Accomplishments of Thermal Neutron Scattering Research at North Carolina State University

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NUCLEAR CRITICALITY SAFETY PROGRAM (NCSP) TECHNICAL PROGRAM REVIEW
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Oak Ridge National Laboratory, Virtual Meeting

Acknowledgment

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

FY 2021 Tasks

Task	Task Title	Budget
ND2	Generation and Benchmarking of Thermal Neutron Scattering Cross Sections in Support of Advanced Nuclear Reactor Concepts	$49 K
ND3	Development and Implementation of an Advanced and Rigorous Computational Platform for Thermal Neutron Scattering Analysis	$99 K
ND5	Development and Implementation of a Modern Doppler Broadening Approach Including Atomic Binding Effects	$89 K
ND10	Development and Implementation of Machine Learning Methods for Thermal Scattering Law Evaluations	$99 K

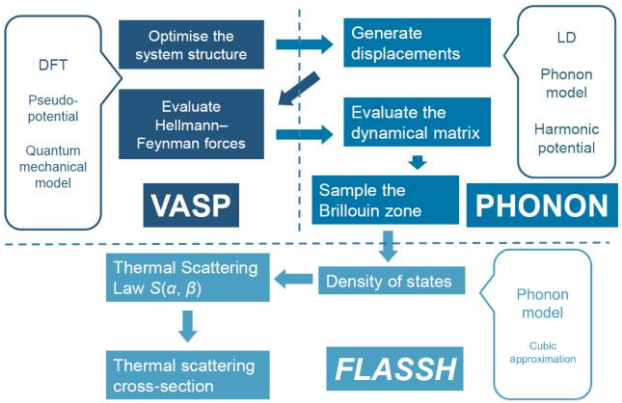
APPENDIX B: Nuclear Data Priorities, Basis Statements, and Milestones

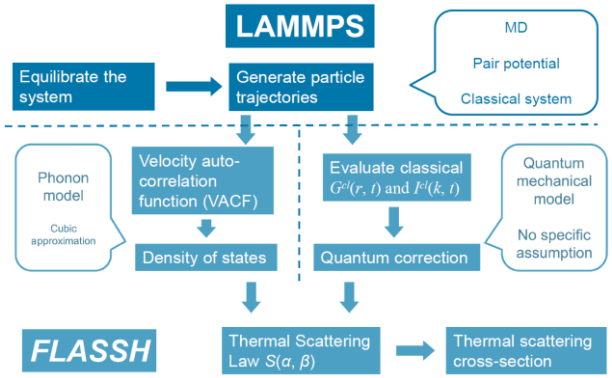
Nuclear Data Evaluations							
Materials	**Pre-FY2022**	**FY2022**	**FY2023**	**FY2024**	**FY2025**	**FY2026**	**Post-FY2026**
Water (H_2O)	LLNL/NCSU	LLNL/NCSU					
Basis	TSL evaluation. Water is this most important moderator and moderating reflector material for criticality safety and light water reactor 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.						
Hydrofluoric Acid (HF)	LLNL/NCSU						
Basis	TSL evaluation. HEU-SOL-THERM-039, "Mixture of Uranium (93%) Hexafluoride and Hydrofluoric Acid (Low H/U Ratio) in a Hot-Water-Reflected Spherical Tank," critical experiments overpredict k-eff from 2-6% regardless of cross-section library or code utilized. An appropriate thermal scattering law for the liquid Hydrofluoric acid (HF) moderator will likely resolve this calculational discrepancy.						
Calcium Hydride (CaH_2)	LLNL/NCSU	LLNL/NCSU					
Basis	TSL evaluation. Calcium hydride is a solid moderator material used in proposed advanced and micro reactor designs. Emergent need requested by micro reactor community.						
Reactor Grade Graphite (20% Porosity)	LLNL/NCSU	LLNL/NCSU					
Basis	TSL evaluation. Graphite is a moderator/reflector material used in advanced reactor designs and in fuel cycle facilities. The prior DOE-NE funded work to produce reactor grade graphite with 10% and 30% porosity will be extended to include 20% porosity per CSEWG request.						
Uranium Metal (U)	LLNL/NCSU	LLNL/NCSU					
Basis	TSL evaluation. Requested by the RPI for use in U-235 resonance parameter analysis.						
Uranium Carbide (UC)	LLNL/NCSU	LLNL/NCSU	LLNL/NCSU				
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.						

Contributed TSL Evaluations

Material	Motivation	NCSP 5 Year Plan	
		Expected	Actual
Liquid hydrogen fluoride (hydrogen)	NCSP applications No TSL data in ENDF/B-VIII.0	FY 2021	FY 2020
Light water (hydrogen)	NCSP applications Extended ENDF/B-VIII.0	FY 2021	FY 2020
Polyethylene (hydrogen)	NCSP applications Extended ENDF/B-VIII.0	----	----
Uranium metal	NCSP applications No TSL data in ENDF/B-VIII.0	FY 2022	FY 2021
Uranium carbide	NCSP applications No TSL data in ENDF/B-VIII.0	FY 2023	FY 2021
20% Porous Reactor Graphite	advanced & micro nuclear reactors No TSL data in ENDF/B-VIII.0	FY 2022	FY 2021
Calcium hydride (CaH2)	advanced & micro nuclear reactors No TSL data in ENDF/B-VIII.0	FY 2022	FY 2021
FLiBe (beryllium) **FLiBe (fluorine)** **FLiBe (lithium)**	advanced & micro nuclear reactors No TSL data in ENDF/B-VIII.0	----	FY 2021
Sapphire (Al in Al2O3) **Sapphire (O in Al2O3)**	Neutron science / Research Reactors No TSL data in ENDF/B-VIII.0 (cryogenic temperatures)	----	FY 2021

