Progress of Thermal Neutron Scattering Research at North Carolina State University

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Department of Nuclear Engineering
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Raleigh, North Carolina, USA

NUCLEAR CRITICALITY SAFETY PROGRAM (NCSP) TECHNICAL PROGRAM REVIEW
February 21-23, 2023
Sandia National Laboratory, Albuquerque, NM

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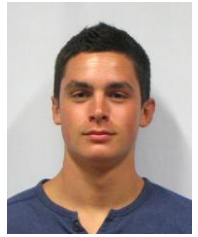
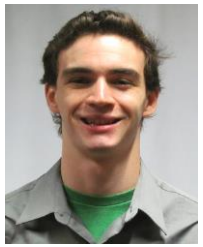
Acknowledgement

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



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FY 2022 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

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

FY 22
5 Year
Execution
Plan

Nuclear Data Evaluations							
Materials	**Pre-FY2022**	**FY2022**	**FY2023**	**FY2024**	**FY2025**	**FY2026**	**Post-FY2026**
	improve the inelastic scattering cross sections and to correct issues with the URR evaluation implemented in ENDF/B-VIII.0 (under DOE-SC funding).						
Water (H_2O)	LLNL/NCSU	LLNL/NCSU					
Basis	TSL evaluation. Water is this most important moderator and moderating reflector material for criticality safety and light water reactor physics. Problems with evaluations submitted by CAB at elevated temperatures (that were noticed during the ENDF/B-VIII.0 evaluation process) warrant re-evaluating this essential material using the latest methods developed under LLNL ND2, ND3.						
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Basis	TSL evaluation. A common fissile compound under consideration for high-temperature advanced nuclear reactor fuel. A thermal scattering law for UC will improve Doppler broadening using advanced methods currently under development as LLNL ND5.						
Paraffin (C_nH_{2n+2})		LLNL/NCSU	LLNL/NCSU	LLNL/NCSU			
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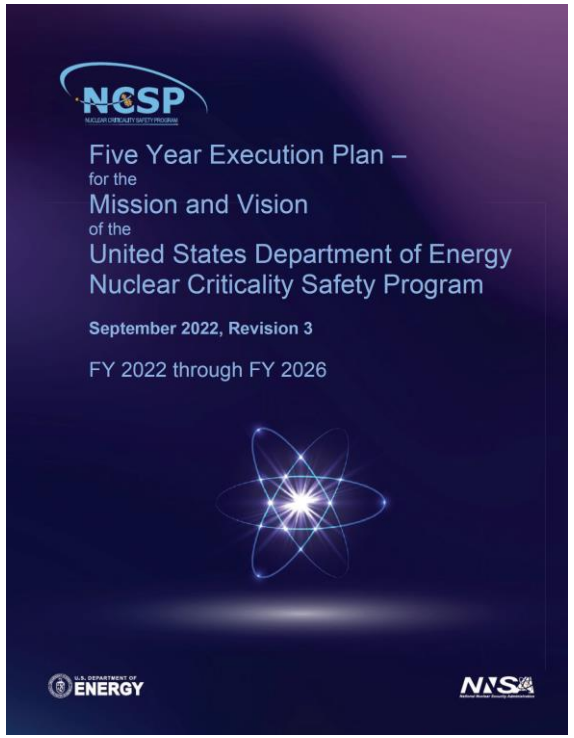

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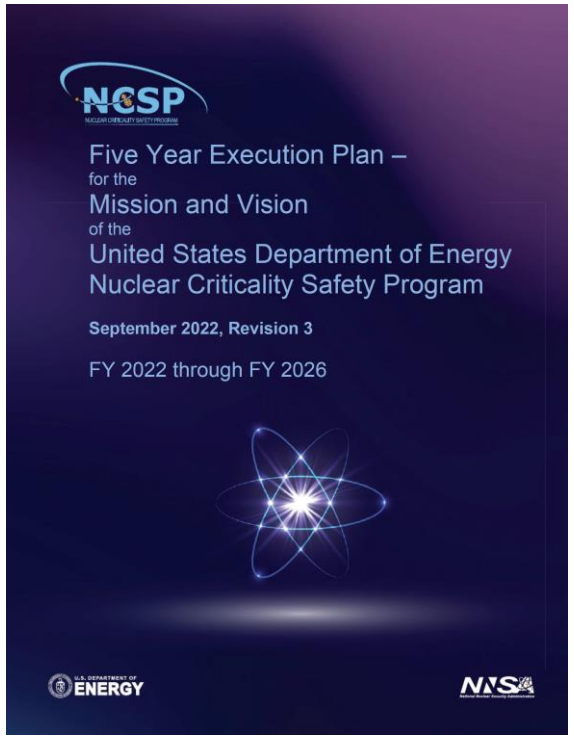

