND2	Generation and Benchmarking of Thermal Neutron Scattering Cross Sections in Support of Advanced Nuclear Reactor Concepts
ND5	Development and Implementation of a Modern Doppler Broadening Approach Including Atomic Binding Effects
ND10	Development and Implementation of Machine Learning Methods for Thermal Scattering Law Evaluations

APPENDIX B: Nuclear Data Priorities, Basis Statements, and Milestones

FY 23/24 5 Year Execution Plan

Nuclear Data Evaluations							
Materials	**Pre-FY2024**	**FY2024**	**FY2025**	**FY2026**	**FY2027**	**FY2028**	**Post-FY2028**
Uranium Metal (U)	LLNL/NCSU						
Basis	TSL evaluation. Requested by the RPI for use in U-235 resonance parameter analysis.						
Paraffin (C_nH_{2n+2})	LLNL/NCSU	LLNL/NCSU					
Basis	TSL evaluation. A common moderator and moderating reflector material for which there are numerous critical benchmarks in the ICSBEP Handbook. A thermal scattering law for paraffin will improve simulations through higher fidelity and reduce uncertainties.						
Plutonium Oxide (PuO_2)	LLNL/NCSU	LLNL/NCSU					
Basis	TSL evaluation. A common fissile compound for which there are critical experiments in the ICSBEP Handbook. A thermal scattering law for PuO_2 will improve Doppler broadening using advanced methods currently under development as LLNL ND12.						
Light Paraffinic Oil (Mineral Oil)		LLNL/NCSU	LLNL/NCSU	LLNL/NCSU			
Basis	TSL evaluation. Mineral oil and other light paraffinic oils are moderators often found in fissile handling areas (FHAs). A thermal scattering law for light paraffinic oils would reduce excessing margins in nuclear criticality safety evaluations for fissile handling areas containing this class of moderator. TSL requested by NNL.						
Uranium Silicide (U_3Si_2)		LLNL/NCSU	LLNL/NCSU	LLNL/NCSU			
Basis	TSL evaluation. A common fissile compound in use in advanced nuclear reactor fuel. A thermal scattering law for U_3Si_2 will improve Doppler broadening using advanced methods currently under development as LLNL ND12.						
Triuranium Octoxide (U_3O_8)			LLNL/NCSU	LLNL/NCSU	LLNL/NCSU		
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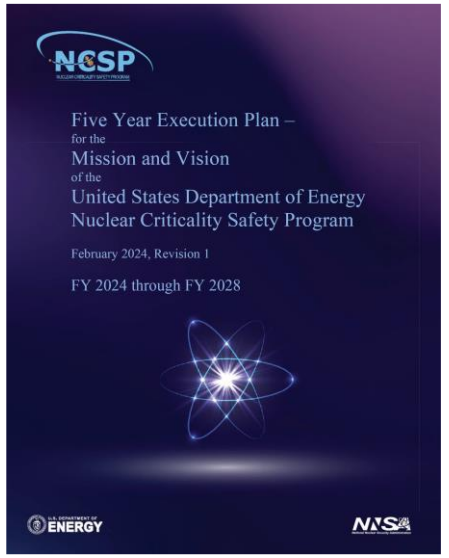