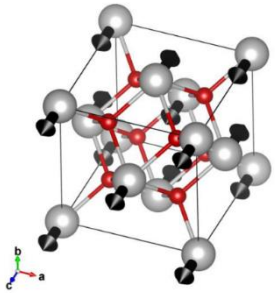
TSL Methodology

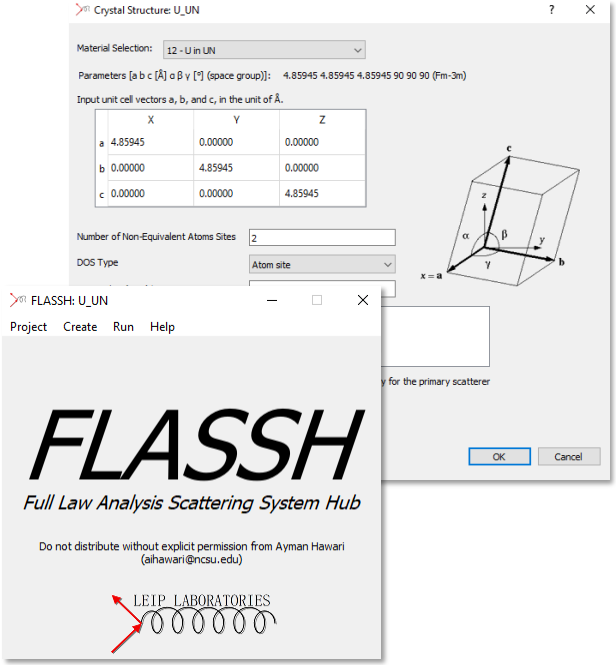


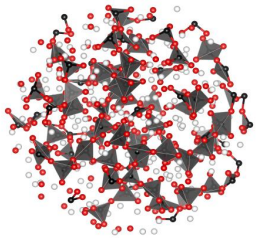


DFT/LD approach

MD approach







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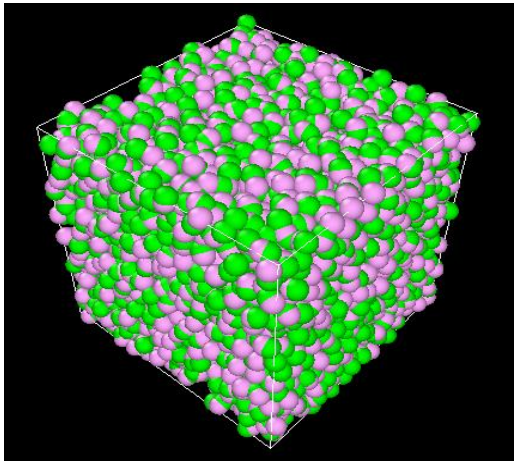
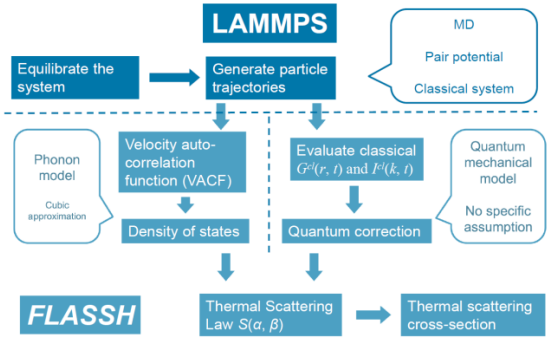
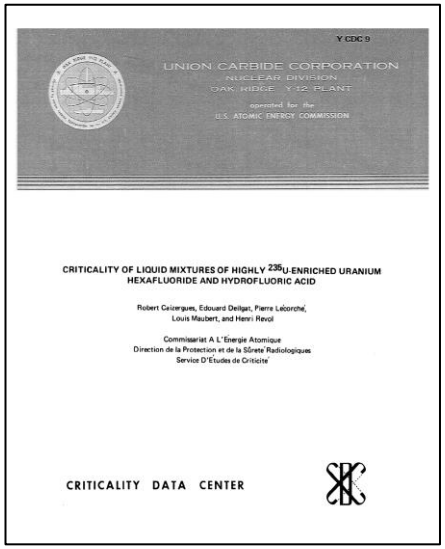





Y CDC 9

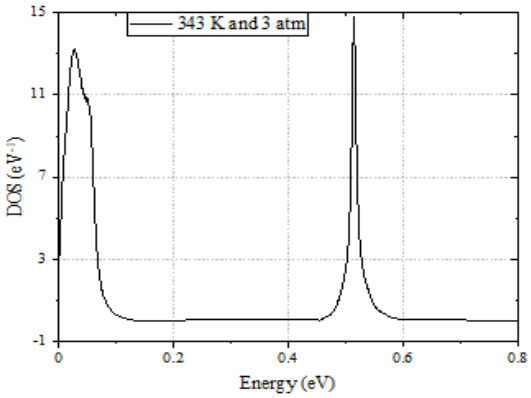
UNION CARBIDE CORPORATION
NUCLEAR DIVISION
OAK RIDGE Y-12 PLANT
operated for the
U.S. ATOMIC ENERGY COMMISSION

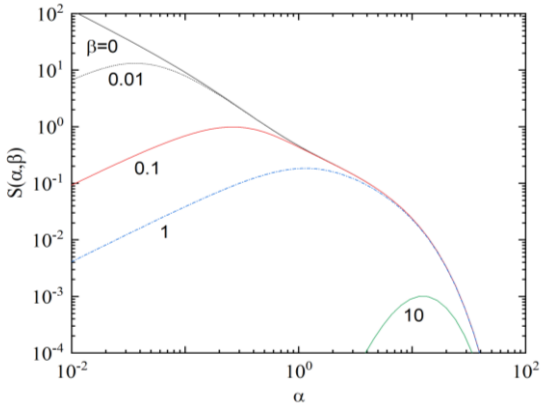
CRITICALITY OF LIQUID MIXTURES OF HIGHLY ^{235}U-ENRICHED URANIUM HEXAFLUORIDE AND HYDROFLUORIC ACID

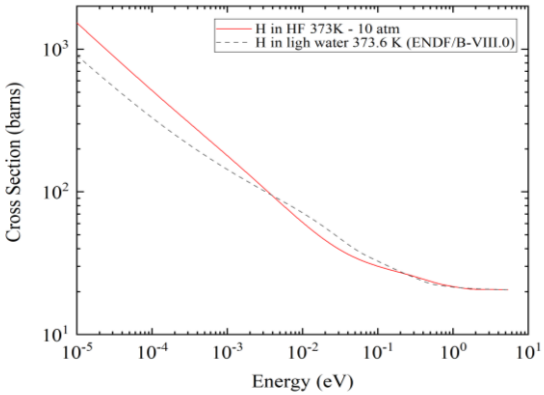
Robert Caicergues, Edouard Deilgat, Pierre Lécorché, Louis Maubert, and Henri Revol

Commissariat A L'Energie Atomique
Direction de la Protection et de la Sûreté Radiologiques
Service D'Études de Criticité

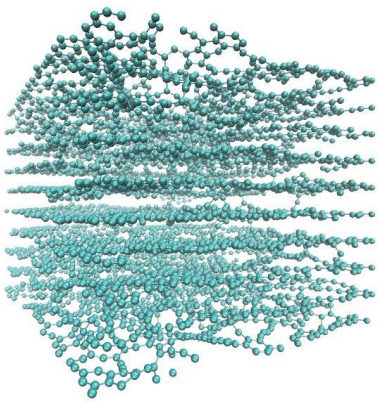
CRITICALITY DATA CENTER

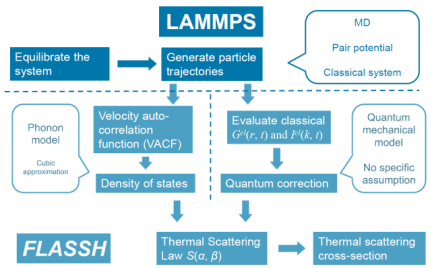


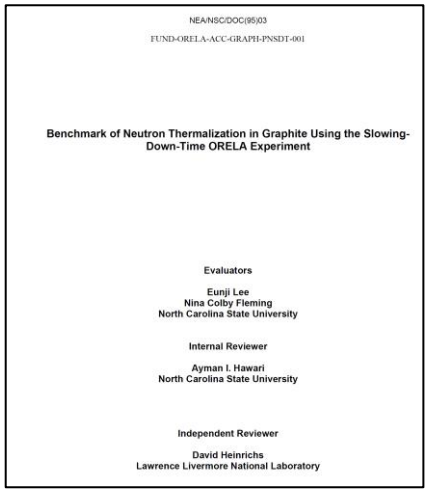




ND2 – New to NNDC
20% Porous Nuclear Graphite







NEA/NSC/DOC(95)03

FUND-ORELA-ACC-GRAPH-PNSDT-001

Benchmark of Neutron Thermalization in Graphite Using the Slowing-Down-Time ORELA Experiment