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FY 23 5 Year Execution Plan

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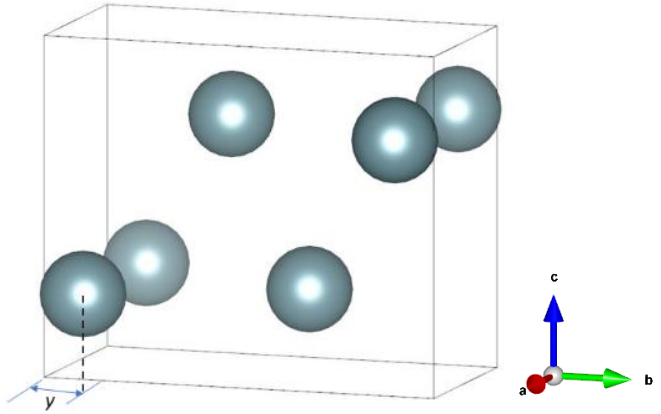
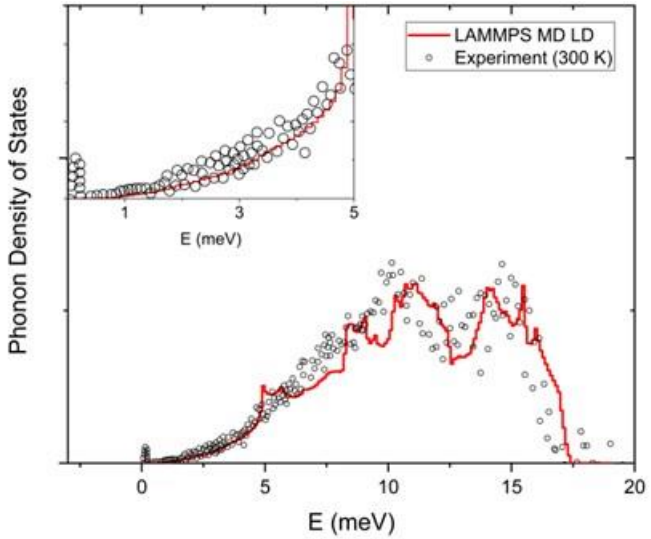
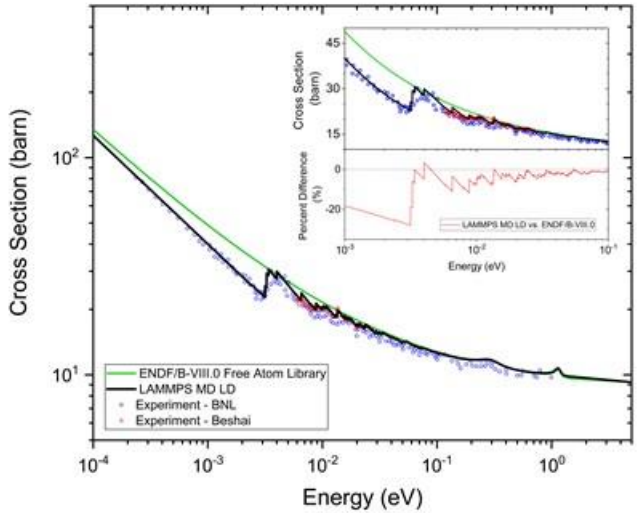
- All completed evaluations have been submitted to NNDC for release as part of ENDF/B-VIII.1.β1
- Additional evaluations were submitted to respond to community needs
- Review process is ongoing

ND2 – Uranium Metal

- Molecular Dynamics / Lattice Dynamics
  - Temperature dependence
  - EAM potential
  - 20x10x10 supercell (20,000 atoms)
  - 0.04Å displacement

