TSL Methods, Evaluations, and Benchmarks at North Carolina State University

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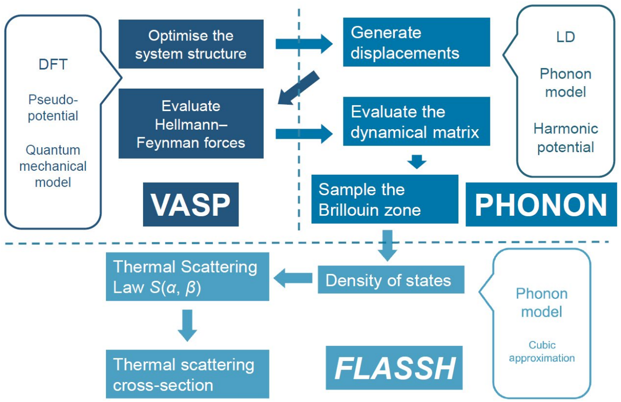
Acknowledgment

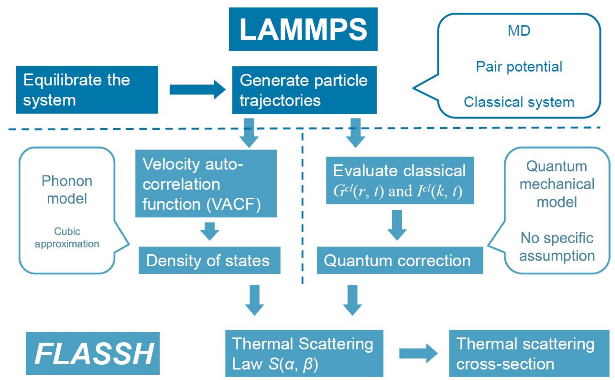
- NNSA Nuclear Criticality Safety Program (NCSP)
  - collaboration with LLNL
- Naval Nuclear Propulsion Program (NNPP)
- Department of Energy - NE
- LEIP team & collaborators

2020 – 2021 Activities

- Generation and benchmark of thermal neutron scattering cross sections in support of various applications including the design advanced and micro nuclear reactors
- Development, implementation, and testing of the *FLASSH* computational platform for thermal neutron scattering (TSL) analysis
- Development and implementation of a modern machine learning approach for TSL analysis
- Measurements in support of TSL analysis

