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Status of TSL Code Development at NCSU

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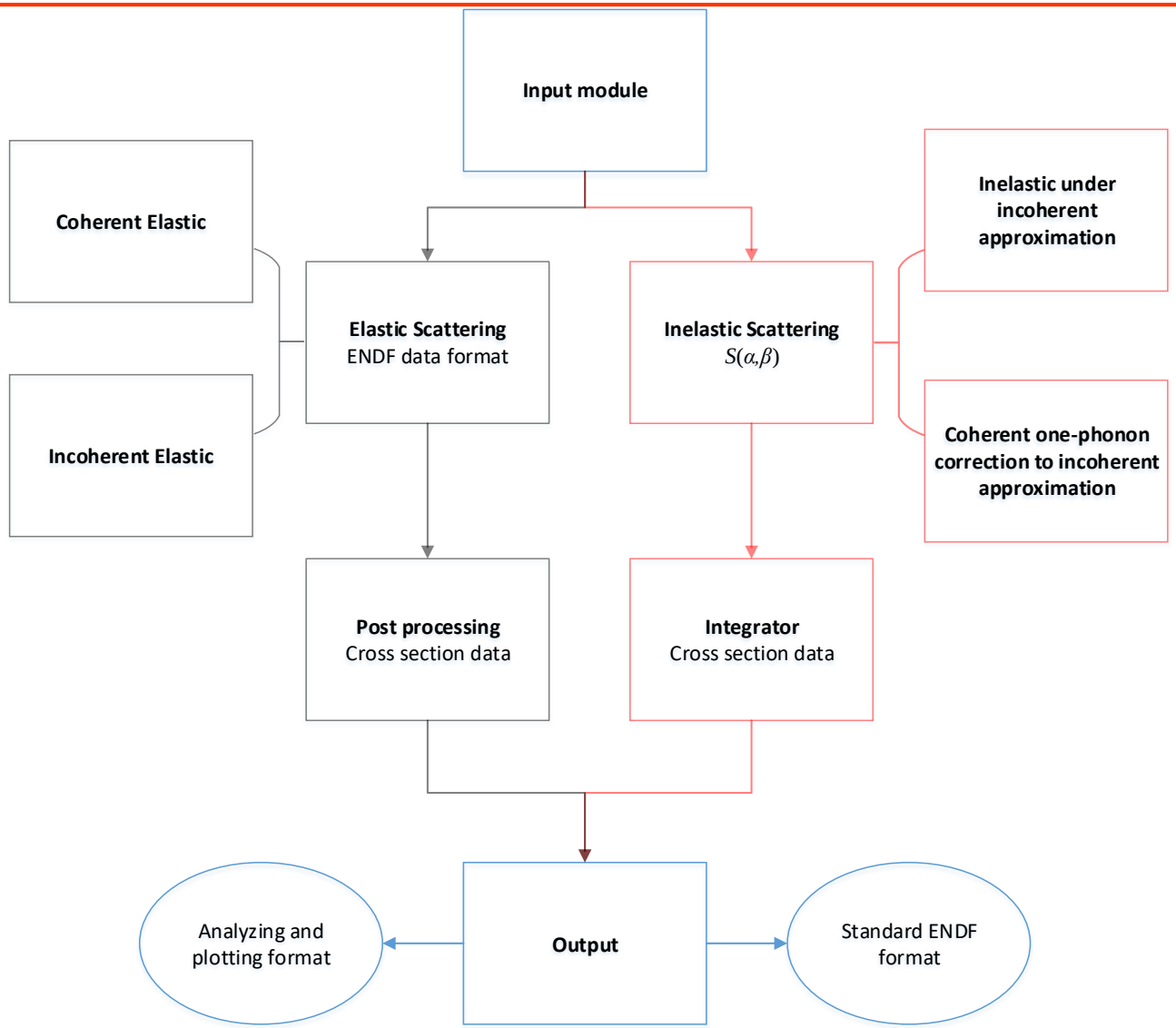
Outline