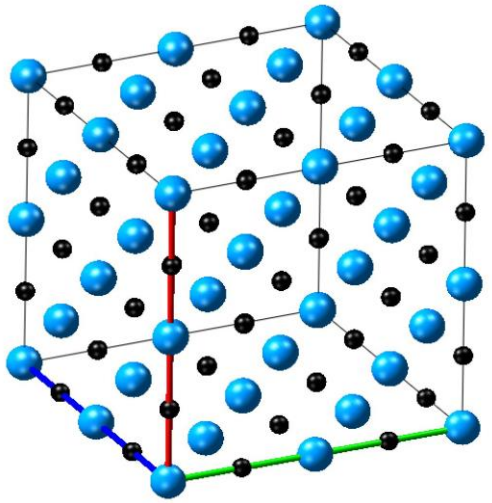


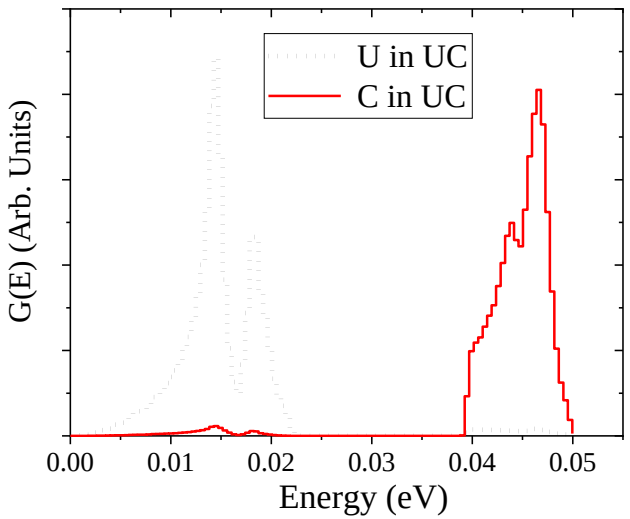


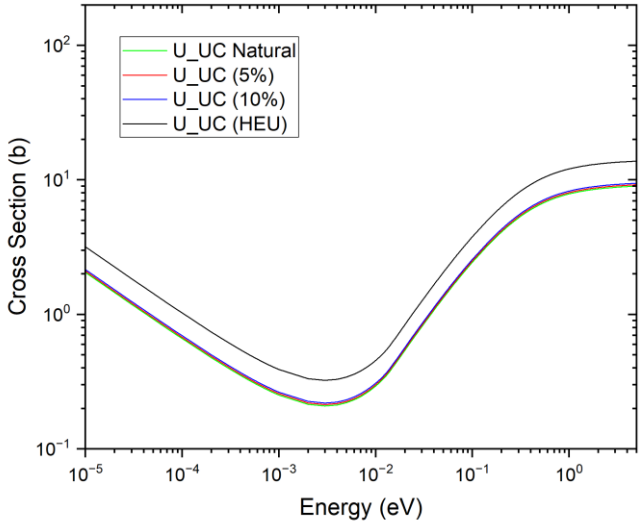


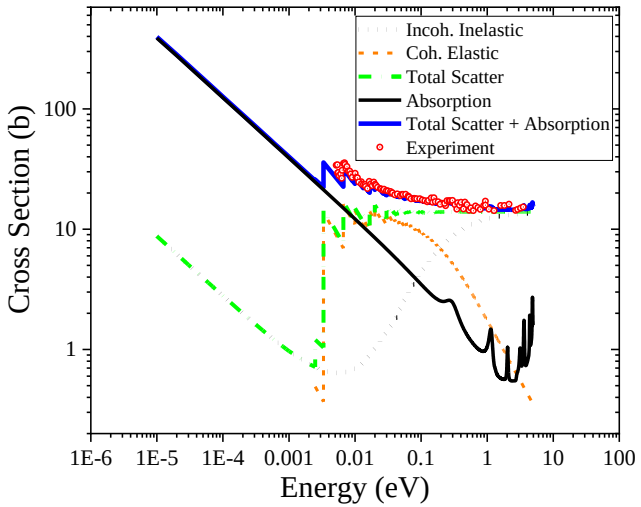
ND2 – Uranium Carbide

- VASP DFT Framework
  - GGA-PBEsol Pseudopotential
  - 1.9 eV Effective Hubbard Term
  - Magnetic Structure Captured with Spin-Orbit-Coupling
  - 2x2x2 supercell (64 atoms)