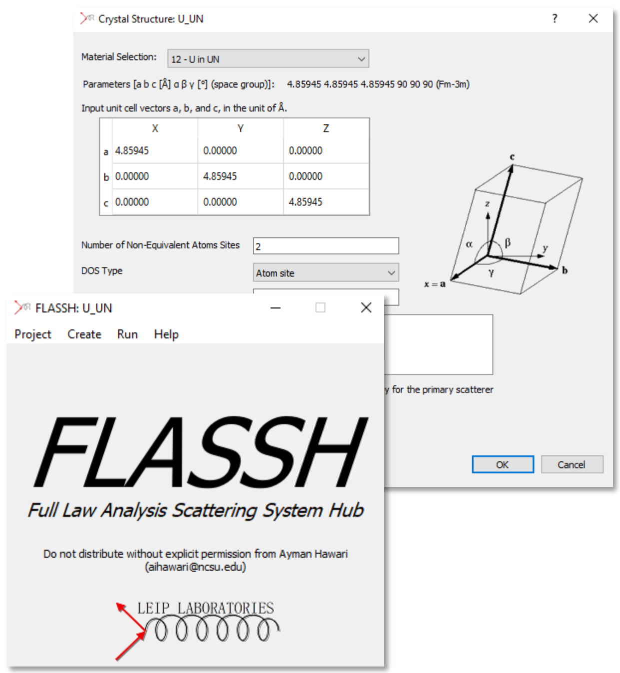
TSL Methodology

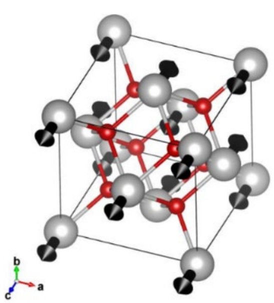


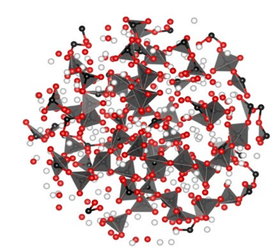


DFT/LD approach

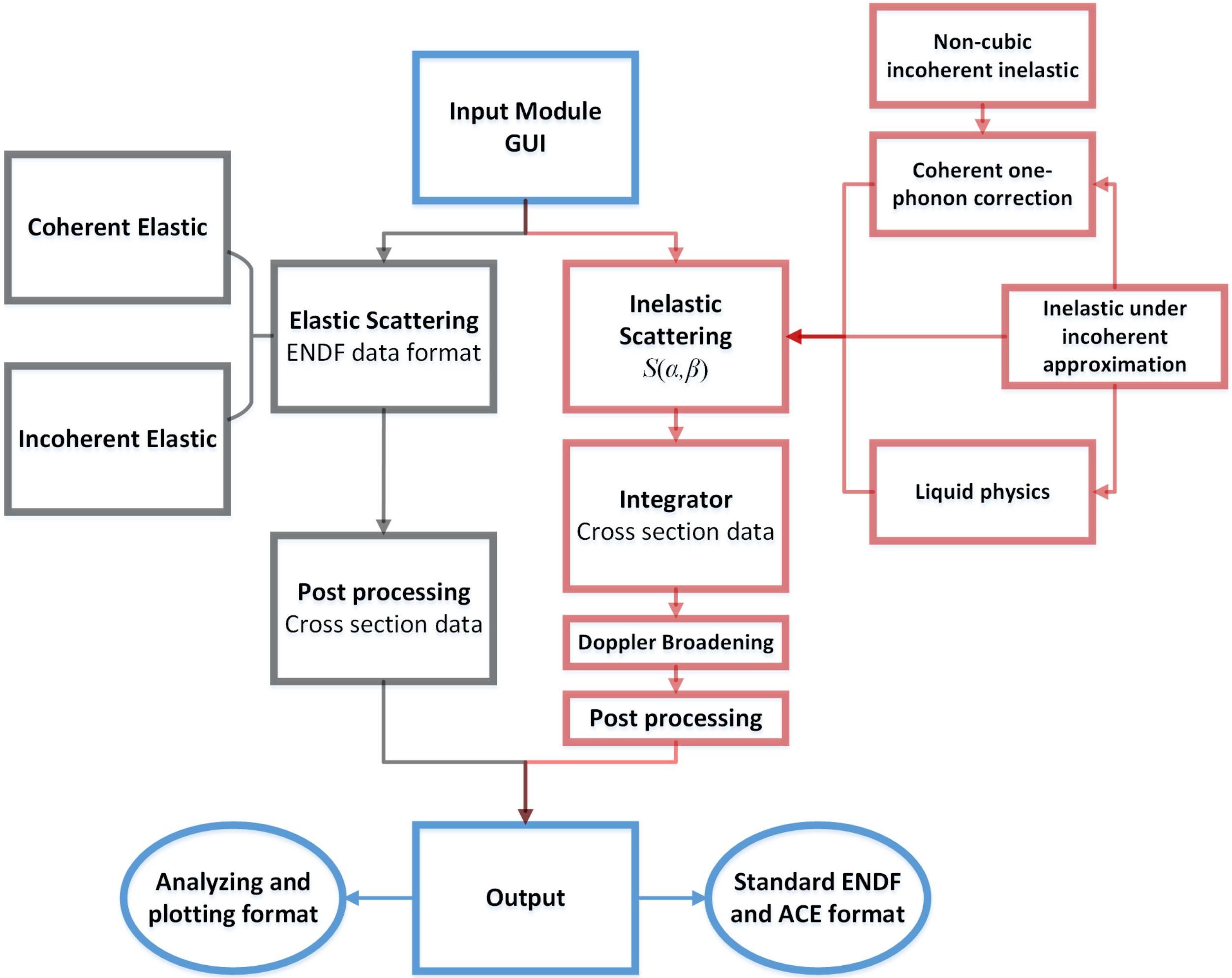
MD approach







FLASSH

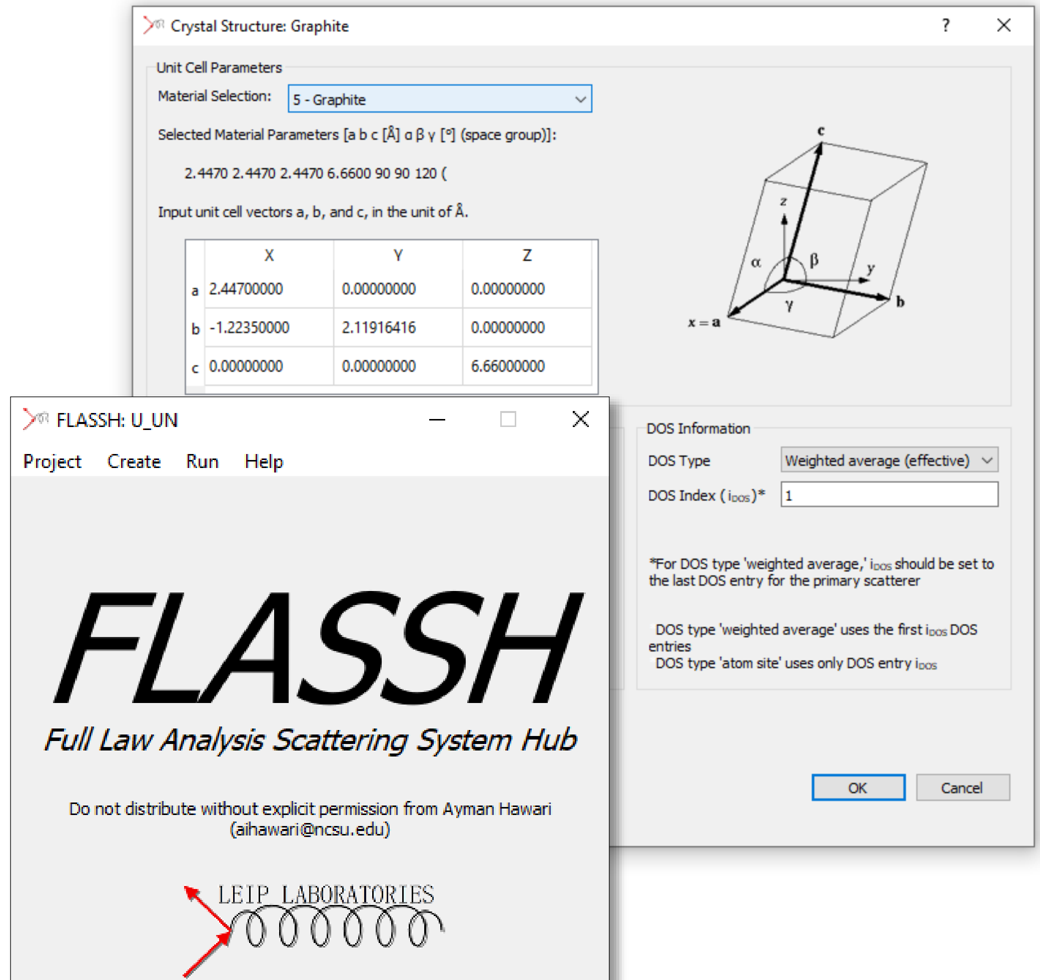

Input Module
GUI
Coherent Elastic
Incoherent Elastic
Elastic Scattering
ENDF data format
Post processing
Cross section data
Inelastic
Scattering
$S(\alpha,\beta)$
Integrator
Cross section data
Doppler Broadening
Post processing
Non-cubic
incoherent inelastic
Coherent one-
phonon correction
Inelastic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

FLASSH

❑ *FLASSH*

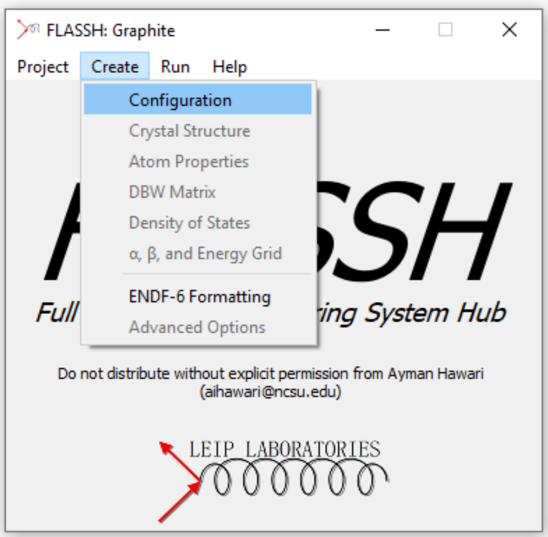
- Calculations and ENDF TSL library formatting modules implemented in FORTRAN 95 using a modular design
- Parallel computing realized by OpenMP 4.0 bindings
- GUI implemented by cross platform QT® C++ API

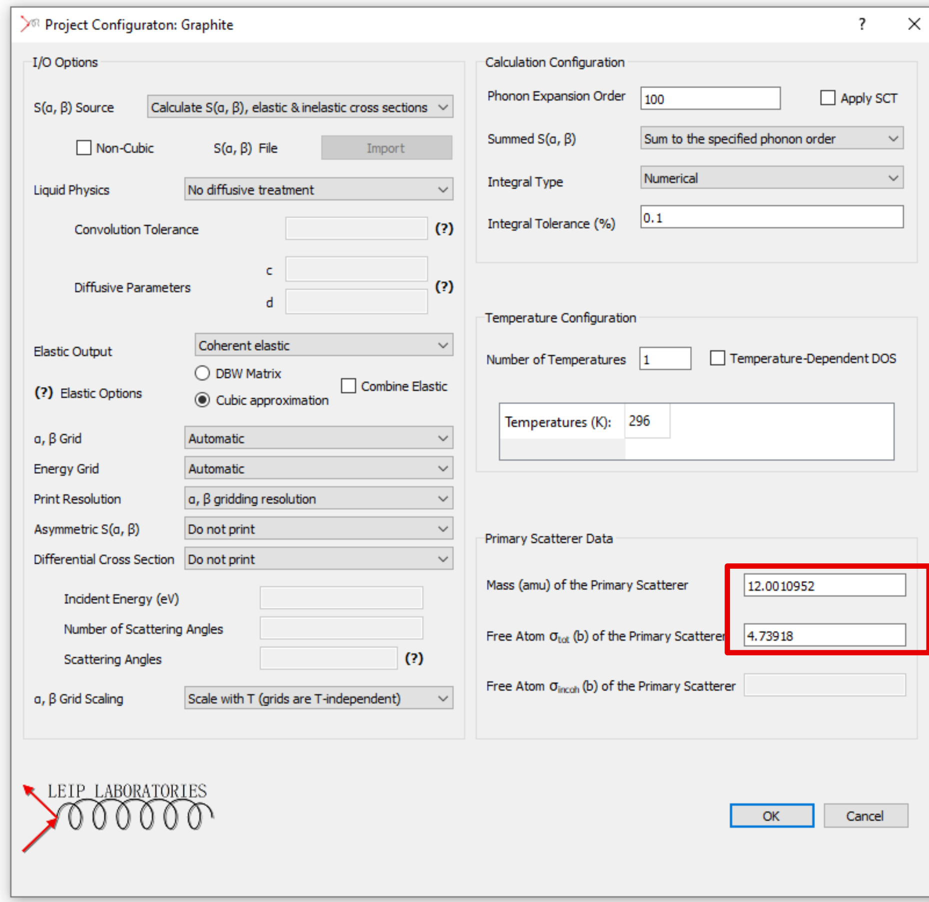
- Error checks
- Input Generator (for both *FLASSH* and NJOY)
- ENDF / ACE Formatting
- Warning Messages Based on Material Physics
- Crystal Structure Dependent Calculation



FLASSH

- ***FLASSH* GUI**
  - Configuration (Defaults Shown)

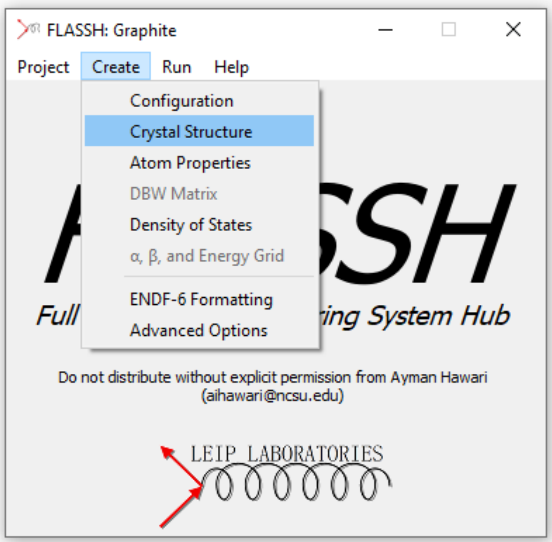




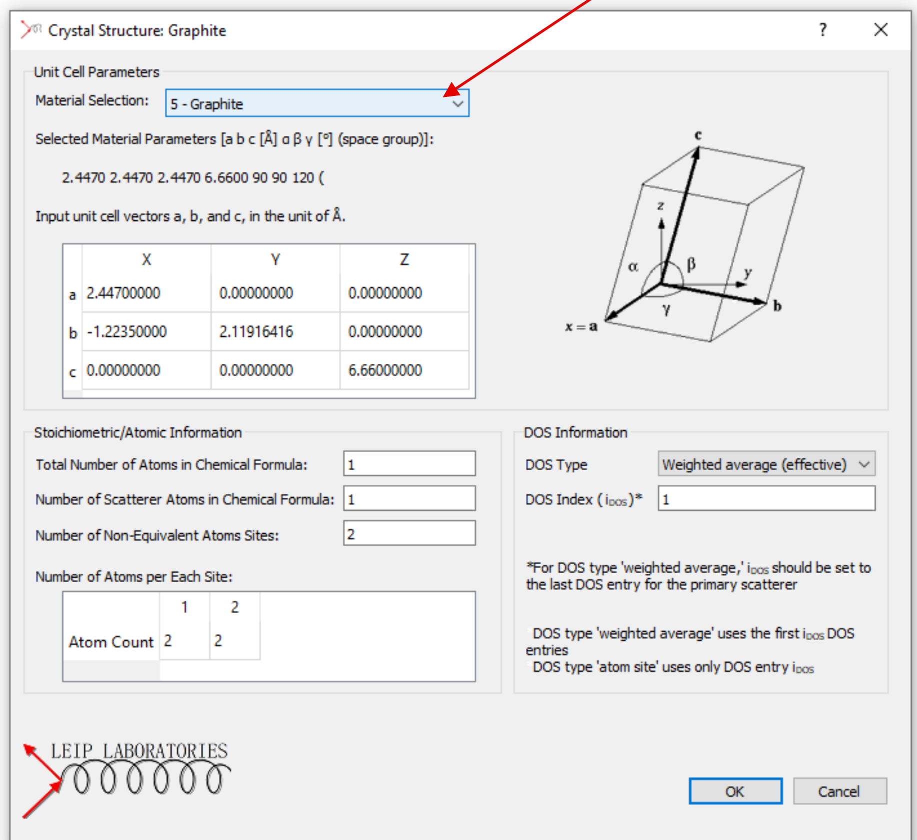
Required User Input

FLASSH

- ***FLASSH* GUI**
  - Crystal Structure (Defaults Shown)