Evaluators

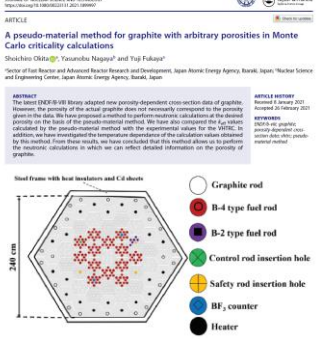
Eunji Lee
Nina Colby Fleming
North Carolina State University

Internal Reviewer

Ayman I. Hawari
North Carolina State University

Independent Reviewer

David Heinrichs
Lawrence Livermore National Laboratory



ARTICLE

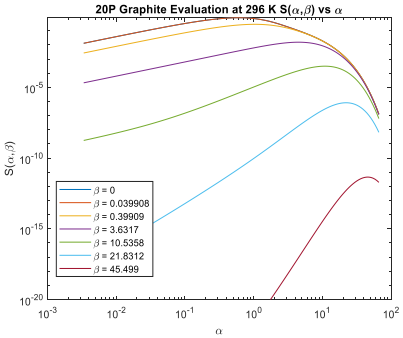
A pseudo-material method for graphite with arbitrary porosities in Monte Carlo criticality calculations

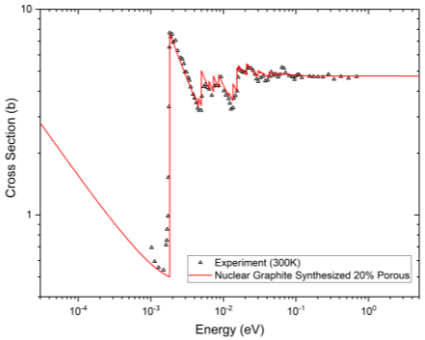
Shoichiro Okita, Yasunobu Nagaya and Tuji Fukaya

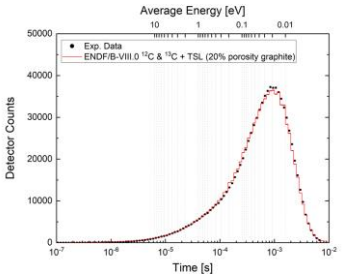
Steel frame with heat insulators and Cd sheets

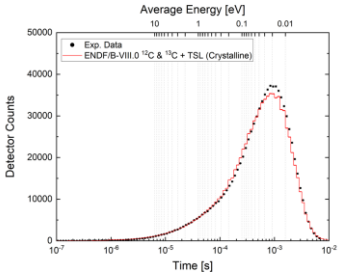
240 cm

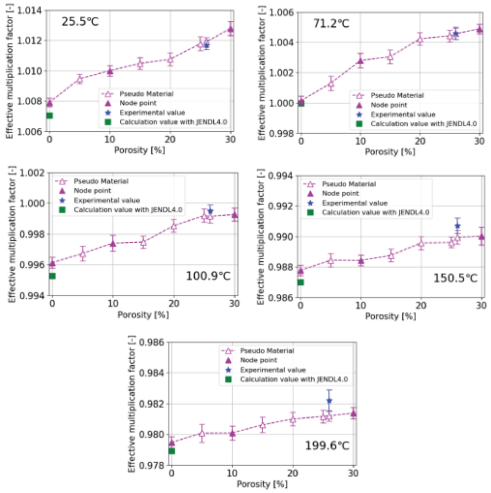
Graphite rod
B-4 type fuel rod
B-2 type fuel rod
Control rod insertion hole
Safety rod insertion hole
BF_3 counter
Heater