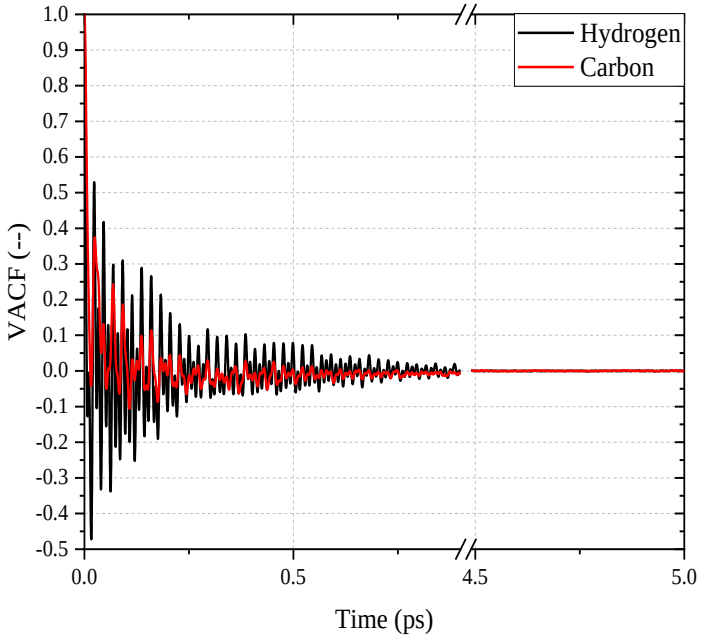


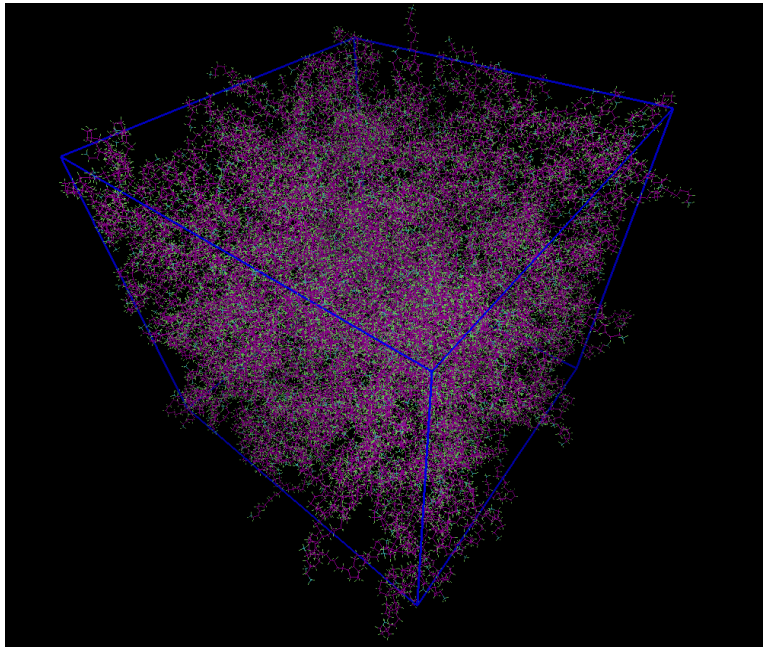




ND2 – Paraffin

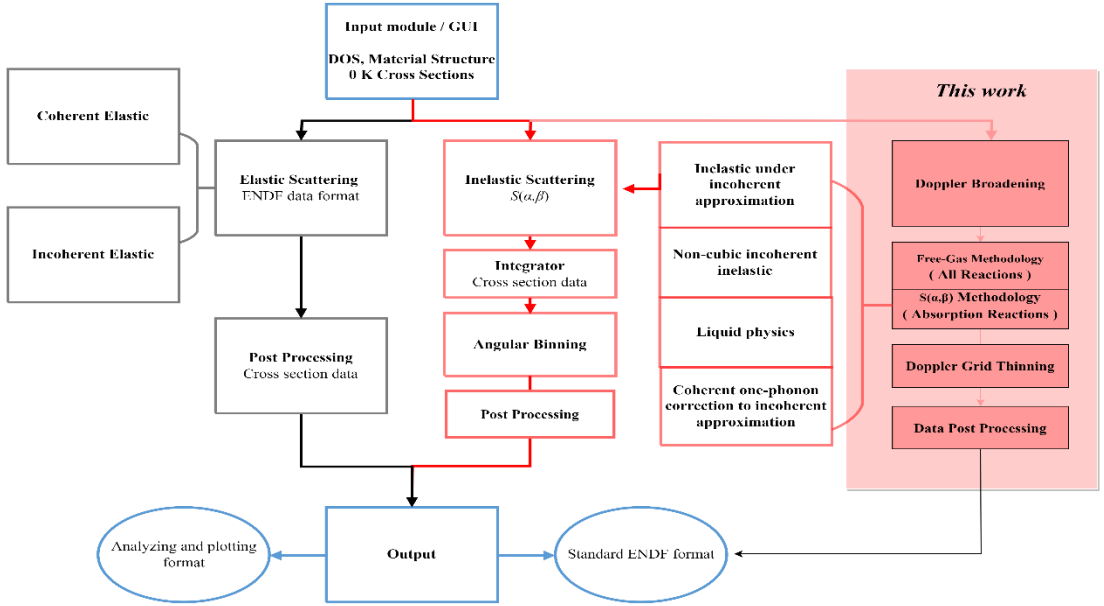
- LAMMPS code using the COMPASS forcefield
  - Tested 10k – 100k atoms
    - Molecular chains
  - 300 K, 1 atm
  - VACF analyzed to obtain DOS for carbon and hydrogen