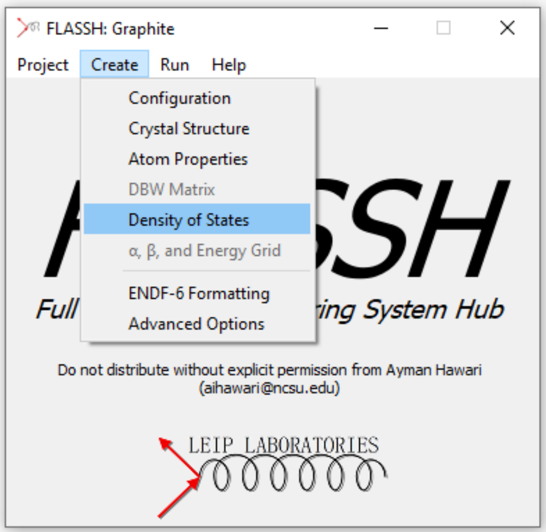
Required
User Input

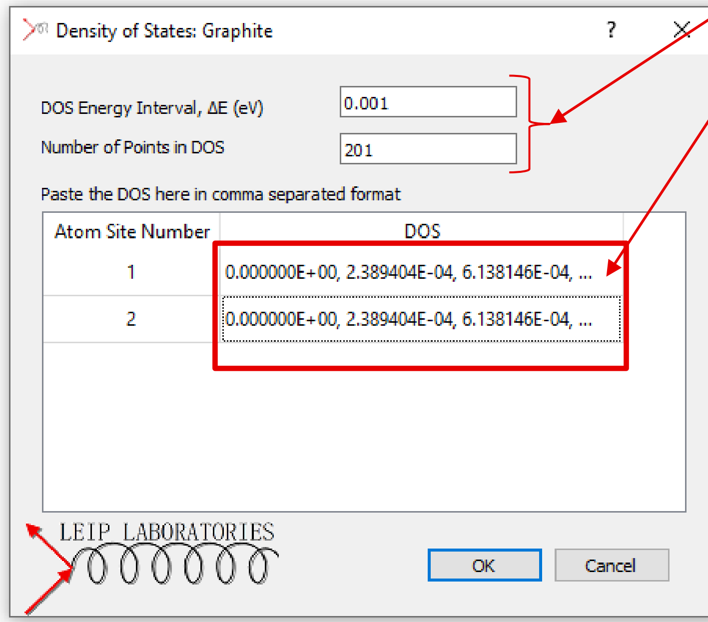


FLASSH

- ***FLASSH* GUI**
  - Density of States

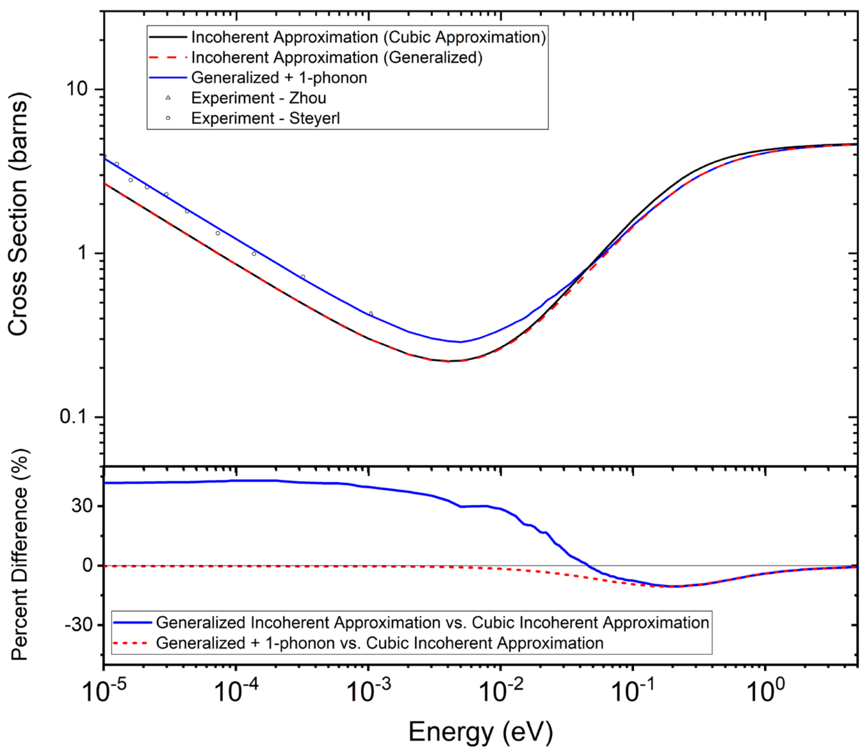
Required User Input



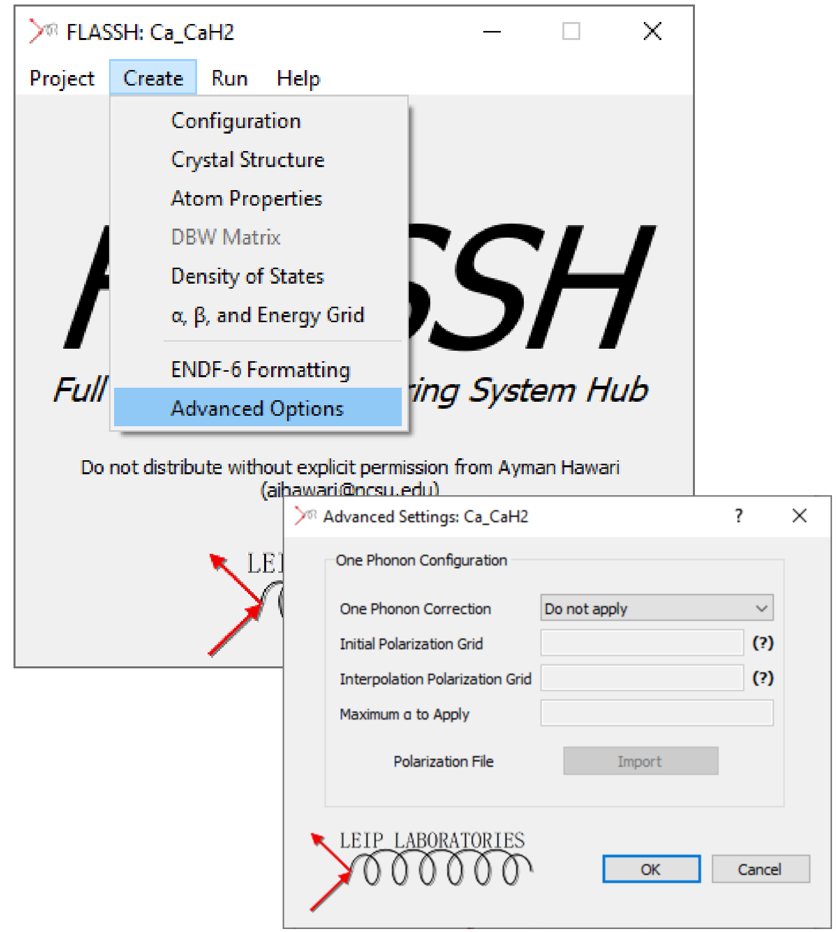


FLASSH

- **Distinct TSL – 1st Order Inelastic**
  - Any material structure
  - Generalized inputs
  - Additional inputs: polarization file