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

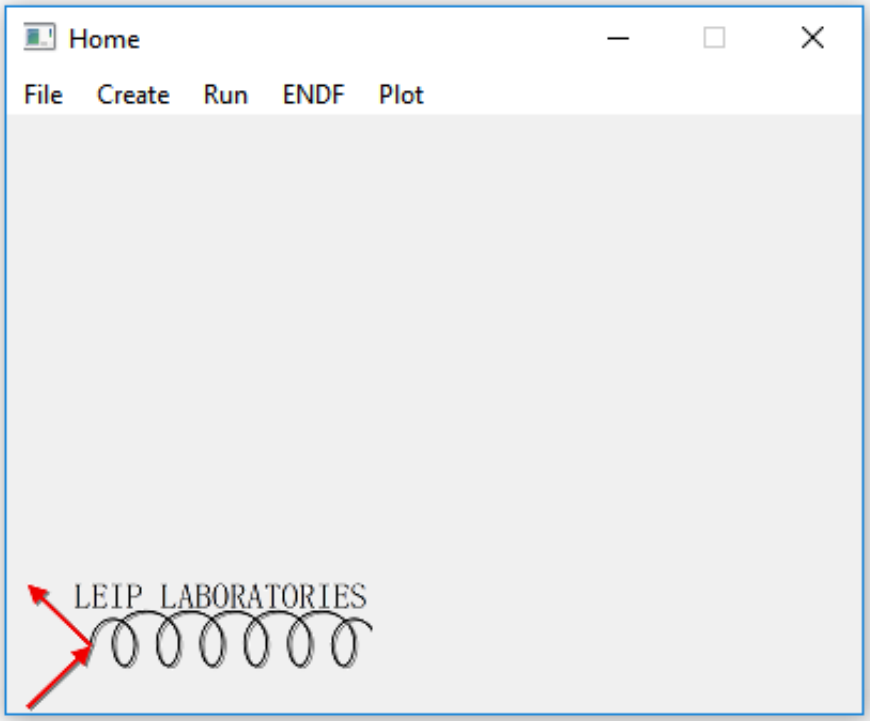
Code Flow

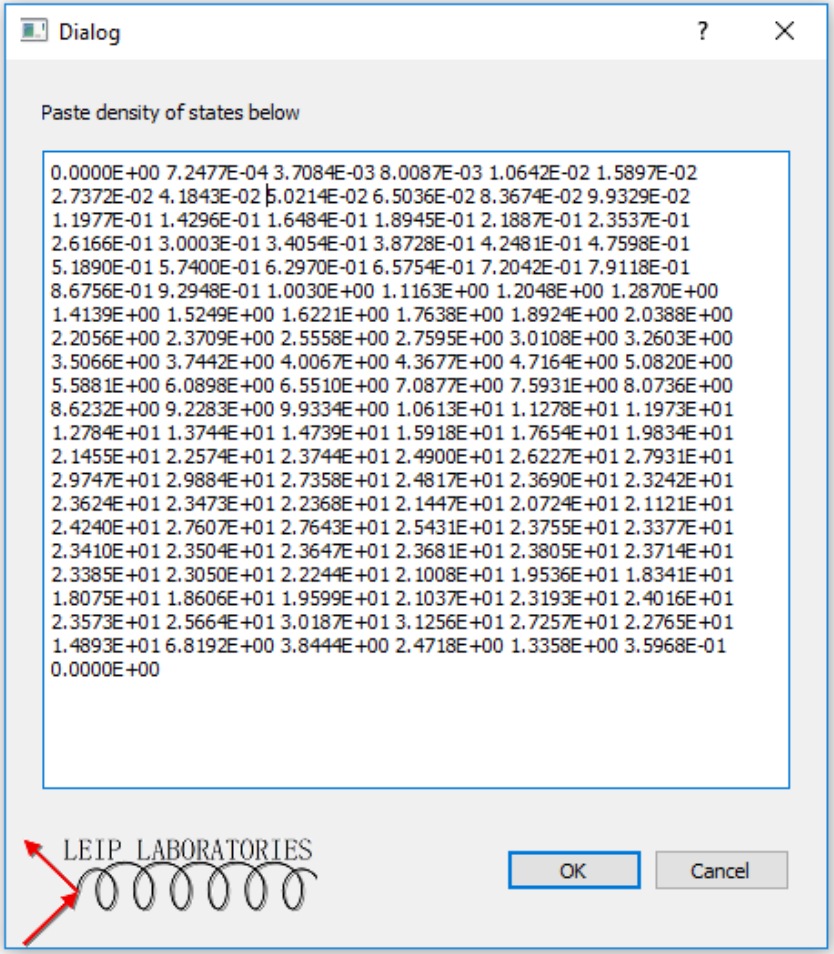

Input module
Coherent Elastic
Incoherent Elastic
Elastic Scattering
ENDF data format
Inelastic Scattering
$S(\alpha,\beta)$
Inelastic under incoherent approximation
Coherent one-phonon correction to incoherent approximation
Post processing
Cross section data
Integrator
Cross section data
Analyzing and plotting format
Output
Standard ENDF format