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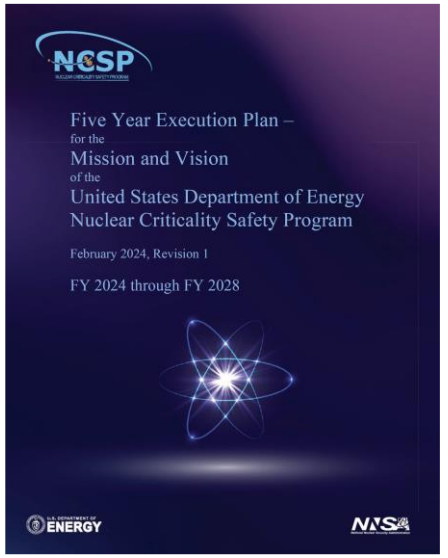
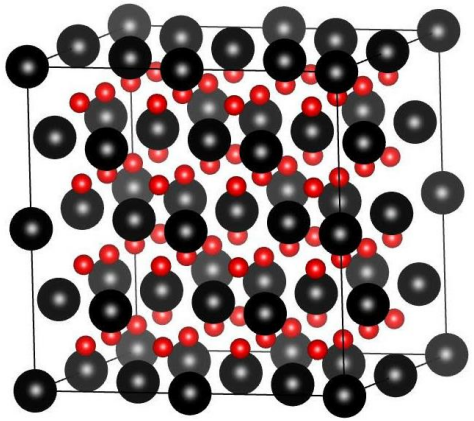
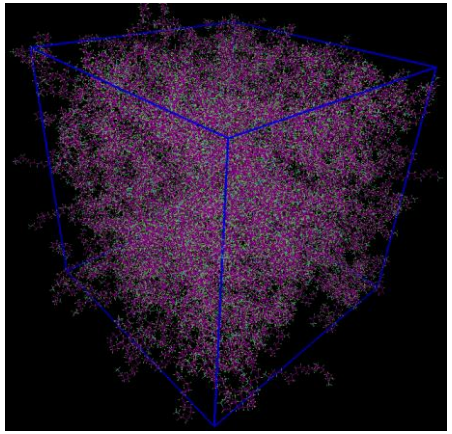
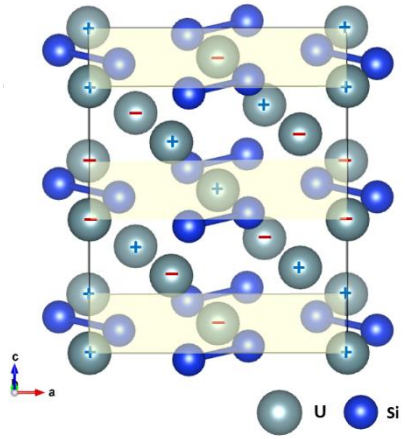


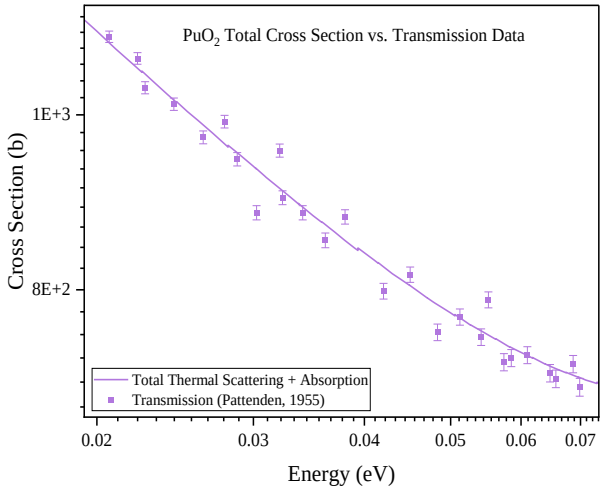
- 66 TSL evaluations were contributed to ENDF/B-VIII.1 for the following materials
  - Al2O3, Be-metal, Be-metal+Sd, BeO, FLiBe, CaH2, CH2, SiC, UC, HF, Paraffinic Oil, UN, PuO2, SiO2, UO2, U-metal, Grph-20P, Grph+Sd