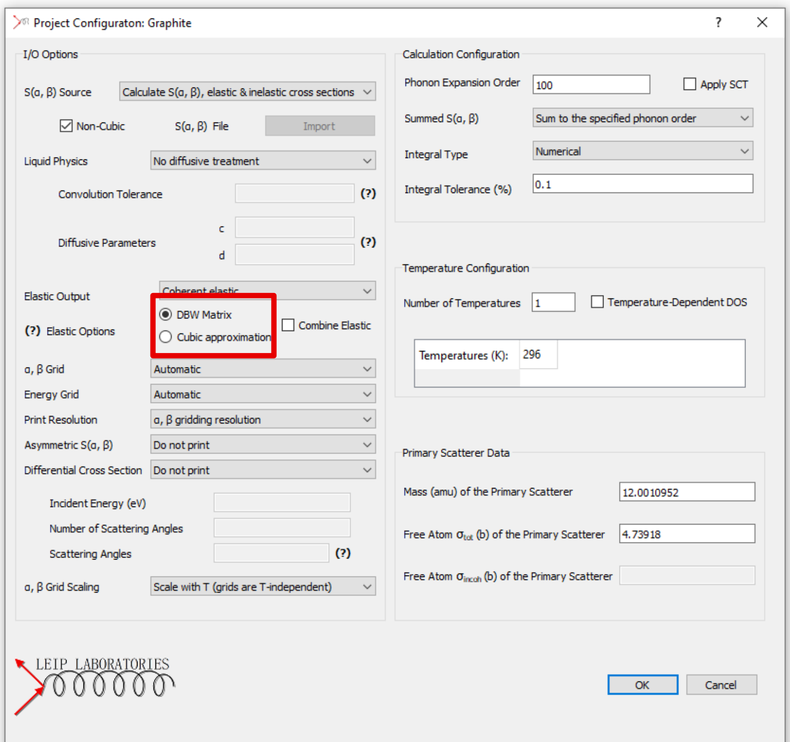


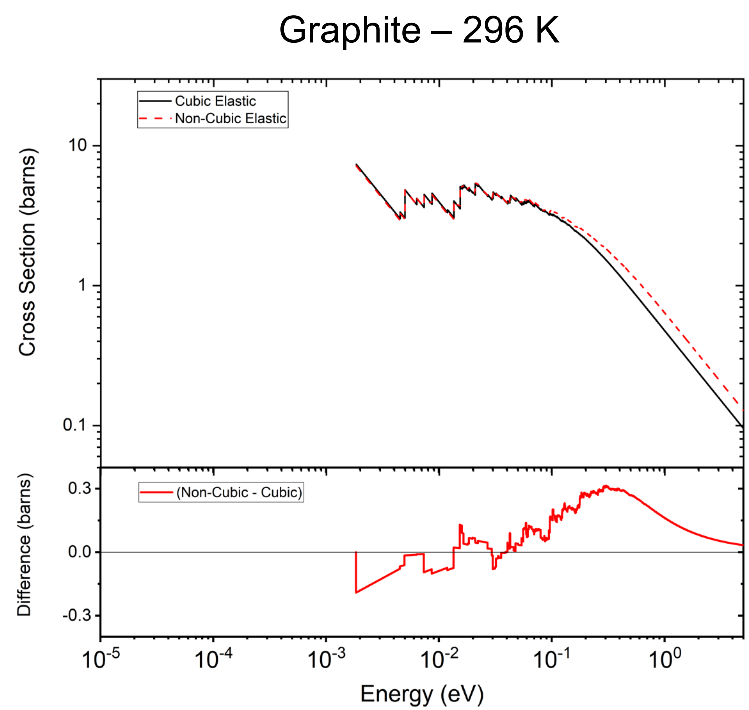
Graphite Cross Section Data



FLASH

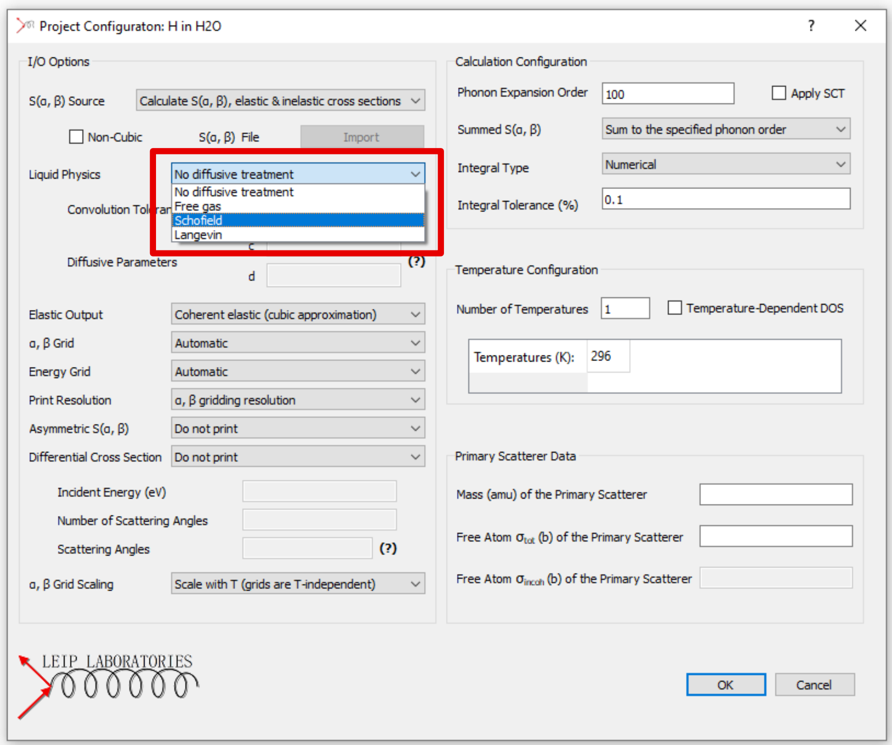
- **Generalized Elastic**
  - Any material structure
- Coherent and Incoherent





FLASSH Liquids

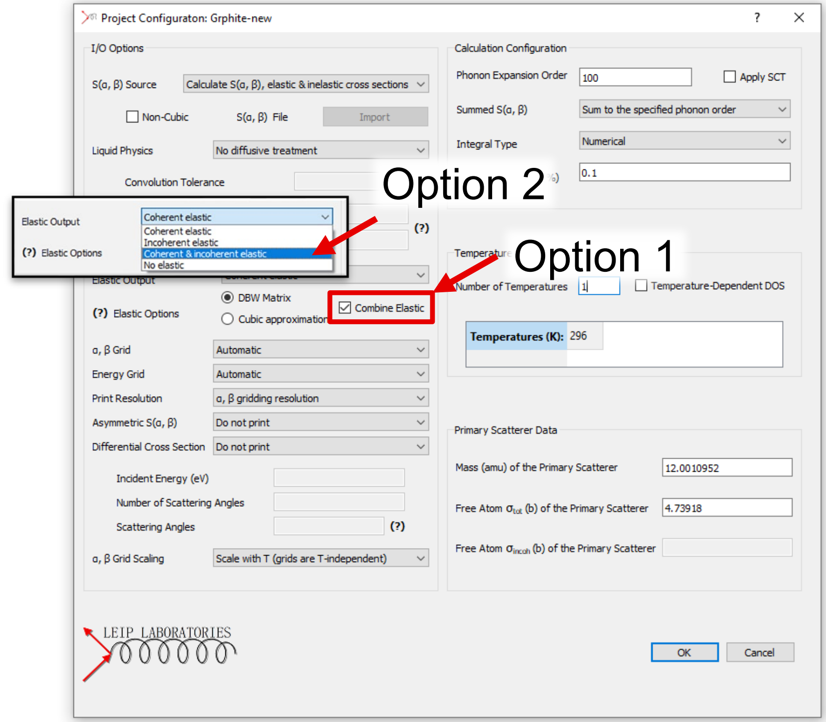
- Results from other codes are improved and even more are made possible with *FLASSH* Liquid Physics (LP)



FLASSH

Elastic Scattering Format Options

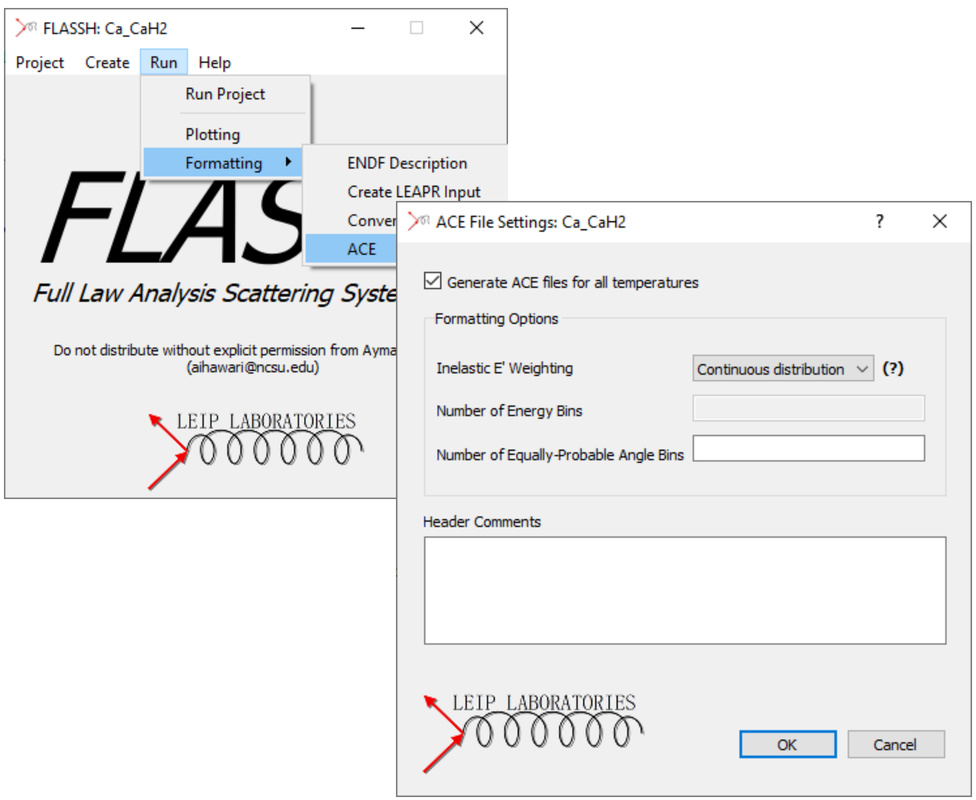
- Compounds and nuclides exhibiting Coherent and Incoherent Elastic
  - Examples: UN
- **Option 1: Current ENDF-6 Format**
  - Calculates the total coherent elastic for the compound and stores the total coherent elastic in the ENDF file for one of the elements
  - Calculates the incoherent elastic and stores the incoherent elastic in the ENDF file for the other element
  - PROS: Works within the current ENDF-6 formatting standards
  - CONS: Must be a compound, element information is lost
- **Option 2: Mixed Elastic Scattering Format**
  - Allows the coherent and incoherent elastic for a given element to be stored in a single ENDF file
  - Updated header options in the ENDF file
  - Print both coherent and incoherent elastic in MF=7, MT=2
  - PROS: Exact information stored with no limits for a give material
  - CONS: Update required to ENDF formatting standard and associated codes which use standard ENDF format inputs



