

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



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	ь 0.00000	4.85945	0.00000				
	c 0.00000	0.00000	4.85945				
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Full L	aw Analysis Sco	attering Sy	stem Hub				
Do no	t distribute without explici (aihawari@	t permission from Incsu.edu)	Ayman Hawari				

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MD approach









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 GUI

Configuration (Defaults Shown)



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LEIP LABORATORIES	OK Cancel	



FLASSH GUI

Crystal Structure (Defaults Shown)

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Project Create Run Help								
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	Cŋ	stal Structure						
Atom Properties								
DBW Matrix								
Density of States								
α, β, and Energy Grid								
Full ENDF-6 Formatting Advanced Options								
								Do not distribute without explicit permission from Ayman Hawari (aihawari@ncsu.edu)
LEIP LABORATORIES								

					Requ User	iired Input		
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FLASSH GUI

Density of States



		Required User Input
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2	0.000000E+00, 2.389404E-04, 6.138146E-04,	
LEIP LABORAT	ORIES	
20000	OK Cancel	



Distinct TSL – 1st Order Inelastic

- Any material structure
- Generalized inputs
- Additional inputs: polarization file







FLASSH

Generalized Elastic

- Any material structure
- Coherent and Incoherent

I/O Options Calculate S(α, β), elastic & inelastic cross sections S(α, β) Source Calculate S(α, β), elastic & inelastic cross sections I Non-Cubic S(α, β) File I Non-Cubic S(α, β) File I Non-Cubic S(α, β) File I Quid Physics No diffusive treatment I Quid Physics No diffusive treatment Convolution Tolerance (?) Diffusive Parameters C C (?) Diffusive Parameters C C (?) Elastic Output Cobsense talestic Cobsense talestic Combine Elastic C(?) Elastic Options Cubic approximation Combine Elastic Print Resolution α, β gridding resolution Asymmetric S(α, β) Io not print Number of Scattering Angles (?) Scattering Angles (?) Scattering Angles (?)	Project Configuraton:	Graphite		? >
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FLASSH Liquids

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

I/O Options Calculator Computation S(α, β) Source Calculate S(α, β), elastic & inelastic cross sections I/O off I/O I/O off Integral Tolerance (%) Integral Tolerance (%) 0.1 Integral Tol	
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Scattering Angles (1)	
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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





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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	6.00000	000000E-09	7.000	00000000E-09	8.	000000000000000000000000000000000000000	-09	9.	000000000	00E-09
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	1.80000	000000E-08	1,900	00000000E-08	2.	0000000000000	-08	2.	100000000	00E-08
	2,20000	000000F-08	2.300	00000000F-08	2.	400000000000	-08	2.	500000000	00F-08
	2.60000	000000E-08	2.700	00000000E-08	2.	800000000000	-08	2.	900000000	00E-08
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	3.80000	000000E-08	3,900	00000000E-08	4.	0000000000000	-08	4.	100000000	00E-08
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	6.60000	000000F-08	6.700	00000000F-08	6.	800000000000	-08	6.	900000000	00F-08
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	7.80000	000000F-08	7,900	00000000F-08	8.	000000000000000000000000000000000000000	-08	8.	100000000	00F-08
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	1.03244	469000F-07	1.036	12882000F-07	1.0	03981296000	-07	1.	043497090	30F-07
	1.04718	123000F-07	1.050	86537000F-07	1.0	05454950000	-07	1.	058233640	00F-07
	1.06191	777000F-07	1.065	60191000F-07	1.	06928604000	-07	1.	072970180	00F-07
	1.07665	432000E-07	1.080	33845000E-07	1.0	08402259000	-07	1	087706720	00E-07
	1.09139	086000E-07	1.095	07500000E-07	1.0	09875913000	-07	1	102443270	00E-07
	1.10304	130000E-07	1.103	63932000E-07	1	10423735000	-07	1.	104835370	00E-07
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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 <i>FLASSH</i>	Ongoing total cross section
Heavy oil (hydrogen)	NCSP/NR applications No TSL data in ENDF/B-VIII.0	MD <i>FLASSH</i>	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 <i>FLASSH</i>	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)









20% Porous Nuclear Graphite (Advanced/Micro Reactors)











Graphite / Slowing-Down-Time Benchmark





Graphite / Slowing-Down-Time Benchmark





Graphite PROTEUS Benchmark





Graphite VHTRC Testing - JAEA

0.996

0.994

Effectiv

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



Check for upda

ARTICLE

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

Shoichiro Okita 100°, Yasunobu Nagaya^b and Yuji Fukaya^a

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ABSTRACT

The latest ENDF/8-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_{atr} values calculated by the pseudo-material method with the experimental values for the VITRC. 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.

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Accepted 26 February 2021 **KEYWORDS** ENDF/b-vili; graphite; porosity-dependent crosssection data; vhtrc; pseudomaterial method





20

Porosity [%]

10









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



(corresponding to lowest temperature)

 Accuracy levels for 2/3-D cases of <1% median deviations and single-digit max % deviations Current model size describing full T range is ~100kB compared to tens of MBs for typical, discrete T evals.



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



Measurements at PULSTAR Reactor

NPDF – Dual Purpose:

Diffraction/PDF Measurements: 15 New Position Encoding Modules (PEM) – improved diffraction measurement resolution ∆d/d of 2.9x10⁻³ 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, Al 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