ND5 – Advanced Methods

$$S(\alpha,\beta) = S_s(\alpha,\beta) + S_d^1(\alpha,\beta)$$

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 1.000000+0 5.000000+0           0          0         12          8 28 1451
 0.000000+0 0.000000+0           0          0         39          3 28 1451
Graphite+Sd LEIP LAB  EVAL-Dec20 N.C. Fleming, A.I. Hawari          28 1451
                      DIST-                                         28 1451
----ENDF/B-VIII       MATERIAL  28                                  28 1451
-----THERMAL NEUTRON SCATTERING                                     28 1451
------ENDF-6 FORMAT                                                 28 1451
                                                                    28 1451
  Temperatures = 296 400 500 600 700 800 1000 1200 1600 2000 K      28 1451
                                                                    28 1451
 HISTORY                                                            28 1451
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 This library was produced by the Low Energy Interaction Physics    28 1451
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 are included in this evaluation using directional information      25 1451
 derived from the Be-metal AILD structure. Ten temperatures are     25 1451
 available in this library. The Full Law Analysis Scattering        25 1451
 System Hub (FLASSH) system was used to produce File 7 MT = 2, 4    25 1451
 data for Be-metal + Sd [3]. The coherent elastic data were         25 1451
 prepared using the cubic approximation. MAT=25 and ZA=125 are      25 1451
 used for Be-metal with distinct effects.                           25 1451
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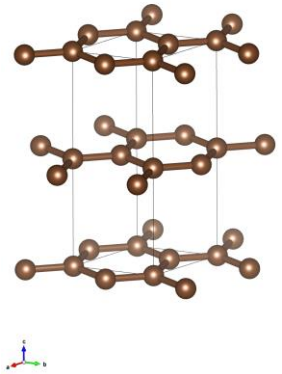
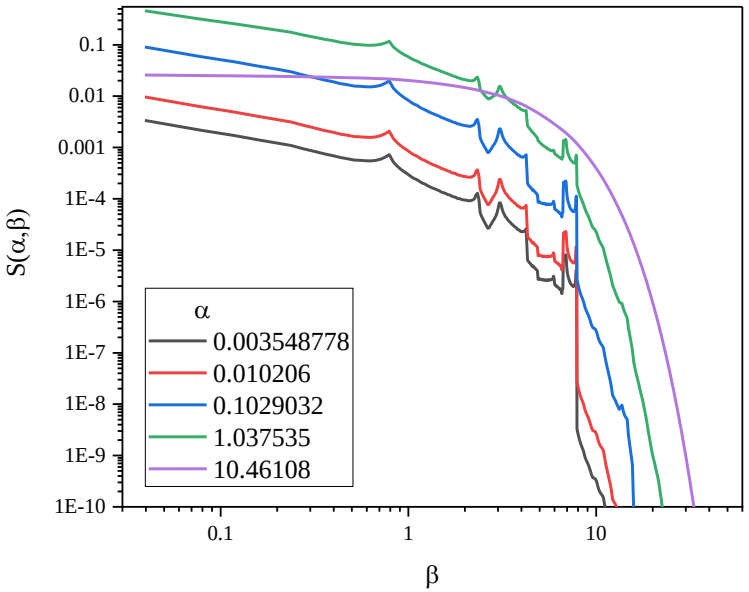
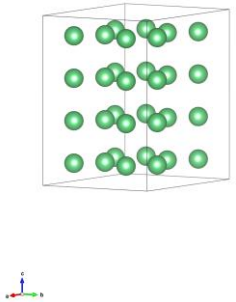
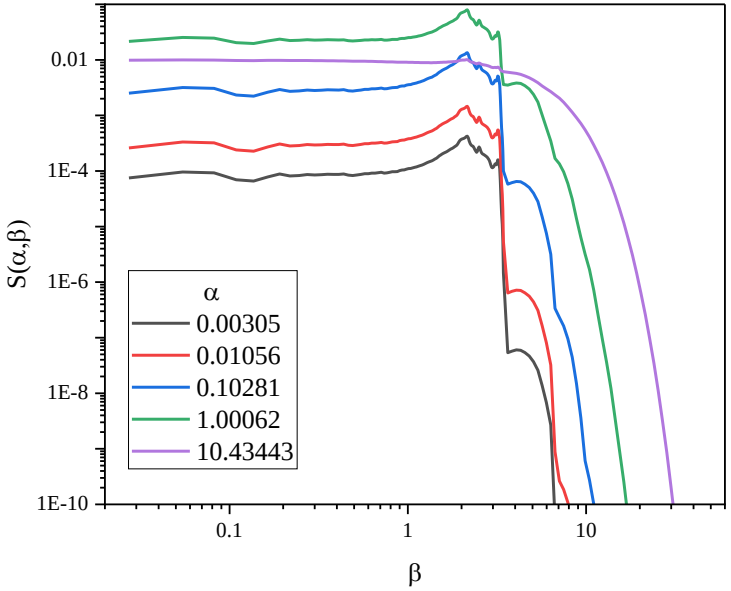
ND10 – Deep Learning and Artificial Neural Networks