FLASSH

ACE Output Capability

- *FLASSH* generated ACE files are directly compatible with codes such as MCNP
- High resolution cross sections without requiring transfer of files




```
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      0         0.     0         0.     0         0.     0         0.
      0         0.     0         0.     0         0.     0         0.
      0         0.     0         0.     0         0.     0         0.
   334050        3        15        16         3        15         1         0
        0        0         0         0         0         0         0         0
        1     1146      2290    313458    314603    315747         0         0
        0        0         0         0         0         0         0         0
        0        0         0         0         0         0         0         0
        0        0         0         0         0         0         0         0
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   4.0000000000E-11   5.0000000000E-11   6.0000000000E-11   7.0000000000E-11
   8.0000000000E-11   9.0000000000E-11   1.0000000000E-10   2.0000000000E-10
   3.0000000000E-10   4.0000000000E-10   5.0000000000E-10   6.0000000000E-10
   7.0000000000E-10   8.0000000000E-10   9.0000000000E-10   1.0000000000E-09
   2.0000000000E-09   3.0000000000E-09   4.0000000000E-09   5.0000000000E-09
   6.0000000000E-09   7.0000000000E-09   8.0000000000E-09   9.0000000000E-09
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   1.4000000000E-08   1.5000000000E-08   1.6000000000E-08   1.7000000000E-08
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```
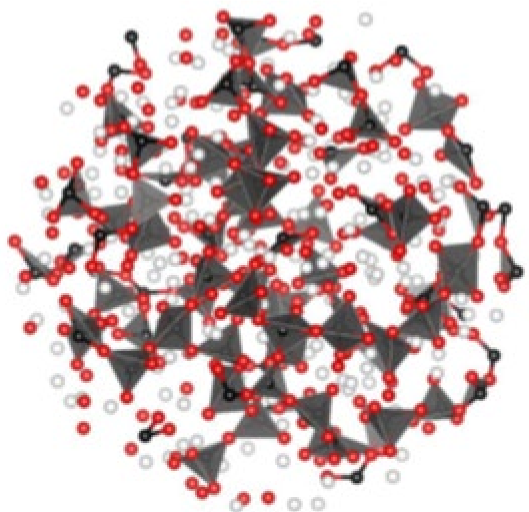
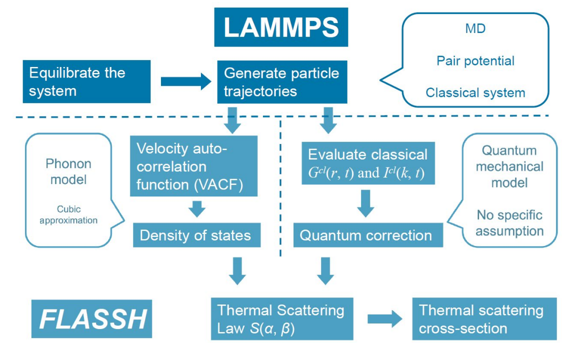
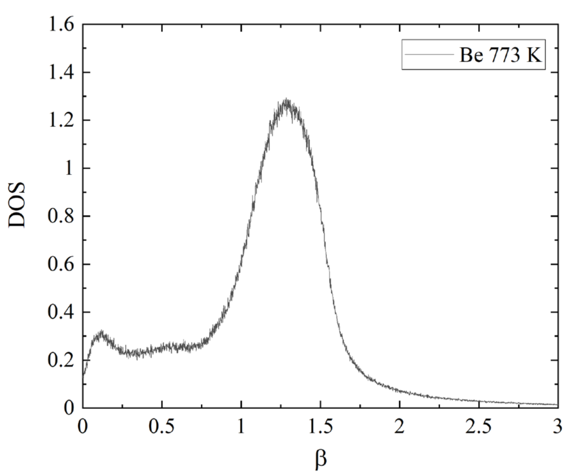

Contributed TSL Evaluations

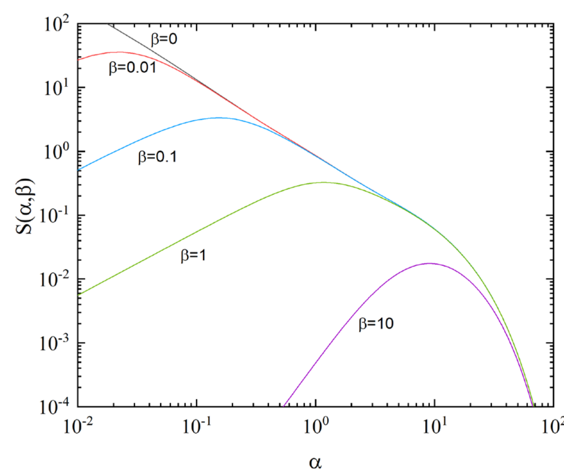