Code Features

	LEAPR+THERMR	New Code
Coherent inelastic	N/A	Implemented
Coherent elastic	Approximate	Exact
Short Scattering Time (SCT) approximation	Yes	No
Integral against α differential cross section	Numerical	**Default: Analytical** Optional: Numerical
α, β gridding	User input	**Default: Automatic grid** Optional: User input
Parallel Computing	N/A	**Yes** Using OpenMP
Graphic User Interface	N/A	Yes

Evaluation Example





Evaluation Example

Input File

Elastic Output	○ Incoherent Elastic	◉ Coherent Elastic with Debye-Waller Matrix method	○ Coherent Elastic with cubic approximation
Output	◉ Output standard phonon summed S(α, β)	○ Output nth phonon order only S(α, β)	
Alpha, Beta Grid	○ Use user input alpha, beta grid	◉ Use automatic alpha, beta grid	
Print Resultion	○ Print full resolution symmetric S(α, β) in output file	◉ Print input grid resolution symmetric S(α, β) in output file	
Print Symmetry	◉ Do not print asymmetry S(α, β)	○ Print asymmetry S(α, β)	
Differential Xsection	◉ Do not print differential cross section	○ Print secondary energy differential cross section	○ Print angular differential cross section
Incident Energy			
Integral Type	◉ Analytical integration	○ Numerical integration	
Scatterer	1		
Maximum Phonon	100		
Number of Temperatures	1		
List of Temperatures	300		
One Phonon Output	○ Do not use one phonon S(α, β) correction	◉ Use one phonon S(α, β) correction	
ENDF Output	○ Do not output ENDF library file	◉ Output ENDF library file	
Material Number	26		
Number of Elements	1	(Number of elements in chemical formula)	
Chemical Formula	1		
AMU Mass	9.012182		
Free Atom Cross Section	6.153875	(Free atom cross section in the unit of barn)	