ND2 – TSL Evaluations

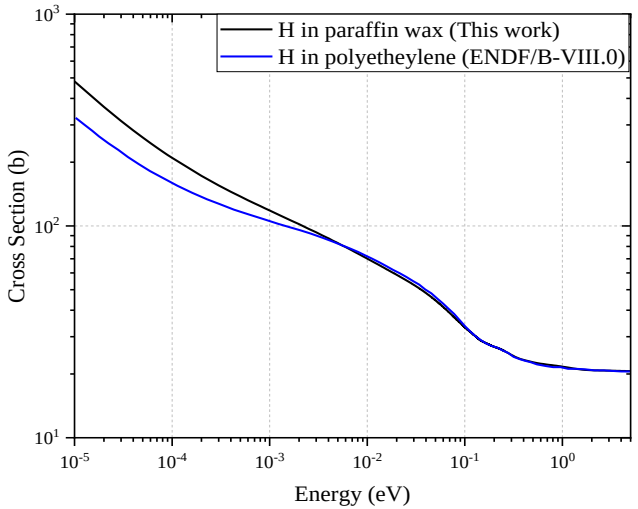




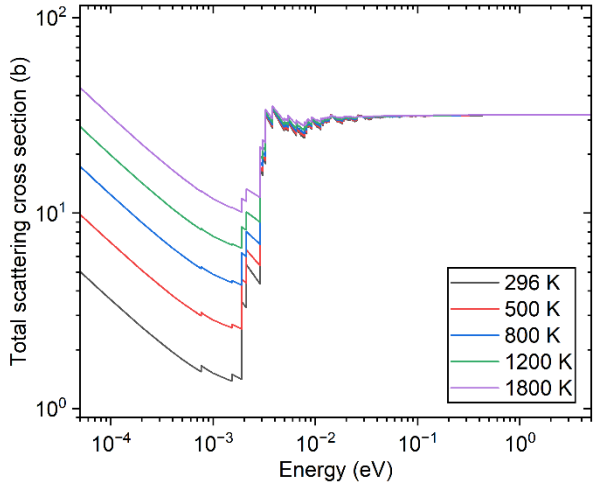




Plutonium dioxide

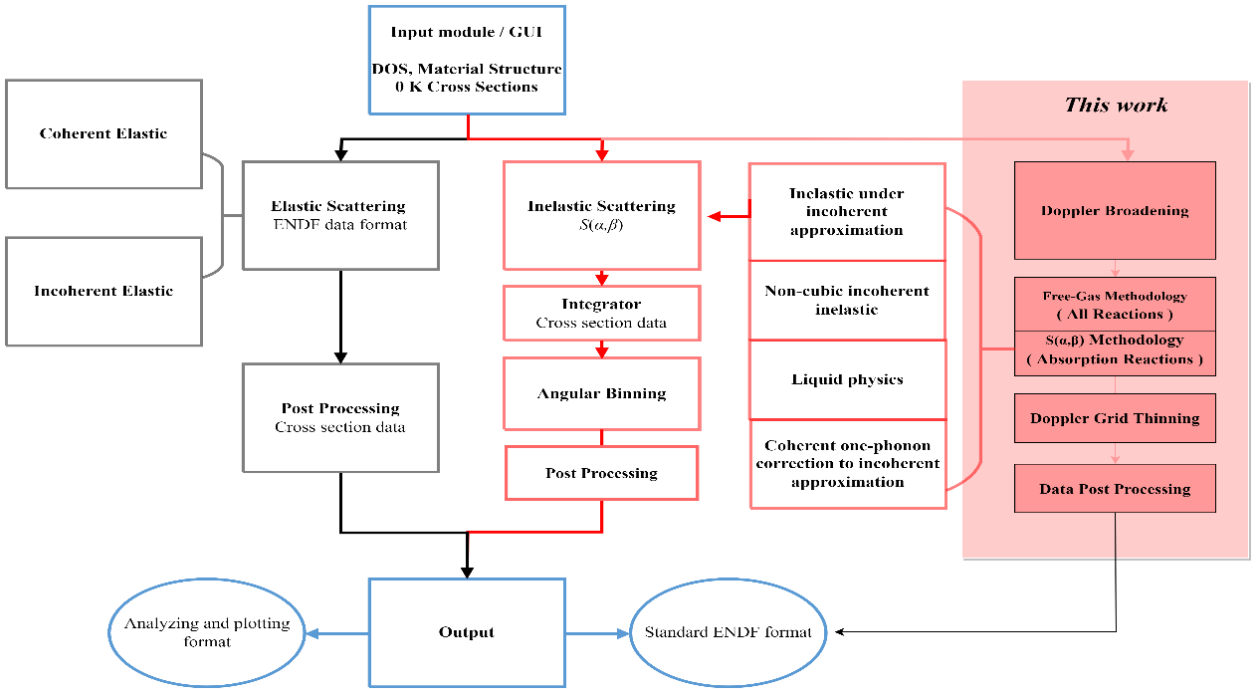


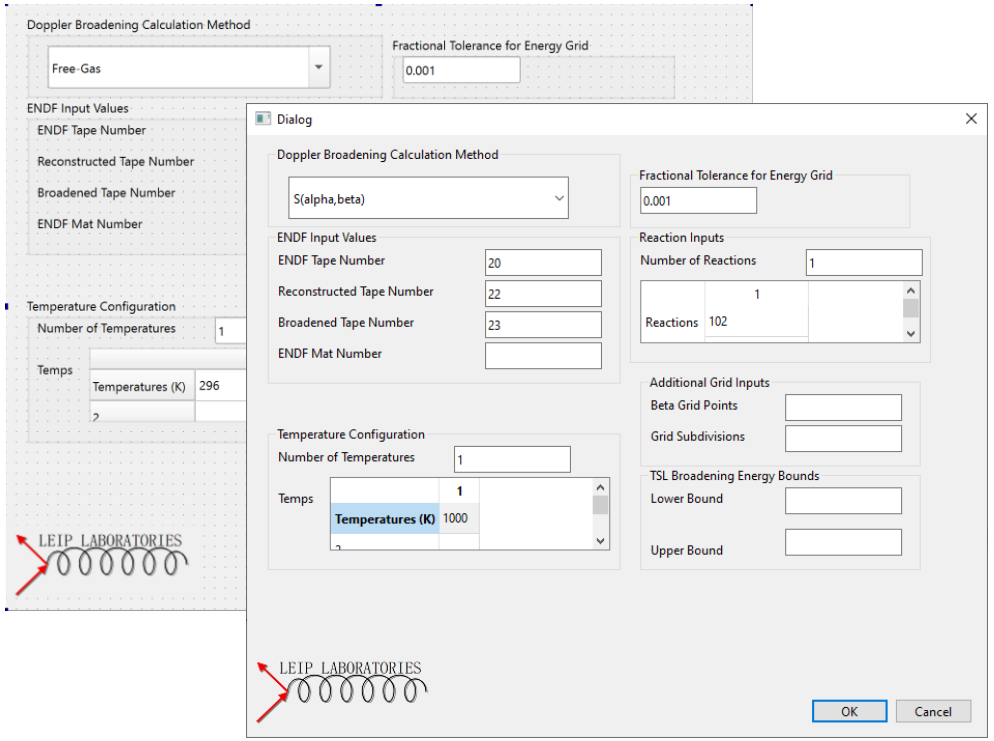
Paraffin



Uranium Silicide

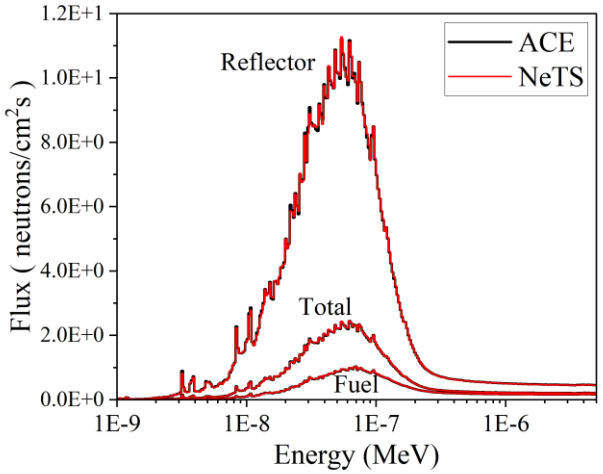
ND5 – Advanced Methods



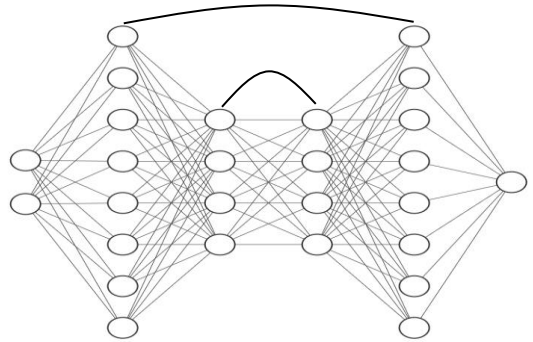


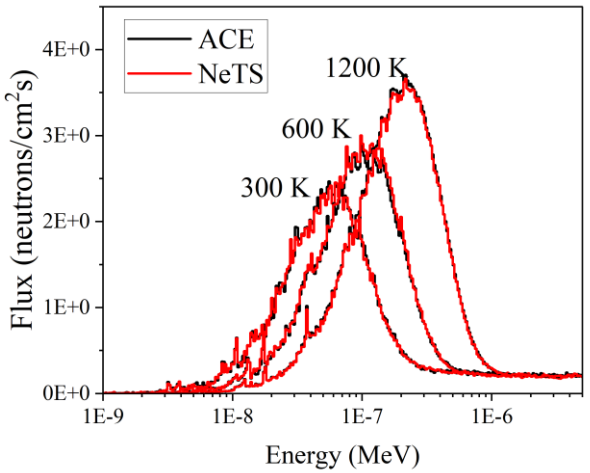
FLASSH Doppler Module

ND10 – Deep Learning and Artificial Neural Networks



TREAT neutron spectra
steady-state
296K





NeTS working with Serpent

TREAT neutron spectra
with
varying temperatures

Dataset	Mean APD [%]	Med. APD [%]	Max APD [%]
NeTS (64-32-32-64 neurons / layer, 25 KB)			
Train	0.0778	0.0573	0.8046
Validation	0.0802	0.0589	0.9559
Test	0.0827	0.0600	0.8305

Publications