Material	Motivation	Theory	Validation
FLiBe (beyllium) **FLiBe (flourine)** **FLiBe (lithium)**	DOE NE Advanced nuclear reactors No TSL data in ENDF/B-VIII.0	MD *FLASSH*	Ongoing against IRPhEP benchmark
Liquid hydrogen fluoride (hydrogen)	NCSP applications No TSL data in ENDF/B-VIII.0	MD *FLASSH*	Ongoing total cross section
Heavy oil (hydrogen)	NCSP/NR applications No TSL data in ENDF/B-VIII.0	MD *FLASSH*	Ongoing total cross section
Sapphire (Al in Al2O3) **Sapphire (O in Al2O3)**	Neutron science / Research Reactors No TSL data in ENDF/B-VIII.0 (cryogenic temperatures)	DFT/LD *FLASSH*	Total cross section
Polyethylene (hydrogen)	NCSP applications Extended ENDF/B-VIII.0 to cryogenic temperature	MD *FLASSH*	Total cross section & benchmarks

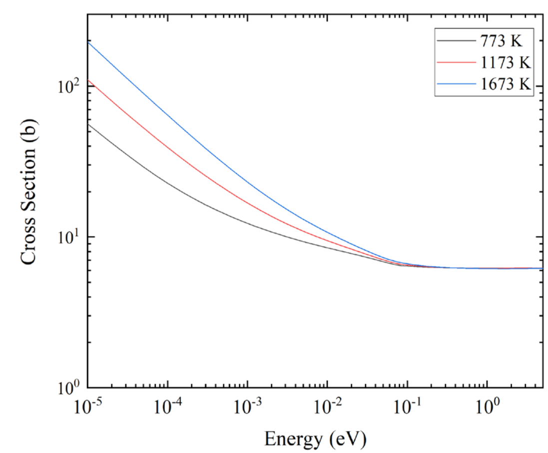
Molten Salt FLiBe Data
(Advanced/Micro Reactors)











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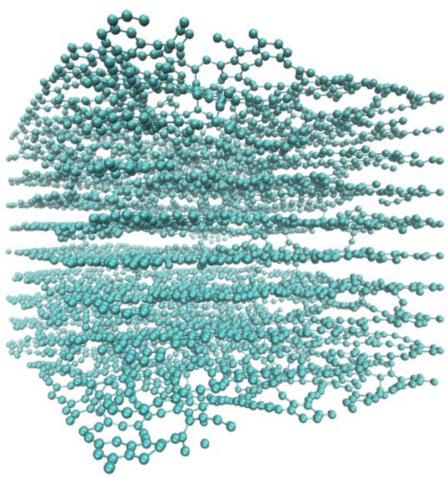
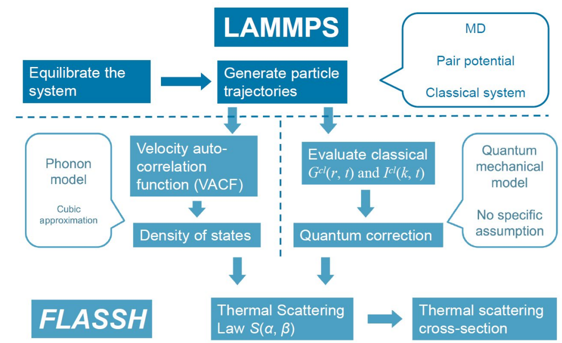
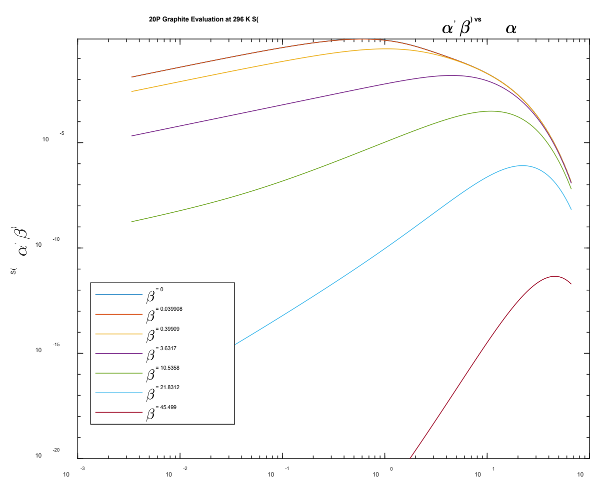
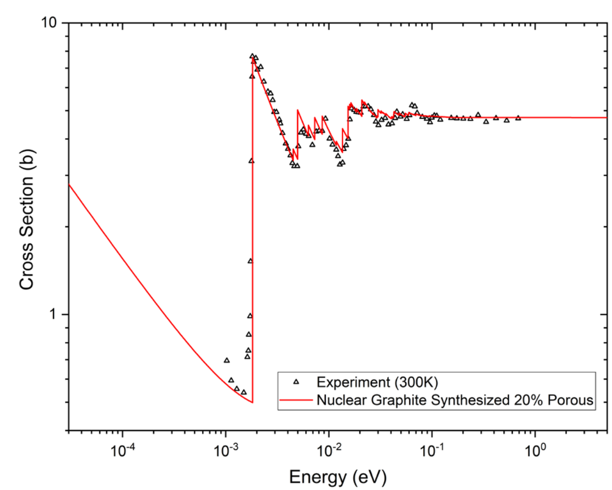
20% Porous Nuclear Graphite
(Advanced/Micro Reactors)









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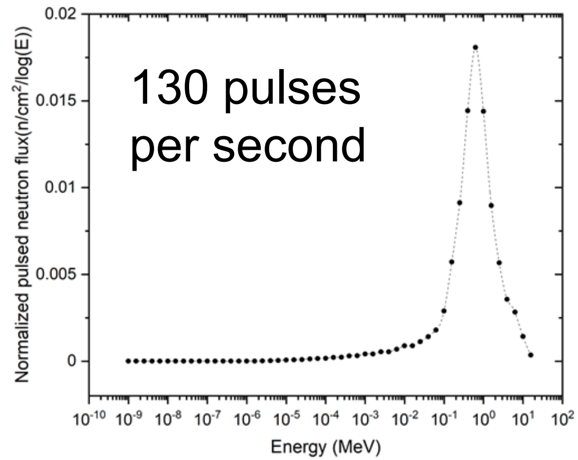
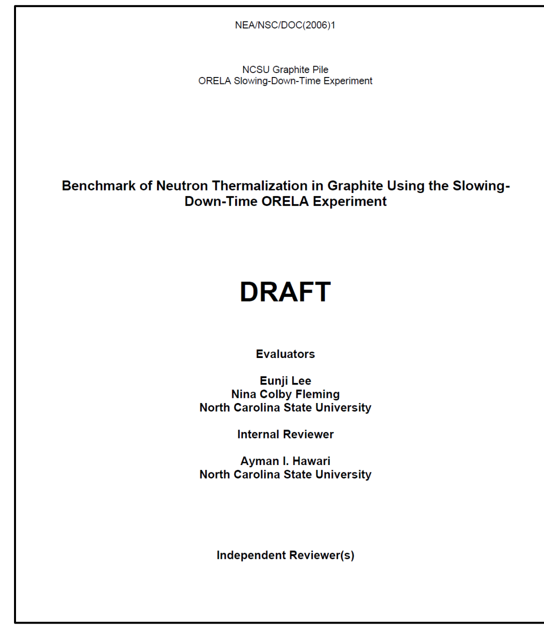
Graphite Slowing-Down-Time Benchmark





NEA/NSC/DOC(2006)1

NCSU Graphite Pile
ORELA Slowing-Down-Time Experiment

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

DRAFT

Evaluators

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Internal Reviewer

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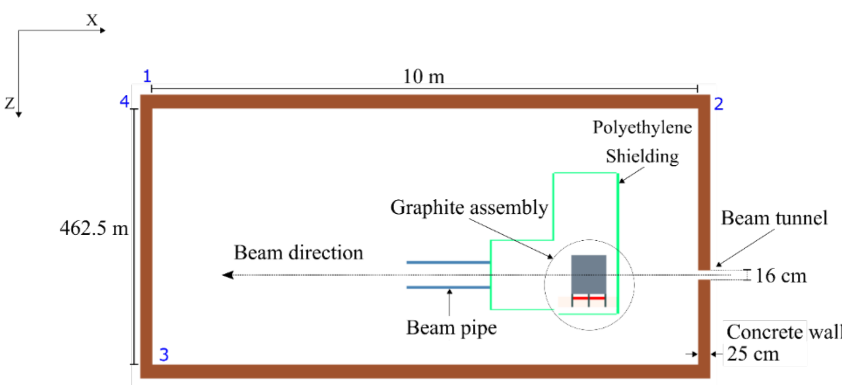
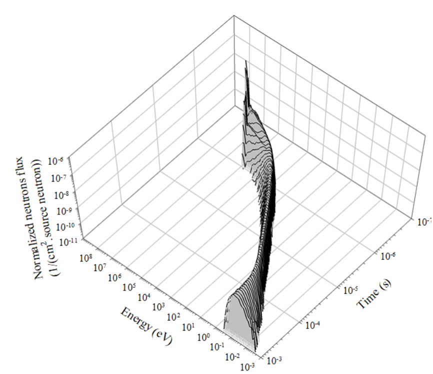
Independent Reviewer(s)





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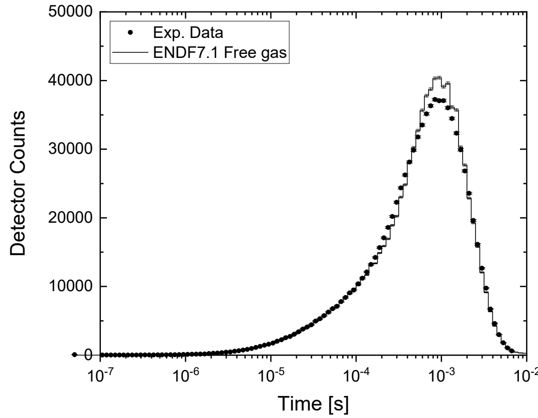
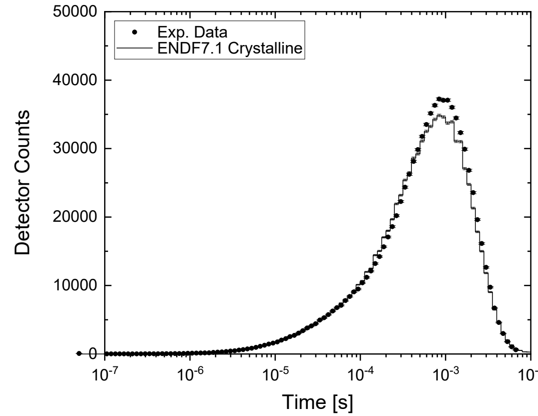
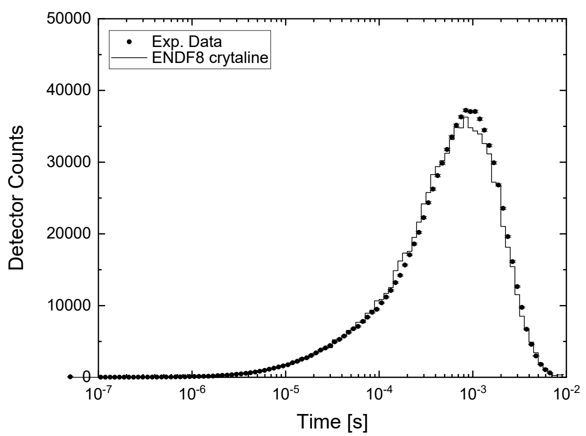