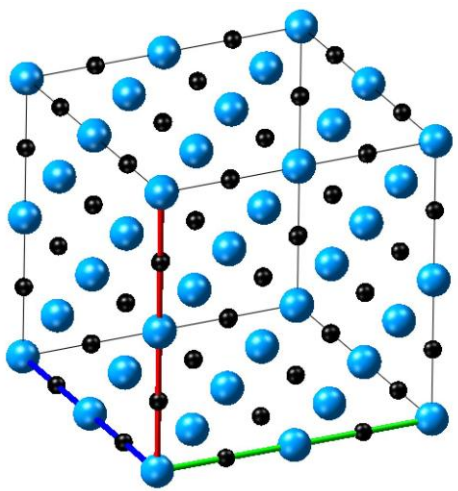


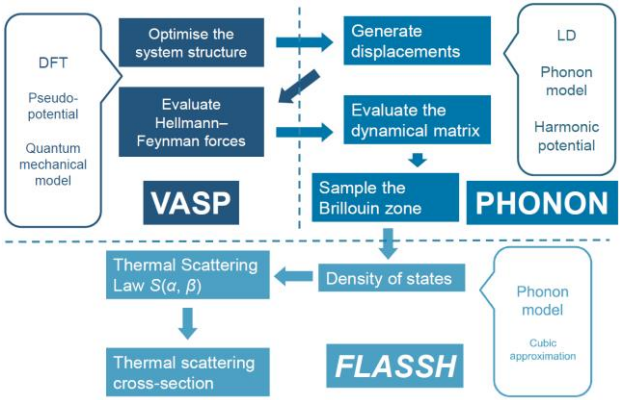


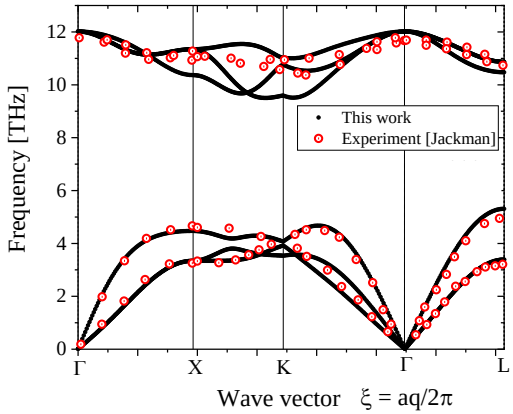


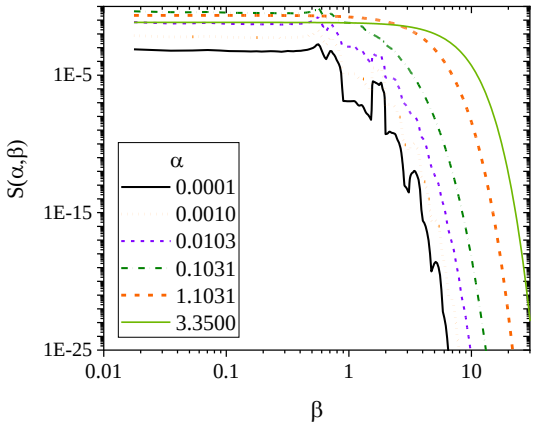


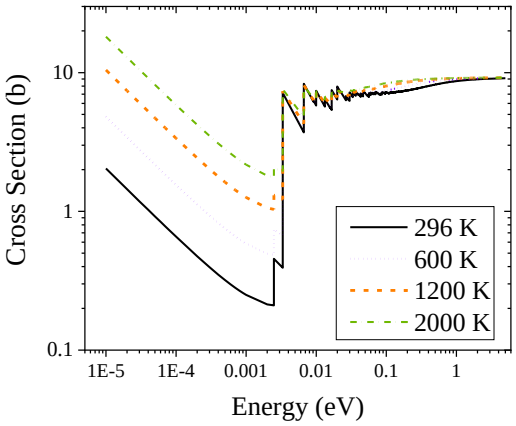
ND2 – New to NNDC Uranium Carbide











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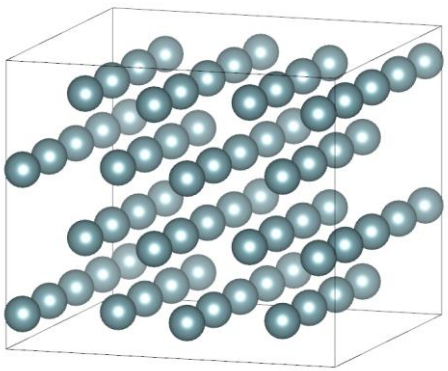
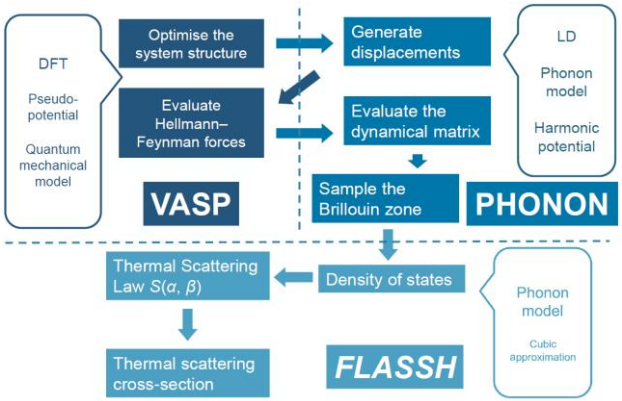
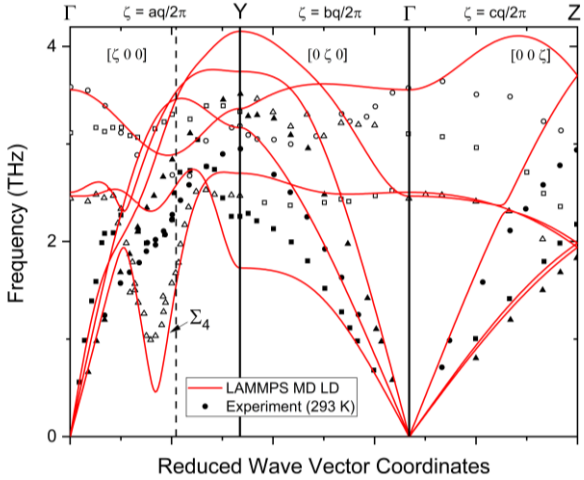
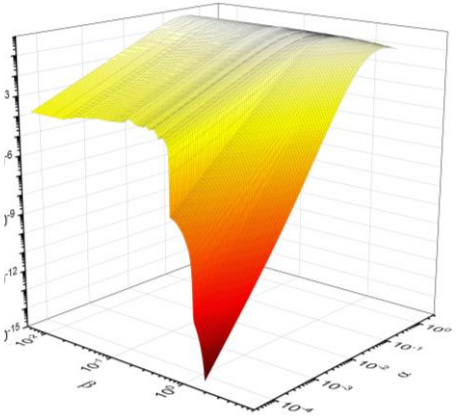
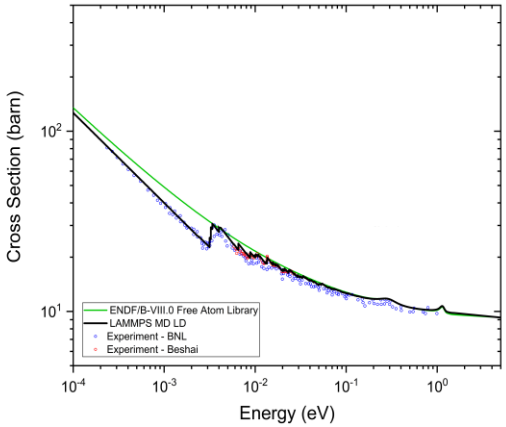
Uranium Metal



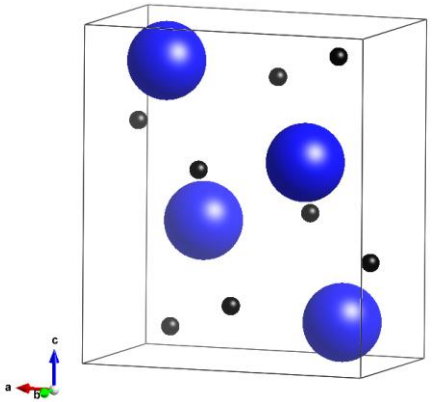


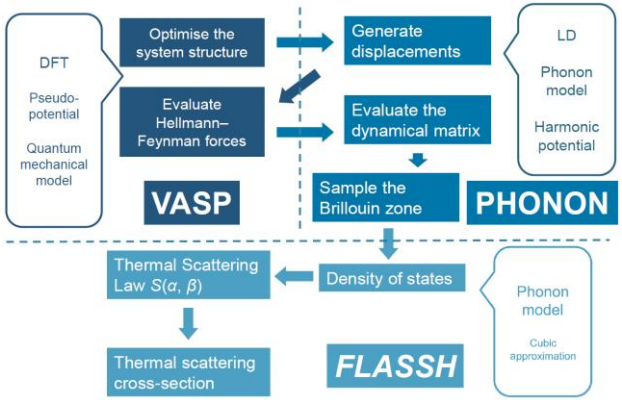


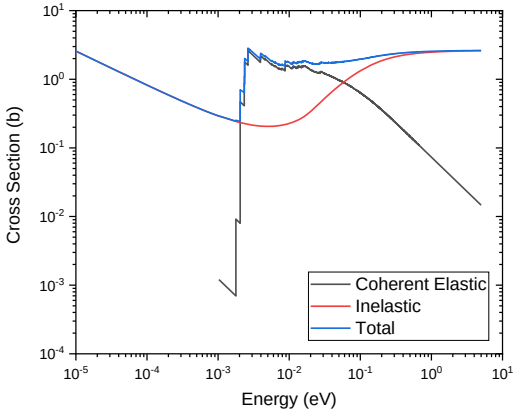


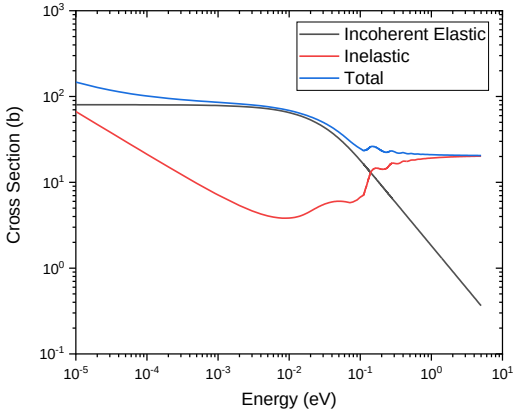


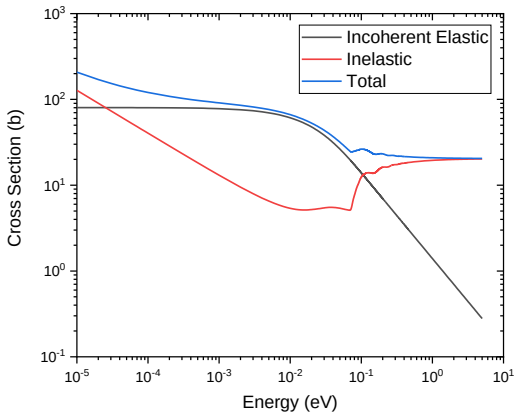
ND2 – New to NNDC
Calcium Hydride (CaH_2)