OK Cancel

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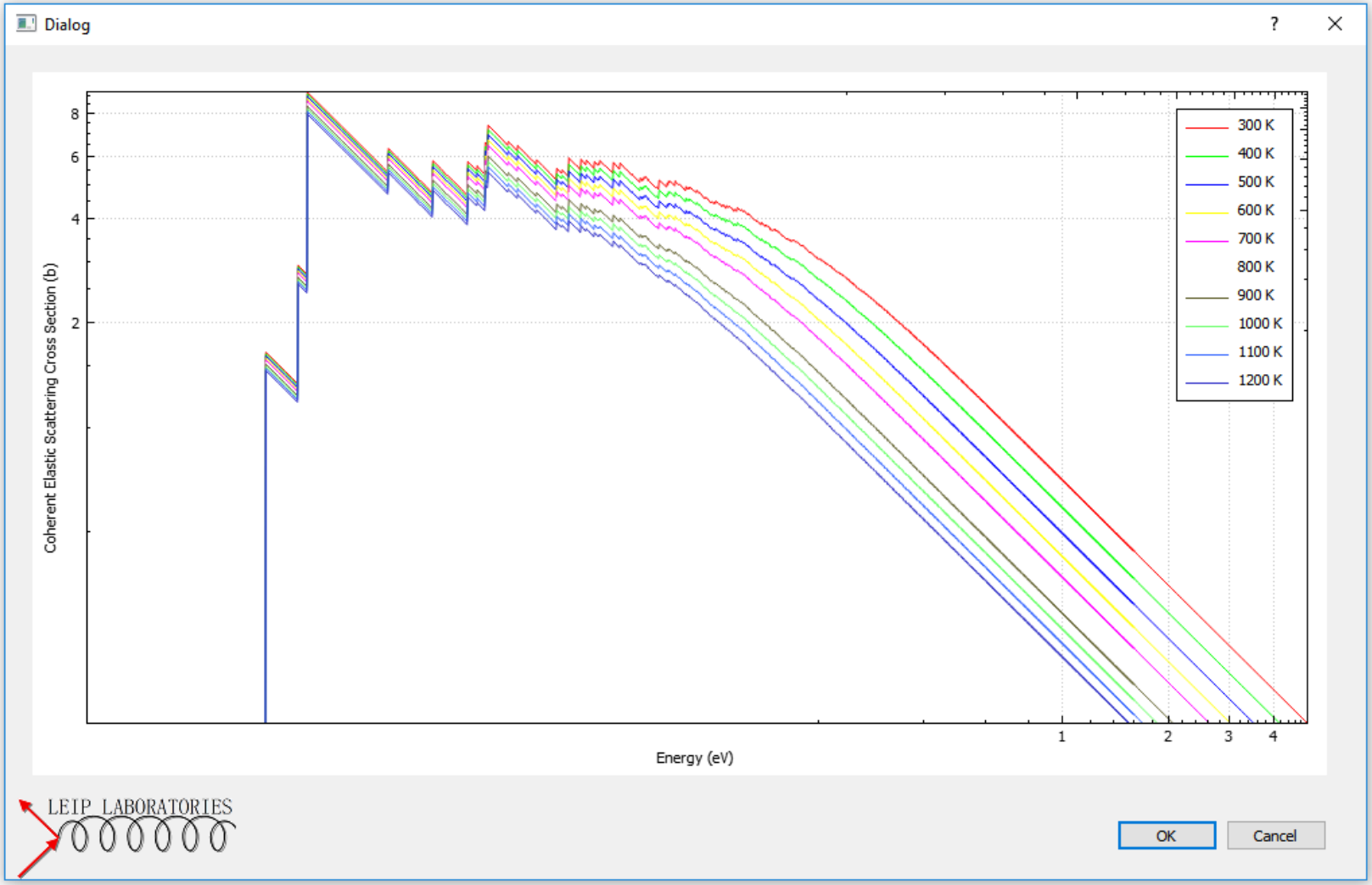
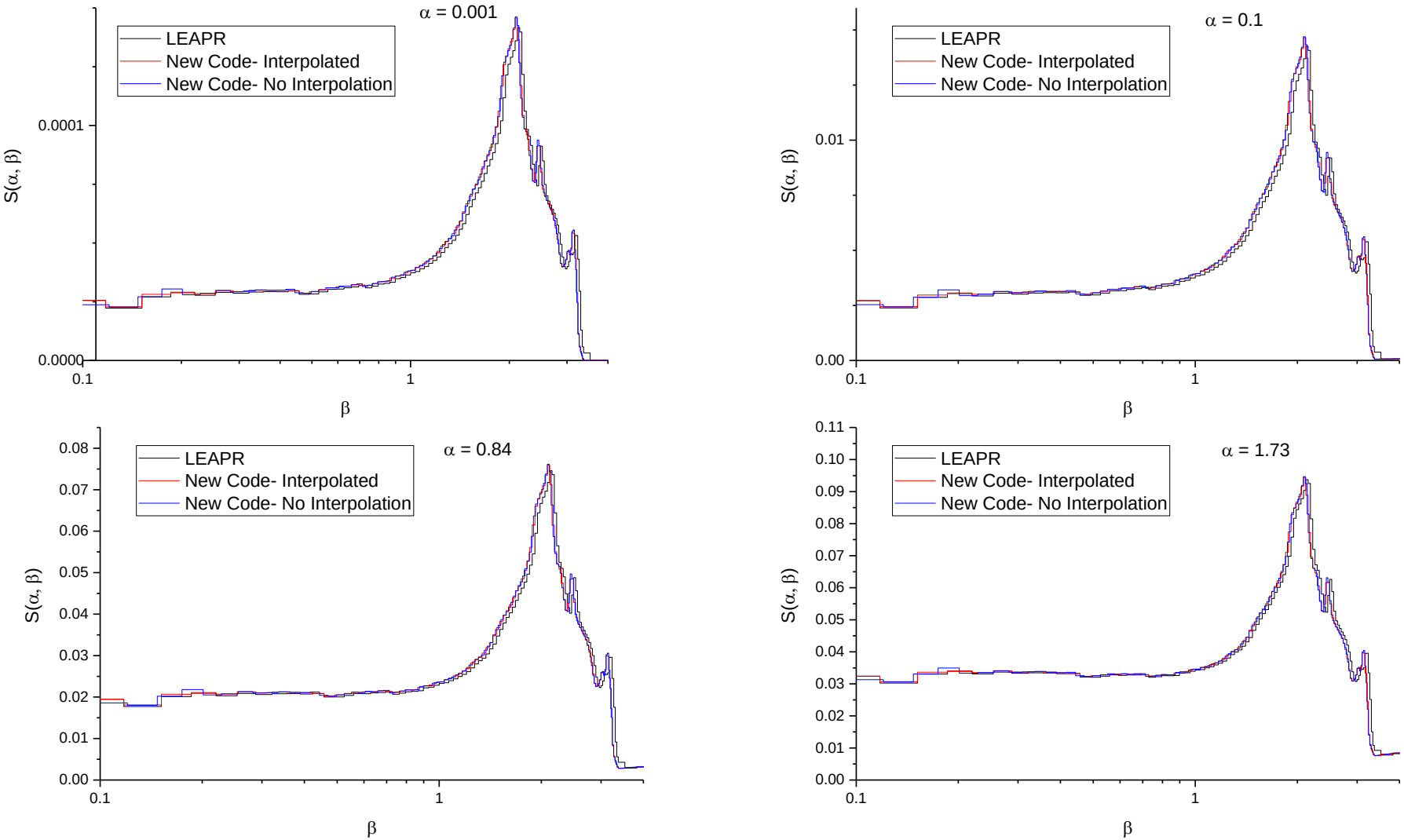
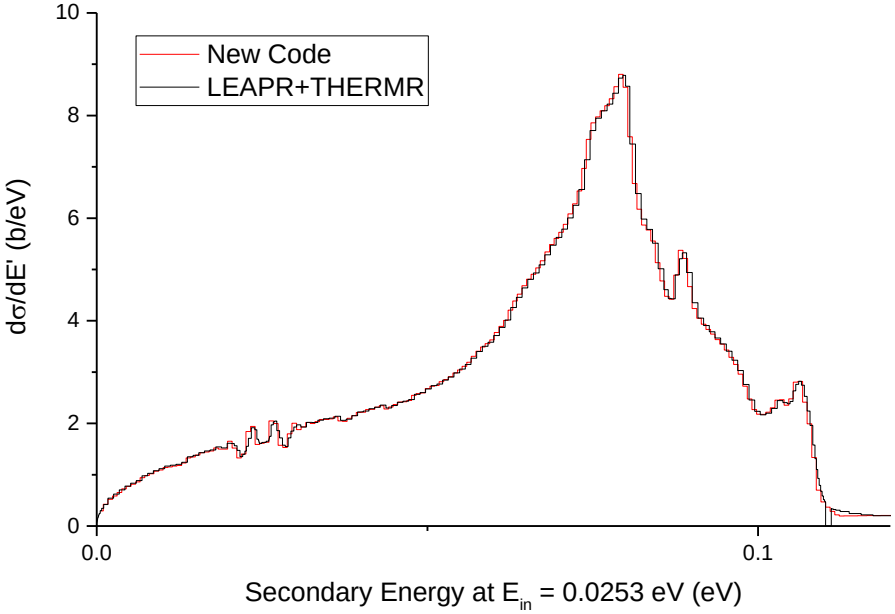
Evaluation Example