1. E. Lee, N. C. Fleming, A. I. Hawari, "Benchmark of Neutron Thermalization in Graphite Using a Pulsed Slowing-Down-Time Experiment," *Nuclear Science and Engineering*, https://doi.org/10.1080/00295639.2022.2162789 , 2023
2. N. C. Fleming, C. A. Manring, B. K. Laramee, J. P. W. Crozier, E. Lee, A. I. Hawari, "*FLASSH* 1.0: Thermal Scattering Law Evaluation and Cross Section Generation for Reactor Physics Applications," *Nuclear Science and Engineering*, https://doi.org/10.1080/00295639.2023.2194195 , 2023.
3. J.P.W. Crozier, A. I. Hawari, "Phonon-Informed Neural Thermal Scattering (NeTS) Optimization for Crystalline Graphite and Beryllium Metal," *Transactions of the American Nuclear Society*, 128, 2023.
4. J. Gil, A. I. Hawari, "Evaluation of Thermal Neutron Scattering Cross Section of Uranium Silicide with Ab Initio Lattice Dynamics," *Transactions of the American Nuclear Society*, 129, 2023.
5. J. P. W. Crozier, A. I. Hawari, "Ab Initio Evaluation of Plutonium Dioxide $S(\alpha,\beta)$ and Thermal Neutron Cross Sections," *Transactions of the American Nuclear Society*, 129, 2023.
6. T. Ahmed, B.K. Laramee, A. I. Hawari, "Thermal Scattering Law Data Development for Paraffin Wax," *Transactions of the American Nuclear Society*, 129, 2023.
7. A. Bauyrzhan, A. I. Hawari, "Investigation of the Impact of TSL Data Libraries on the MSRE Benchmark," *Transactions of the American Nuclear Society*, 129, 2023.

FY 2024 several papers accepted for PHYSOR 2024 and others are in preparation for journal submissions

Summary

- Meeting and exceeding all NCSP ND2 objectives
  - Significant number of evaluations contributed to ENDF/B-VIII.1
- Innovative methods (ND5 and ND10 tasks) significant progress including
  - Doppler module integration into *FLASSH* code
  - ML TSL approach integration into Serpent MC code.

NC STATE UNIVERSITY

Thank You