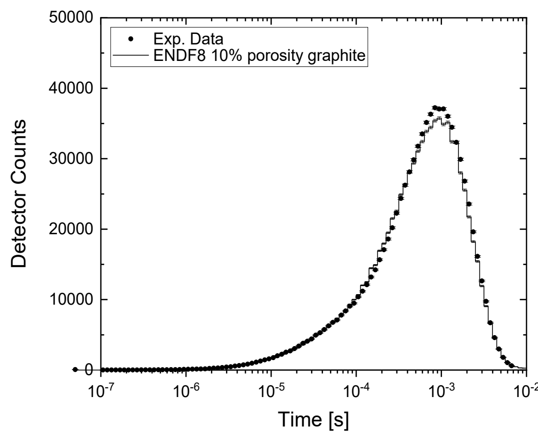
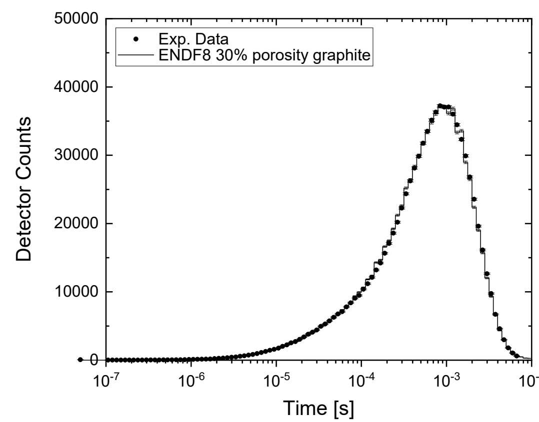
Graphite Slowing-Down-Time Benchmark



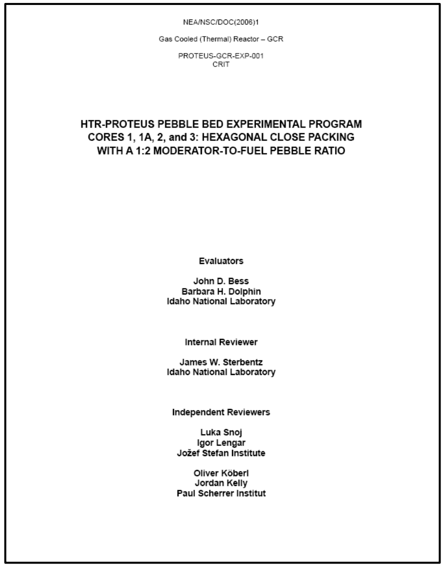








Graphite
PROTEUS Benchmark


NEA/NSC/DOC(2006)1
Gas Cooled (Thermal) Reactor – GCR
PROTEUS-GCR-EXP-001
CRIT

HTR-PROTEUS PEBBLE BED EXPERIMENTAL PROGRAM
CORES 1, 1A, 2, and 3: HEXAGONAL CLOSE PACKING
WITH A 1:2 MODERATOR-TO-FUEL PEBBLE RATIO

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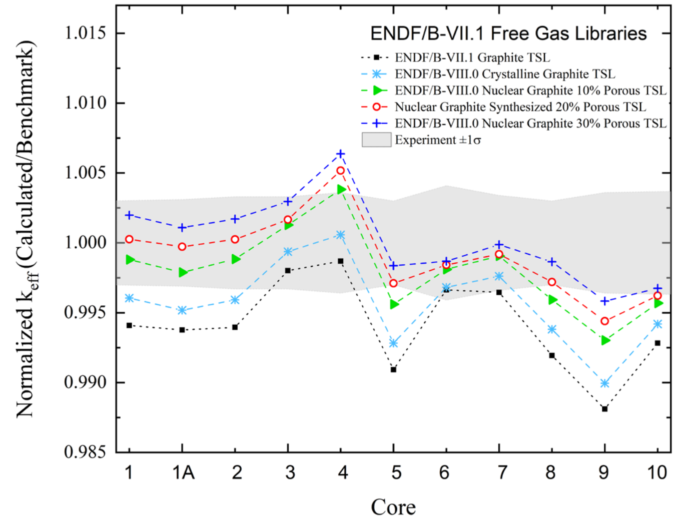

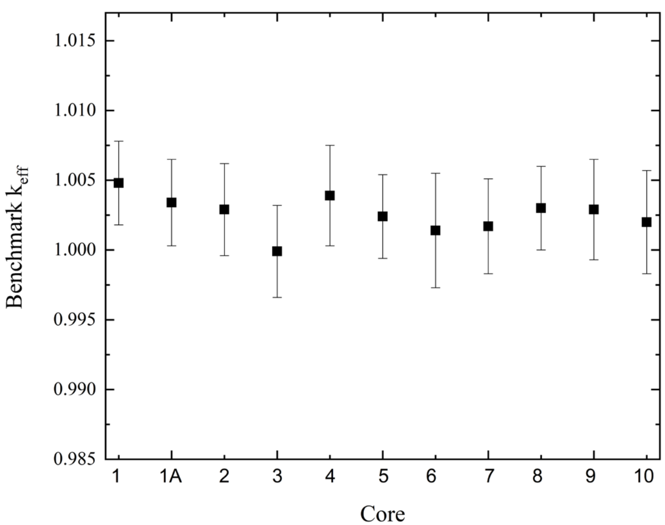

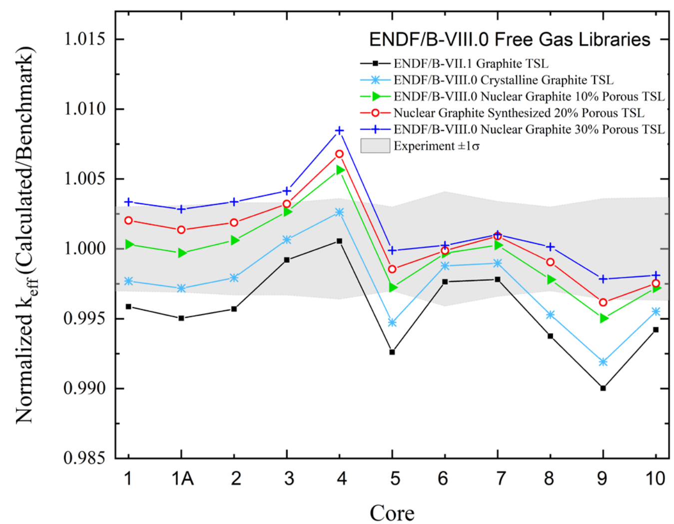

Graphite
VHTRC Testing - JAEA

JOURNAL OF NUCLEAR SCIENCE AND TECHNOLOGY
https://doi.org/10.1080/00223131.2021.1899997

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ARTICLE

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

Shoichiro Okita[a], Yasunobu Nagaya[b] and Yuji Fukaya[a]

[a]Sector of Fast Reactor and Advanced Reactor Research and Development, Japan Atomic Energy Agency, Ibaraki, Japan; [b]Nuclear Science and Engineering Center, Japan Atomic Energy Agency, Ibaraki, Japan

ABSTRACT

The latest ENDF/B-VIII library adapted new porosity-dependent cross-section data of graphite. However, the porosity of the actual graphite does not necessarily correspond to the porosity given in the data. We have proposed a method to perform neutronic calculations at the desired porosity on the basis of the pseudo-material method. We have also compared the k_{eff} values calculated by the pseudo-material method with the experimental values for the VHTRC. In addition, we have investigated the temperature dependance of the calculation values obtained by this method. From these results, we have concluded that this method allows us to perform the neutronic calculations in which we can reflect detailed information on the porosity of graphite.