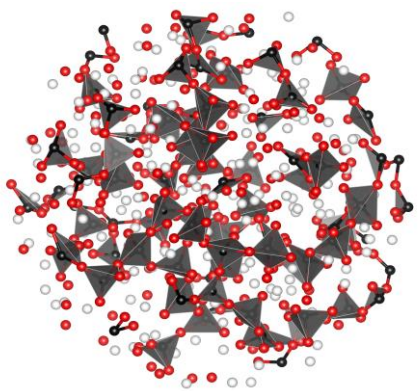


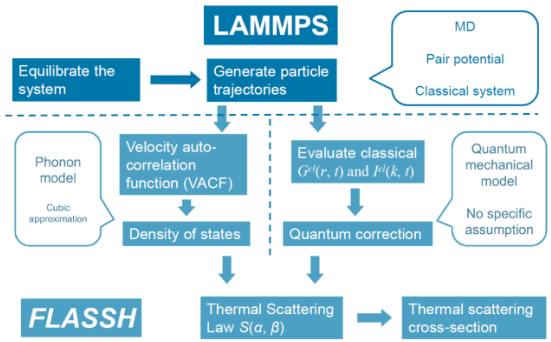


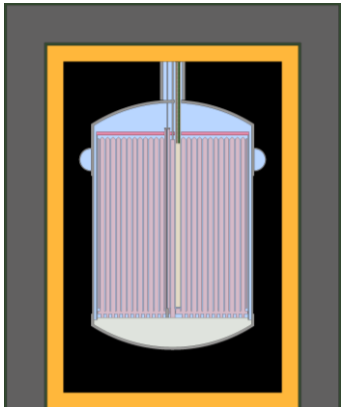




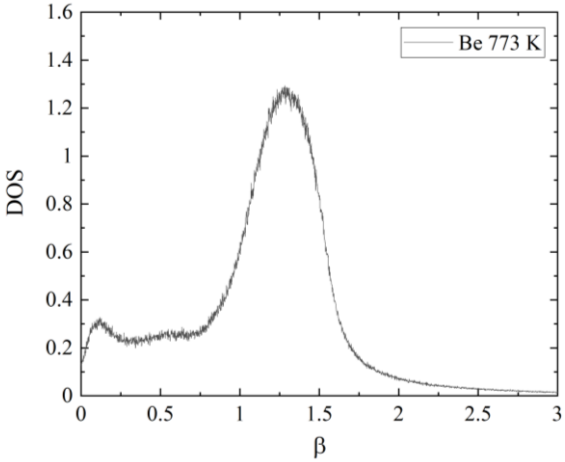
New to NNDC
Molten Salt FLiBe – DOE NE

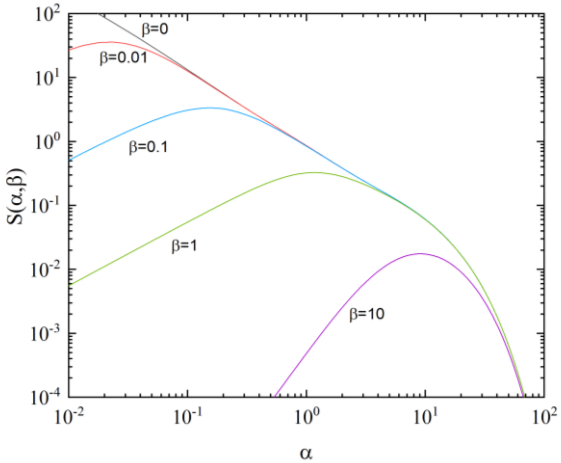


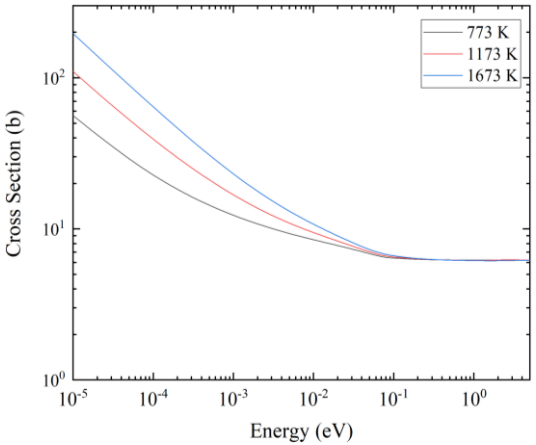




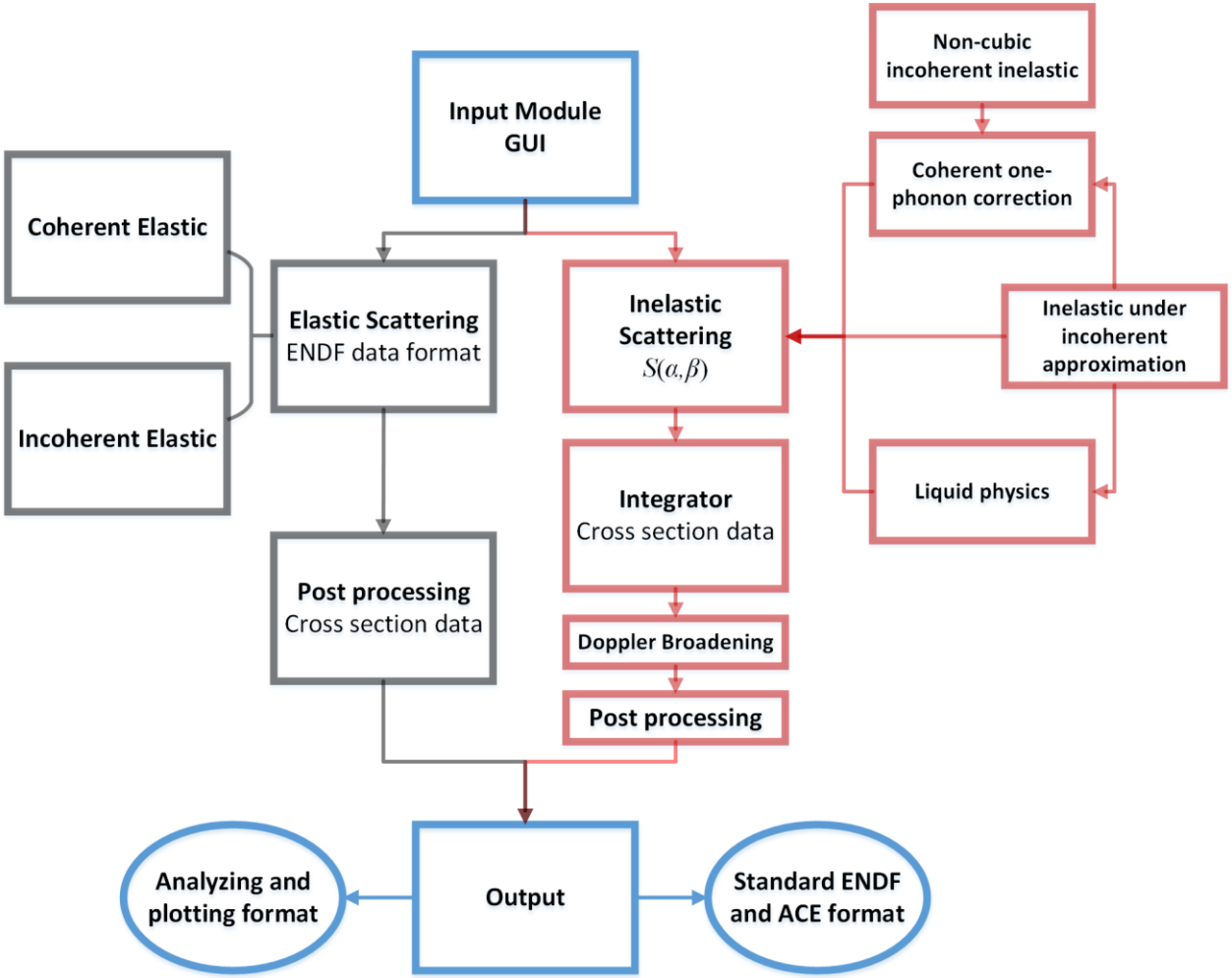
MSRE-MSR-EXP-001





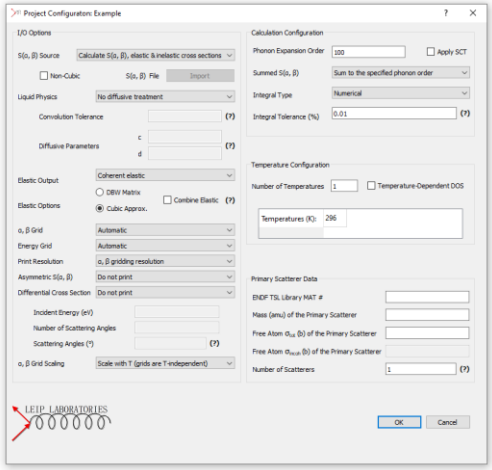


ND3 – *FLASSH*

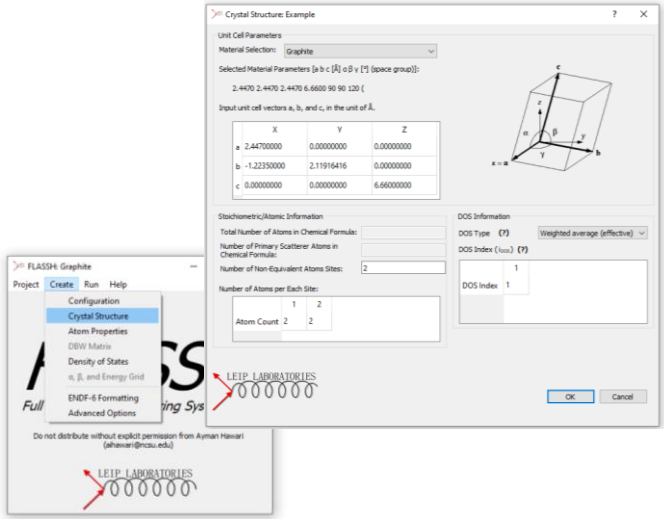

Input Module
GUI
Coherent Elastic
Incoherent Elastic
Elastic Scattering
ENDF data format
Post processing
Cross section data
Inelastic
Scattering
$S(\alpha,\beta)$
Integrator
Cross section data
Doppler Broadening
Post processing
