#### Nuclear Data Week

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#### Status of TSL Code Development at NCSU

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#### Outline

- Overview of Code Development
- □ Inelastic Scattering under Incoherent Approximation
- Coherent Inelastic Scattering with One-phonon Correction
- Coherent Elastic Scattering with Debye-Waller matrix
- □ Summary

#### Code Flow



#### Code Features

	LEAPR+THERMR	New Code
Coherent inelastic	N/A	Implemented
Coherent elastic	Approximate	Exact
Short Scattering Time (SCT) approximation	Yes	Νο
Integral against a differential cross section	Numerical	<b>Default: Analytical</b> Optional: Numerical
a, β gridding	User input	Default: Automatic grid Optional: User input
Parallel Computing	N/A	<b>Yes</b> Using OpenMP
Graphic User Interface	N/A	Yes

#### Evaluation Example

	Dialog     ? ×	(
■ Home – □ × File Create Run ENDF Plot	Paste density of states below 0.0000E+00 7.2477E-04 3.7084E-03 8.0087E-03 1.0642E-02 1.5897E-02 2.7272E-03 4.1847E-03 E-0314E-03 6.5036E-03 8.2674E-03 0.0339E-03	
LEIP LABORATORIES	2.7372E-02 4, 1843E-02 6, 0214E-02 6, 5036E-02 8, 3674E-02 9, 9329E-02 1. 1977E-01 1, 4296E-01 1, 6484E-01 1, 8945E-01 2, 1887E-01 2, 3537E-01 2.6166E-01 3, 0003E-01 3, 4054E-01 3, 8728E-01 4, 2481E-01 4, 7598E-01 5, 1890E-01 5, 7400E-01 6, 2970E-01 6, 5754E-01 7, 2042E-01 7, 9118E-01 8.6756E-01 9, 2948E-01 1,0030E+00 1, 1163E+00 1, 2048E+00 1, 2870E+00 1.4139E+00 1, 5249E+00 1, 6221E+00 1, 7638E+00 1, 8924E+00 2, 0388E+00 2.2056E+00 2, 3709E+00 2, 5558E+00 2, 7595E+00 3, 0108E+00 3, 2603E+00 3.5066E+00 3, 7442E+00 4, 0667E+00 4, 3677E+00 4, 7164E+00 5, 0820E+00 5.5881E+00 6, 0898E+00 6, 5510E+00 7, 0877E+00 7, 164E+00 1, 0736E+00 8.6232E+00 9, 2283E+00 9, 9334E+00 1, 0613E+01 1, 1278E+01 1, 1973E+01 1.2784E+01 1, 3744E+01 1, 4739E+01 1, 5918E+01 1, 7654E+01 1, 9834E+01 2.1455E+01 2, 2574E+01 2, 3744E+01 2, 4900E+01 2, 6227E+01 2, 7931E+01 2.9747E+01 2, 9884E+01 2, 7358E+01 2, 4817E+01 2, 3690E+01 2, 3242E+01 2.3624E+01 2, 3473E+01 2, 3647E+01 2, 3681E+01 2, 0724E+01 2, 1121E+01 2.4240E+01 2, 7607E+01 2, 7643E+01 2, 5431E+01 2, 3755E+01 2, 3377E+01 2.3410E+01 2, 3504E+01 2, 3647E+01 2, 3681E+01 2, 3805E+101 2, 3377E+01 2.3385E+01 2, 3050E+01 2, 2244E+01 2, 1008E+01 1, 9536E+01 1, 3841E+01 1.8075E+01 1, 8606E+01 1, 9599E+01 2, 1037E+01 2, 3193E+01 2, 4016E+01 2.3573E+01 2, 5664E+01 3, 0187E+01 3, 1256E+01 2, 7257E+01 2, 2765E+01 1.4893E+01 6, 8192E+00 3, 8444E+00 2, 4718E+00 1, 3358E+00 3, 5968E-01 0,0000E+00	
	LEIP LABORATORIES OK Cancel	

#### Evaluation Example

L' Input File			ŕ ×
			-
Elastic Output	O Incoherent Elastic	Coherent Elastic with Debye-Waller Matrix method	O Coherent Elastic with cubic approximation
Output	Output standard phonon summed S(α, β)	<ul> <li>Output nth phonon order only S(a, β)</li> </ul>	
Alpha, Beta Grid	🔘 Use user input alpha, beta grid	<ul> <li>Use automatic alpha, beta grid</li> </ul>	
Print Resultion	$\bigcirc$ Print full resolution symmetric S(a, $\beta$ ) in output file	Print input grid resolution symmetric S(a, β) in output file	
Print Symmetry	Do not print asymmetry S(α, β)	<ul> <li>Print asymmetry S(α, β)</li> </ul>	
Differential Xsection	Do not print differential cross section	<ul> <li>Print secondary energy differential cross section</li> </ul>	O Print angular differential cross section
Incident Energy			
Indicite Energy			
Integral Type	Analytical integration	<ul> <li>Numerical integration</li> </ul>	
Scatterer	1		
Maximum Phonon	100		
Plaximant Honor	100		
Number of Temperatures	1		
hander of reliperatored	1		
List of Temperatures	300		
	300		
One Phonon Output	$\bigcirc$ Do not use one phonon S(a, B) correction	O Use one phonon S(a, β) correction	
ENDF Output	O Do not output ENDF library file	Output ENDF library file	
	,	<u> </u>	
Material Number	26		
Number of Elements	1 (Number of elements in chem	nical formula)	
	[] ``		
Chemical Formula	1		
AMU Mass	9.012182		
Free Atom Cross Section	6.153875 (Free atom cross section in t	he unit of barn)	OK Cancel
LEID LABORATORIE	29		
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/000000	)		

#### Evaluation Example



### Scattering Law $S(\alpha, \beta)$



#### Differential Scattering Cross Section



#### Integrated Cross Section



## Coherent inelastic one-phonon correction routine

	New Code
Supported structure	Any crystal structure
Supported material	Any material
Compound material	Yes
Debye-Waller Factor	Exact
Polarization vector	Exact
Sampling of the full reciprocal space	Yes
Structure Factor	Exact

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# One-phonon Corrected Scattering Law $S(\alpha, \beta)$



#### Coherent Elastic Routine

	LEAPR	New routine
Supported structure	Hexagonal, FCC, BCC	Any crystal structure
Supported material	Graphite, beryllium, beryllium oxide, aluminum, lead, iron	Any material
Compound material	2 elements with ratio 1:1	Any number of elements with any ratio
Cubic Approximation	Yes	Νο
Atom sites approximation	Yes	Νο
Coherent Elastic Scattering Cross Section	Over Ewald Sphere	On every reciprocal lattice point
Need to modify source code if calculating other materials	Yes	Νο

# Coherent Elastic Cross Section of $\alpha$ -SiO<sub>2</sub>



The calculation shows around 15% divergence at low and high energies between the two methods in the cross sections of a-SiO<sub>2</sub>.



#### Code Implementation

- Calculations and ENDF TSL library formatting modules were implemented by FORTRAN 95 using modulus design
- □ MF=1, MT=451 formatting was done by Python
- □ Parallel computing was realized by OpenMP 4.0 bindings
- GUI implemented by cross platform QT® C++ API

#### Summary

- □ The more general coherent elastic and coherent inelastic calculation routines were implemented.
- Approximations such as SCT approximation, cubic approximation, atom site approximation and incoherent approximation were removed or relaxed in the new code.
- Tested the new code by comparing to NJOY result and experimental measurements.
- The new code is designed using modern C++ and FORTRAN95 language with GUI and parallel computation capability.