ARTICLE HISTORY
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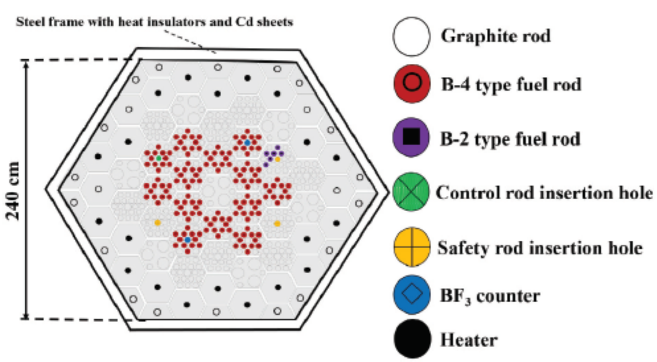
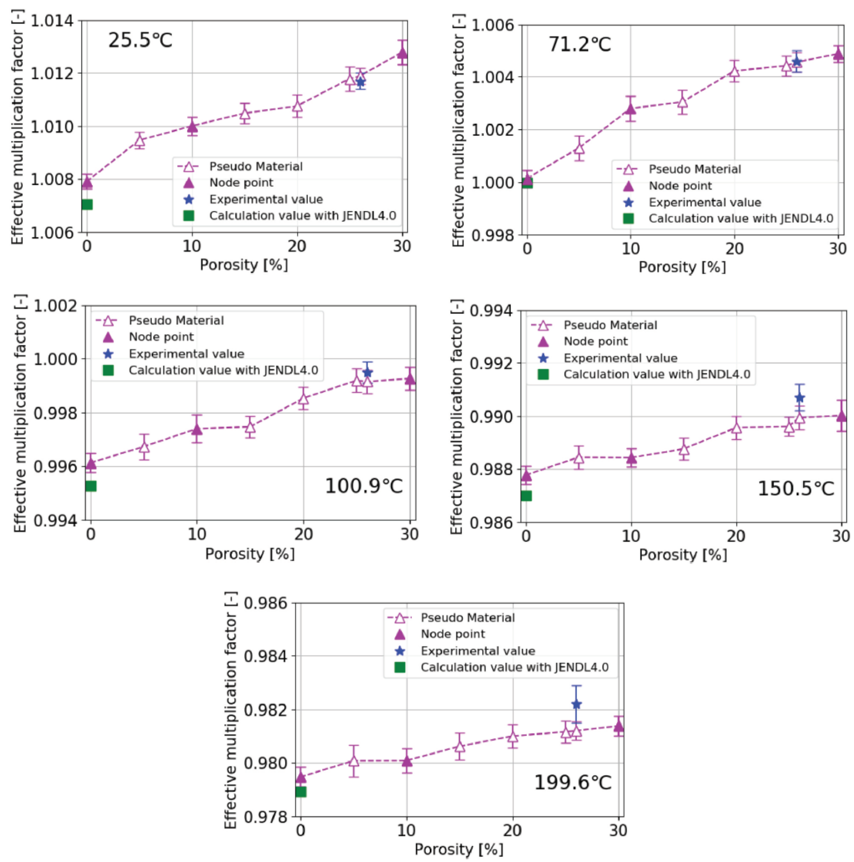
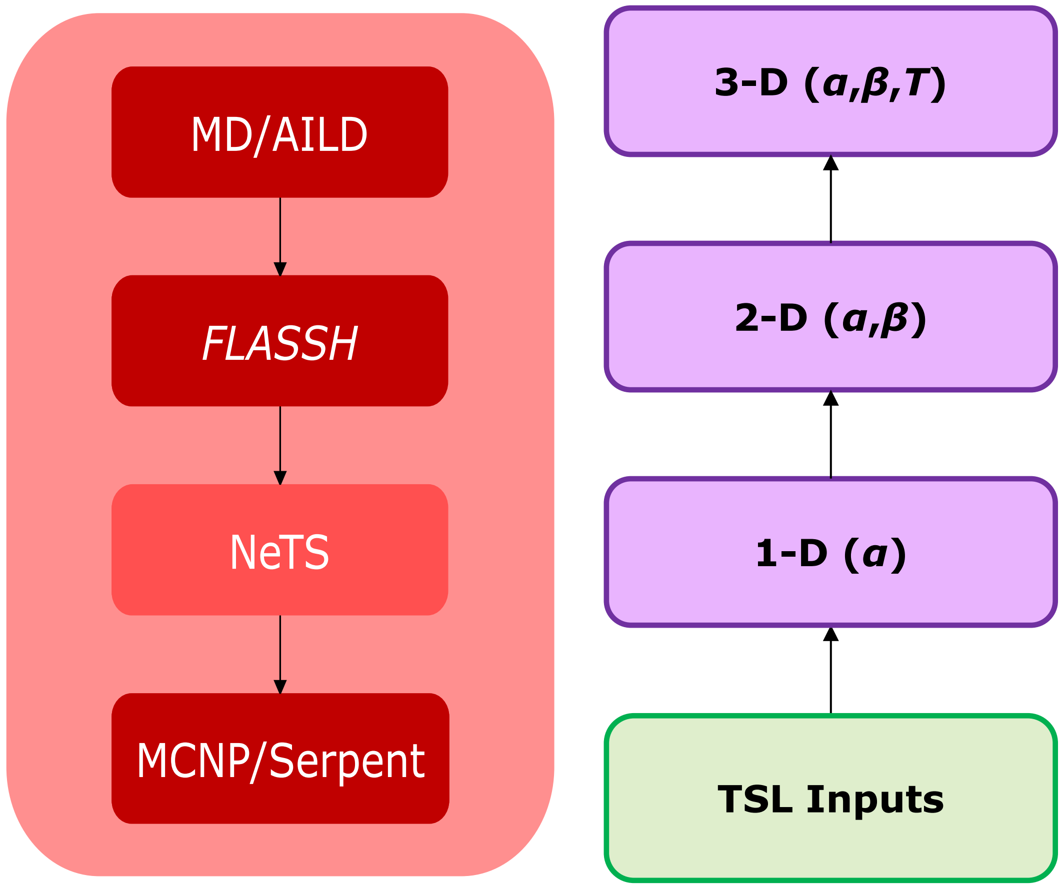
KEYWORDS
ENDF/b-viii; graphite; porosity-dependent cross-section data; vhtrc; pseudo-material method





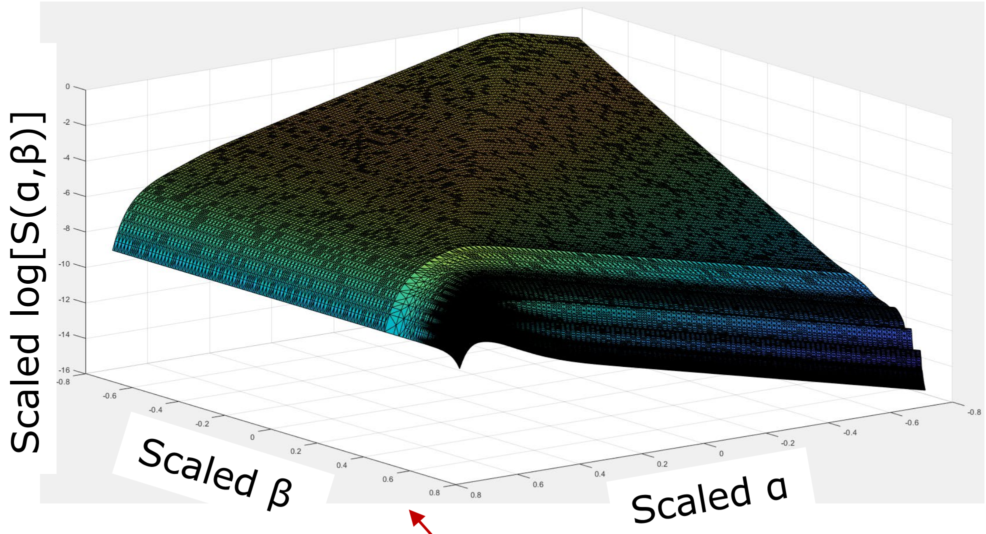
Neural Thermal Scattering (NeTS)

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



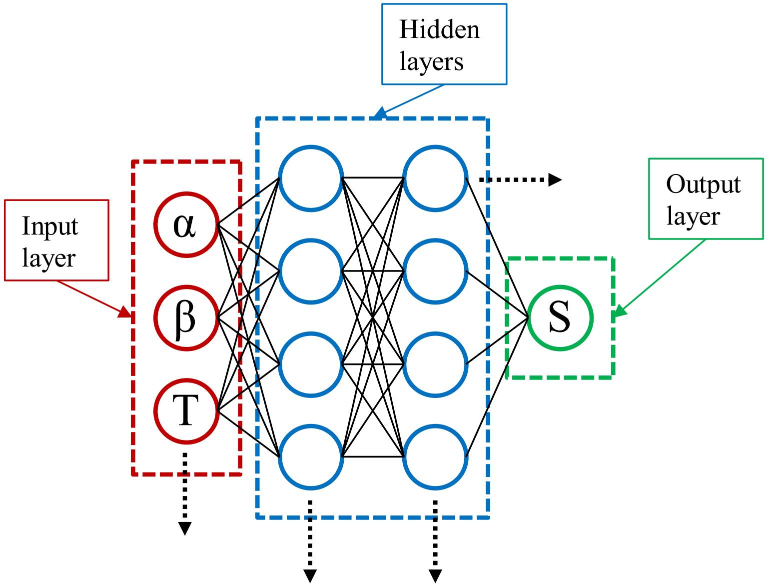
PyTorch

Example NeTS Output



2-D prediction surface
(corresponding to lowest temperature)

- Current model size describing full T range is ~100kB compared to tens of MBs for typical, discrete T evals.



- Accuracy levels for 2/3-D cases of <1% median deviations and single-digit max % deviations

- Optimizing network architecture (activation, hidden layers, etc.)

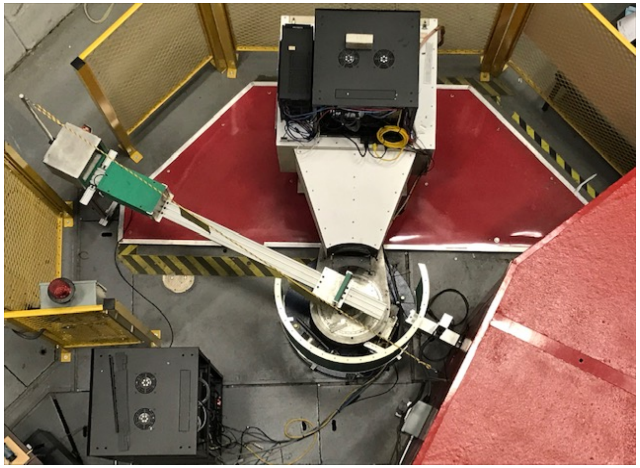
LEIP LABORATORIES

Measurements at PULSTAR Reactor

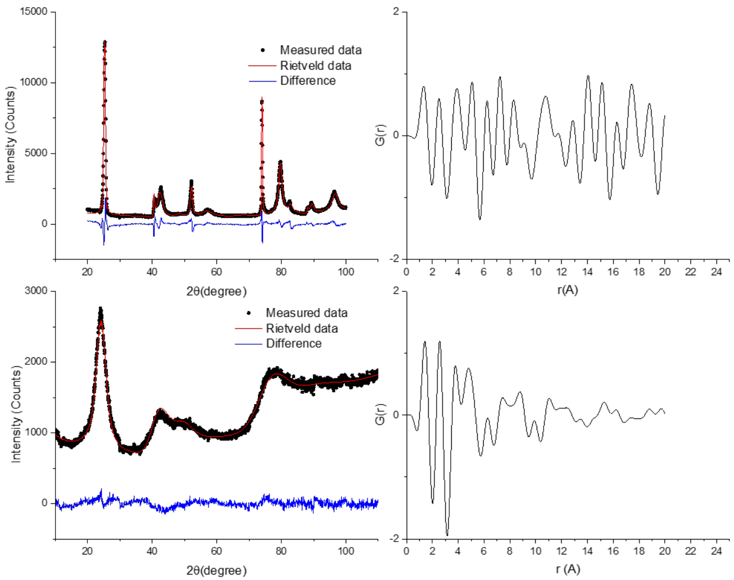
NPDF –Dual Purpose:

- **Diffraction/PDF Measurements:**

  15 New Position Encoding Modules (PEM) – improved diffraction measurement resolution Δd/d of 2.9×10^{-3} for 3mm holder



- **Transmission Measurement Capabilities:**
  - Monochromator capable of providing beam wavelengths of 1.085 Å, 1.180 Å, 1.479 Å, and 1.762 Å
  - Transmission Detection Apparatus with collimator.



❖ Facilities for Nano Materials Examination at the PULSTAR Reactor, AI Hawari, M Liu, Q Cai, PHYSOR 2020

Summary

- TSL activities continue including evaluations and methods development
- Several evaluations are contributed to NNDC
- *FLASSH* testing in the performance of TSL evaluations is underway
- ML/DL NeTS approach is under testing
- Activities in data measurements and benchmark development are underway at NCSU PULSTAR reactor