Non-cubic
incoherent inelastic
Coherent one-
phonon correction
Inelastic under
incoherent
approximation
Liquid physics
Analyzing and
plotting format
Output
Standard ENDF
and ACE format

FLASSH

- ***FLASSH* Code**
  - Calculations and ENDF TSL library formatting modules implemented in FORTRAN 95 using a modular design
  - Parallel computing realized by OpenMP 4.0 bindings
  - GUI implemented by cross platform QT® C++ API

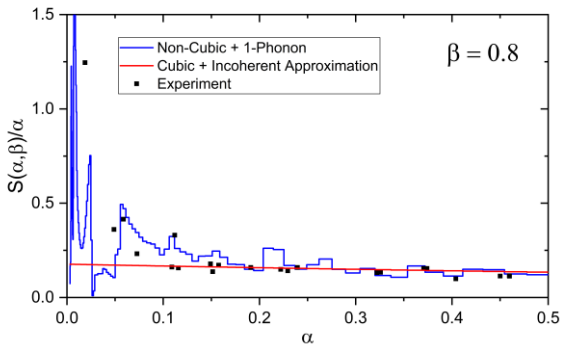


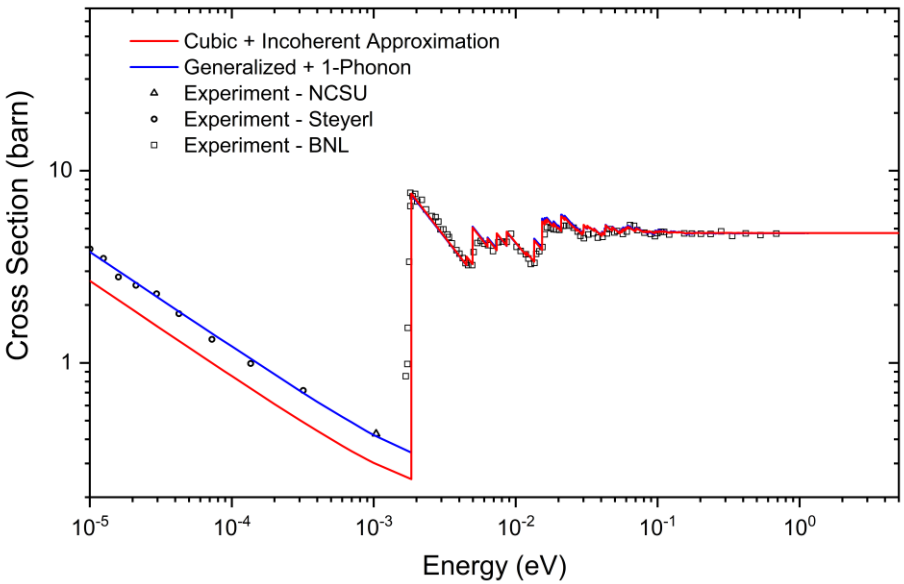
  - Error checks
  - Input Generator (for both *FLASSH* and NJOY)
  - ENDF / ACE Formatting
  - Warning Messages Based on Material Physics
  - Crystal Structure Dependent Calculation