ENDF/B-VIII Material	File 7	Temps
Crystalline Graphite	9 MB	10
Beryllium Metal	3.7 MB	8
NeTS	< 200 KB	Continuous

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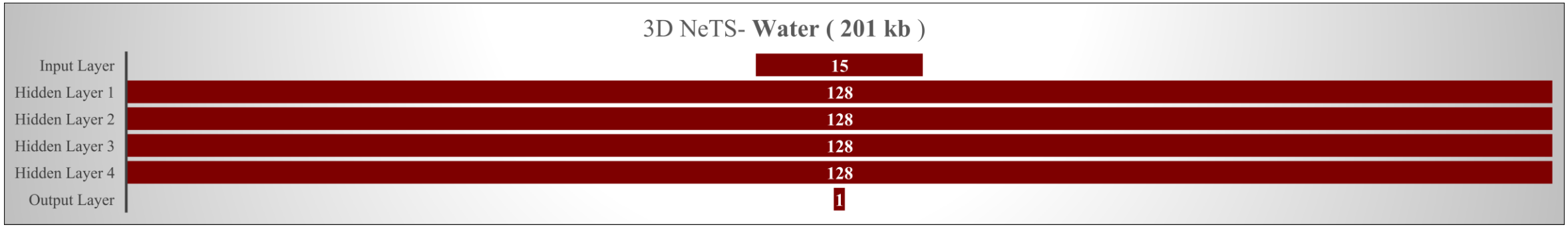
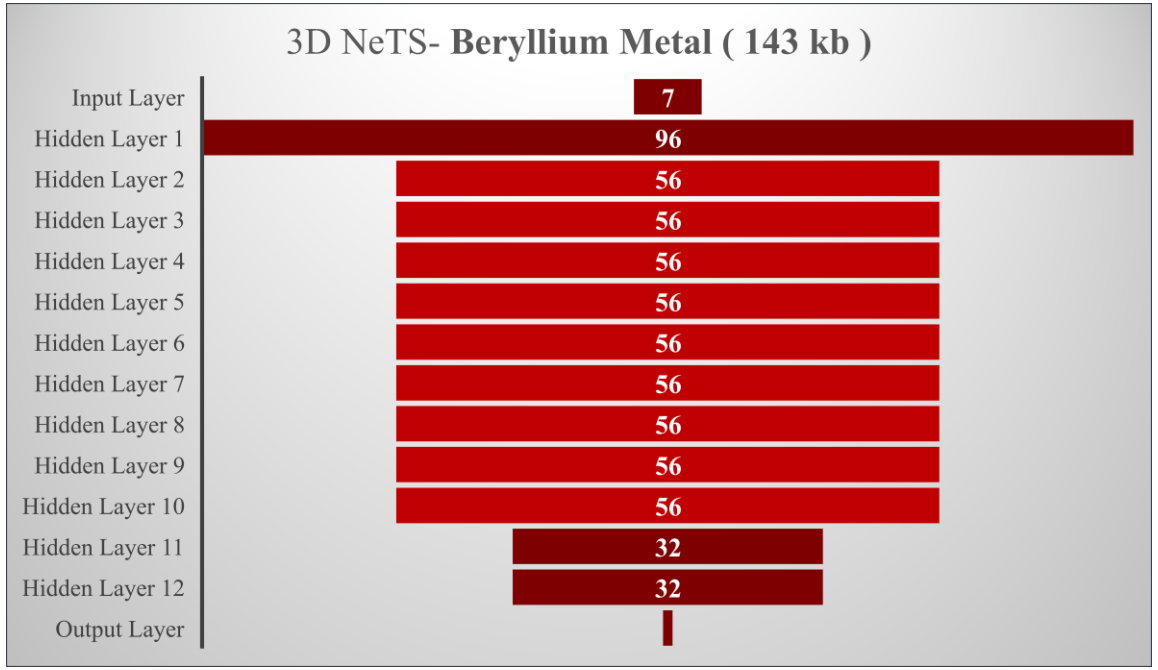
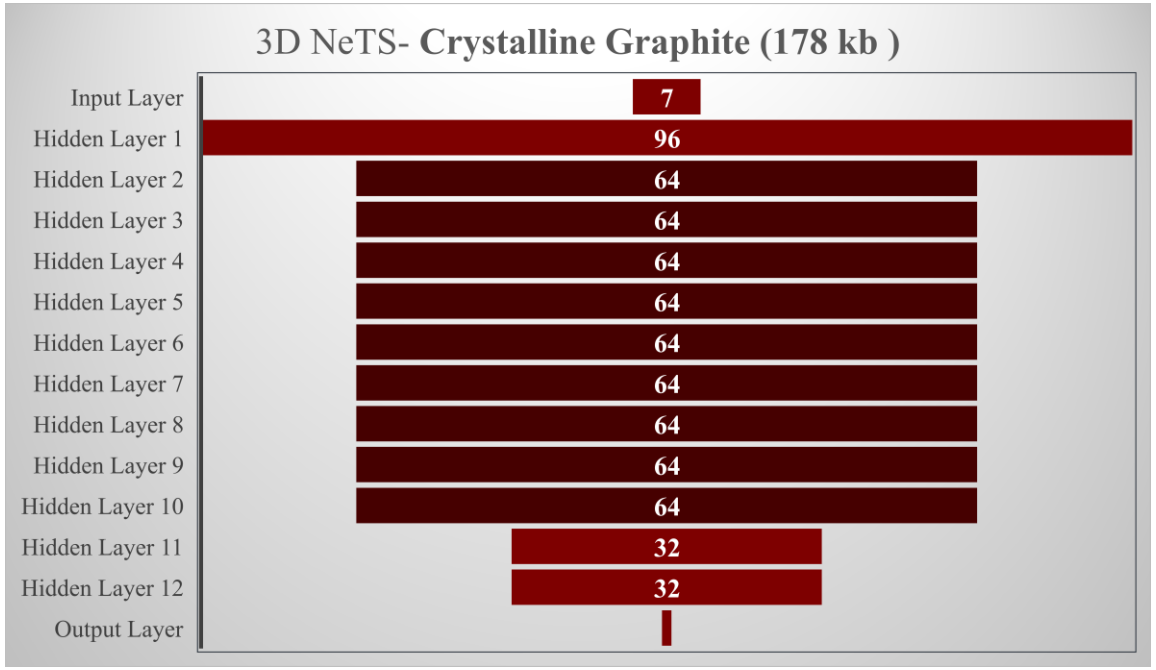
Architecture Visualization / Comparison







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Summary

- Meeting and exceeding all NCSP objectives in FY 2022 (ND2)
- Significant number of evaluations contributed to NNDC
- Innovative methods under development (ND5 and ND10 tasks) including
  - Doppler module integration in *FLASSH* code (under testing)
  - ML methodology development for TSL representation

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Thank You

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