FLASSH

- **Non-Cubic (NC) Elastic and Inelastic**
  - Any material
  - Additional inputs: partial DOSs
- **1-Phonon (Distinct) Contributions**
  - Additional inputs: polarization file





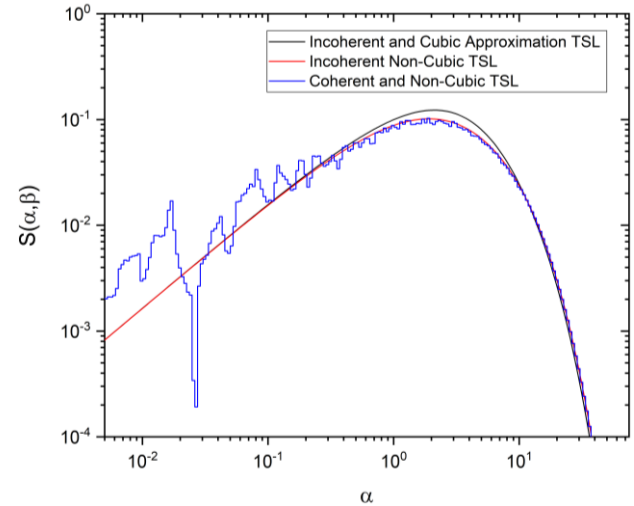
Graphite (296 K) NC and 1-phonon needed to benchmark TSL and cross sections

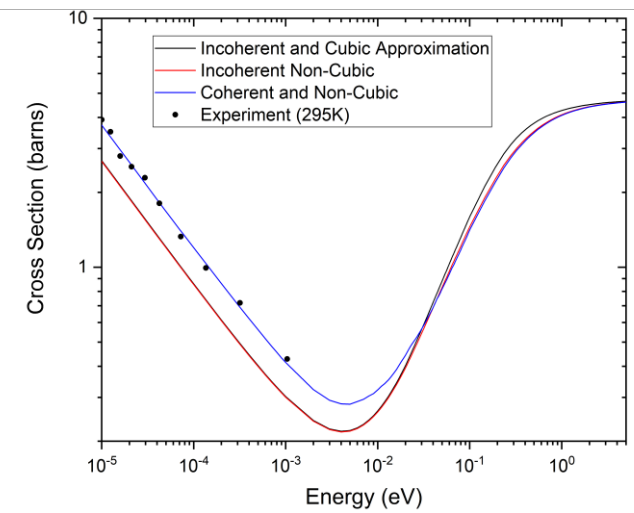
ND5 – Doppler Analysis *FLASSH* Generalized TSL

- Generalized Self and Distinct (Coherent) Evaluation
  - Exact material structure
  - Direction-dependent calculations averaged into α/β space
  - Effects at lowest α-values

2.33E-03	-1.65E-06	2.15E-09
-1.65E-06	2.33E-03	-5.65E-09
2.15E-09	-5.65E-09	1.35E-02

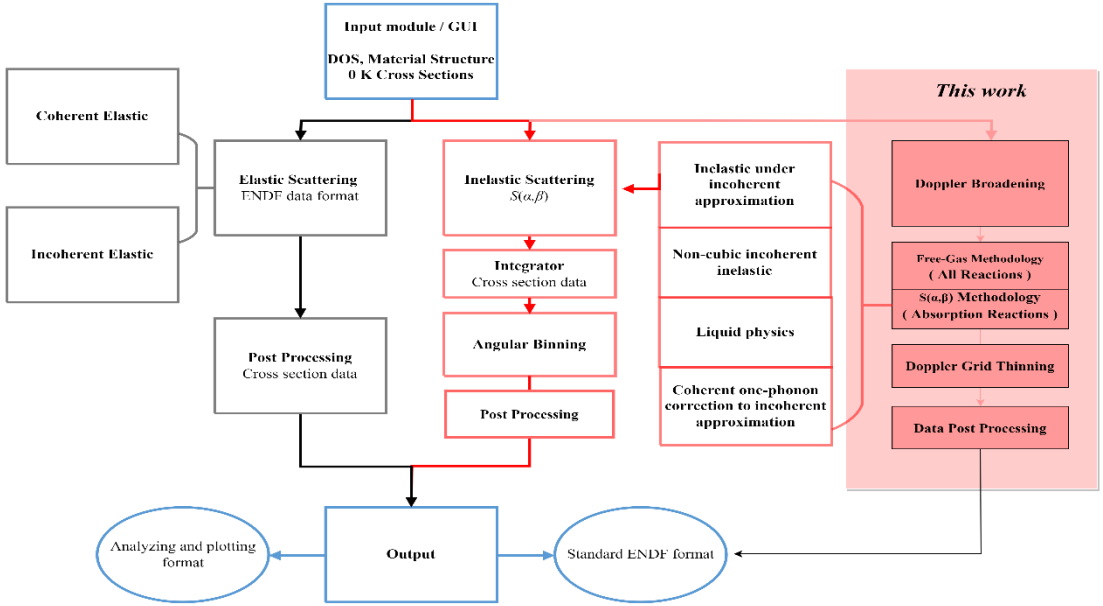
Exact Debye-Waller Matrix

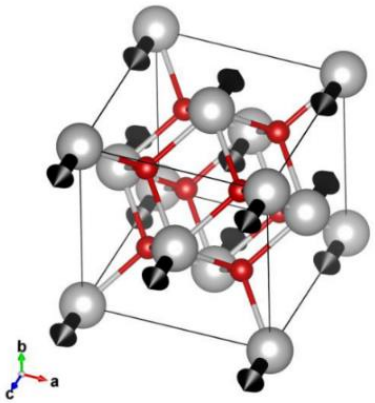


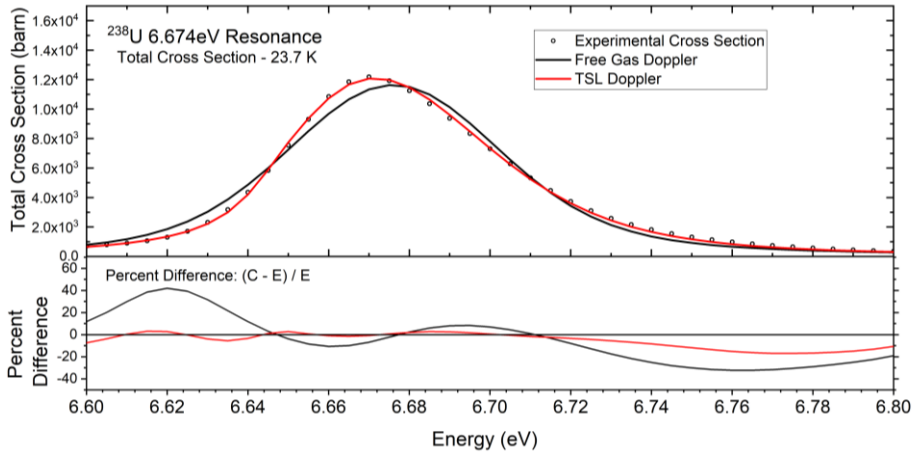


Graphite TSL data and inelastic cross sections comparing incoherent cubic and generalized full TSL impacts at room temperature.

ND5 – Doppler Broadening

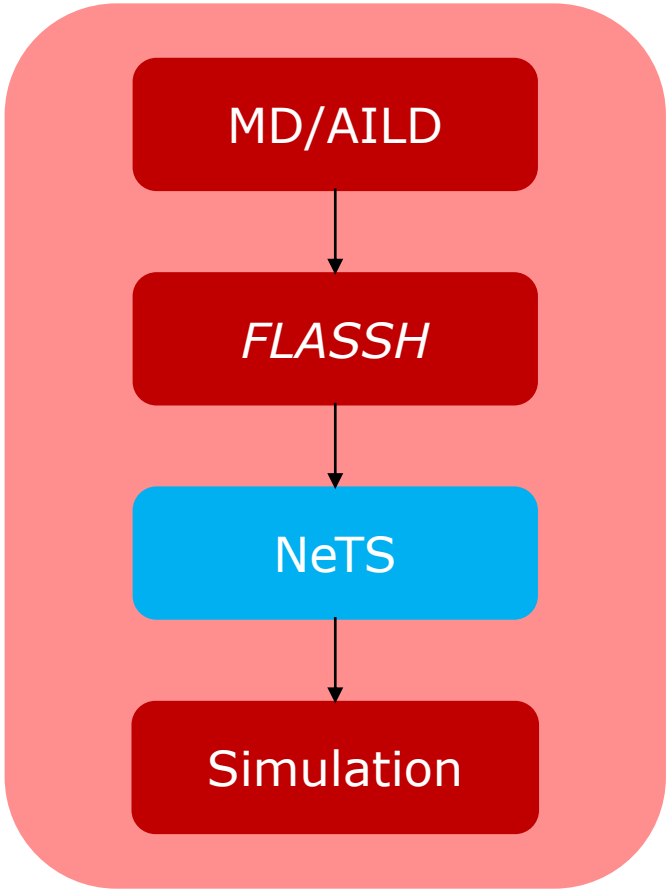






FY 21
ND10 – TSL NeTS

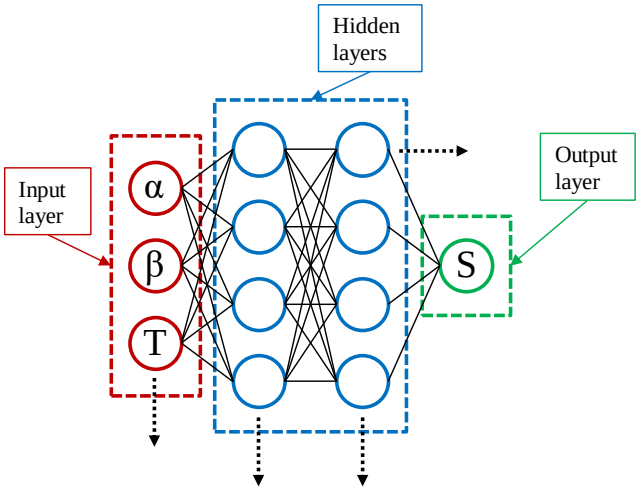
- New TSL paradigm
  - ML/DL **Neural Thermal Scattering (NeTS) modules**
  - Completed NeTS for H_2O
- See papers and presentations
  - ANS 2019 Winter Meeting, Washington, DC, USA
  - PHYSOR 2020 Meeting, Cambridge, UK
  - PHYSOR 2022 Meeting, Pittsburgh, PA



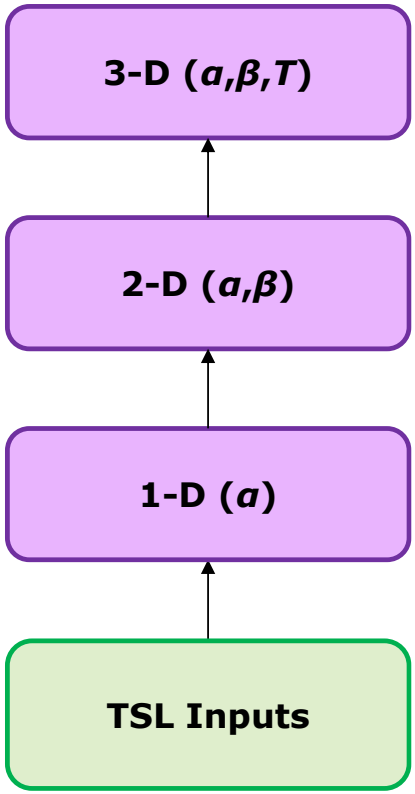
FY 21

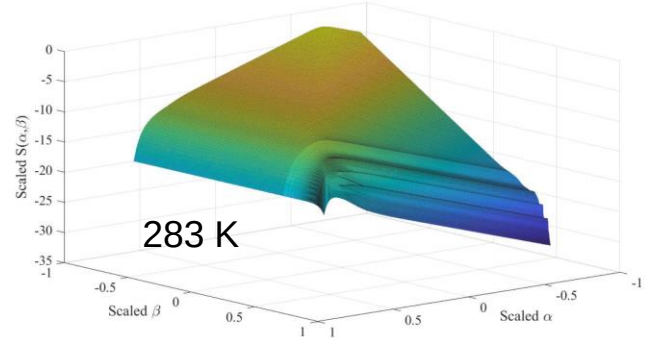
ND10 – TSL NeTS H_2O

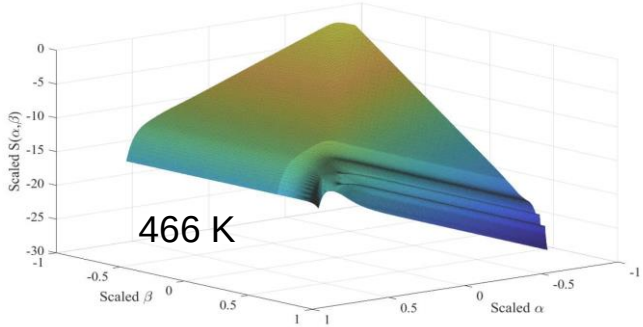
- **Start simple**
- **Adaptive iteration**
- **Less than 0.5% deviation**
- **300 kB data needs for H_2O NeTS**

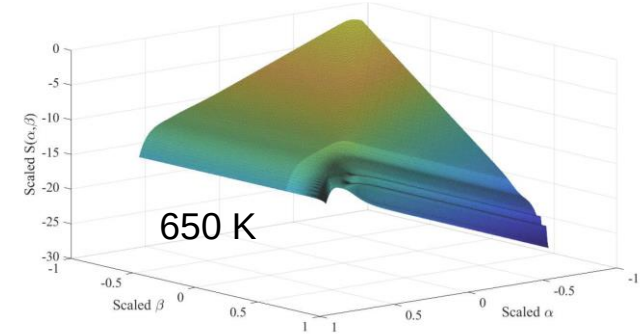


PyTorch









Summary

- Thermal neutron scattering law (TSL) data evaluations have been completed and contributed to ENDF
  - New evaluations are underway
- *FLASSH* is developing as a modern platform for thermal neutron data analysis
  - Enhanced user experience and low learning overhead
- Advanced TSL techniques in combination with Doppler analysis have been developed
  - Incorporated into *FLASSH*
- ML/DL NeTS method development initiated
- Experimental capabilities for validation have been developed at the PULSTAR reactor

Thank You
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