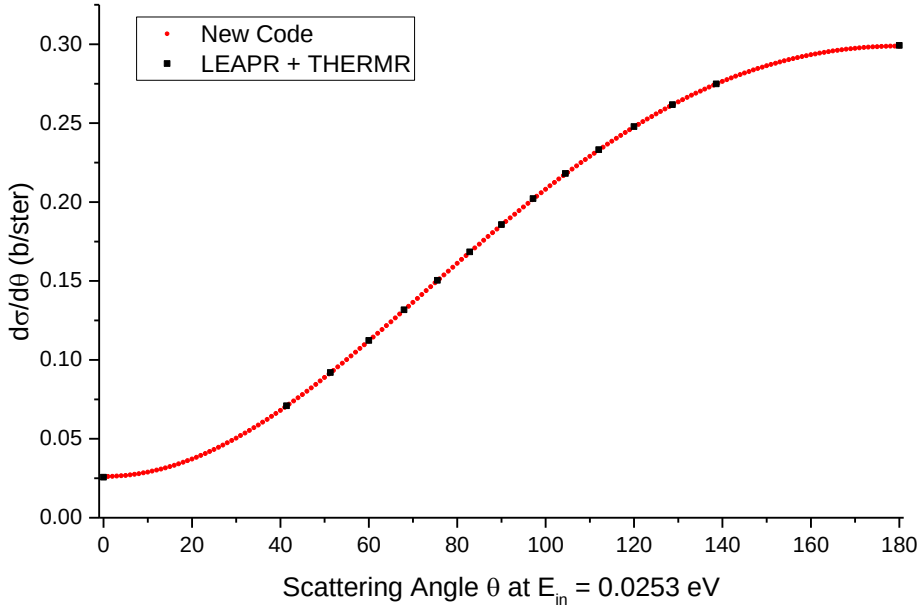


Scattering Law $S(\alpha, \beta)$

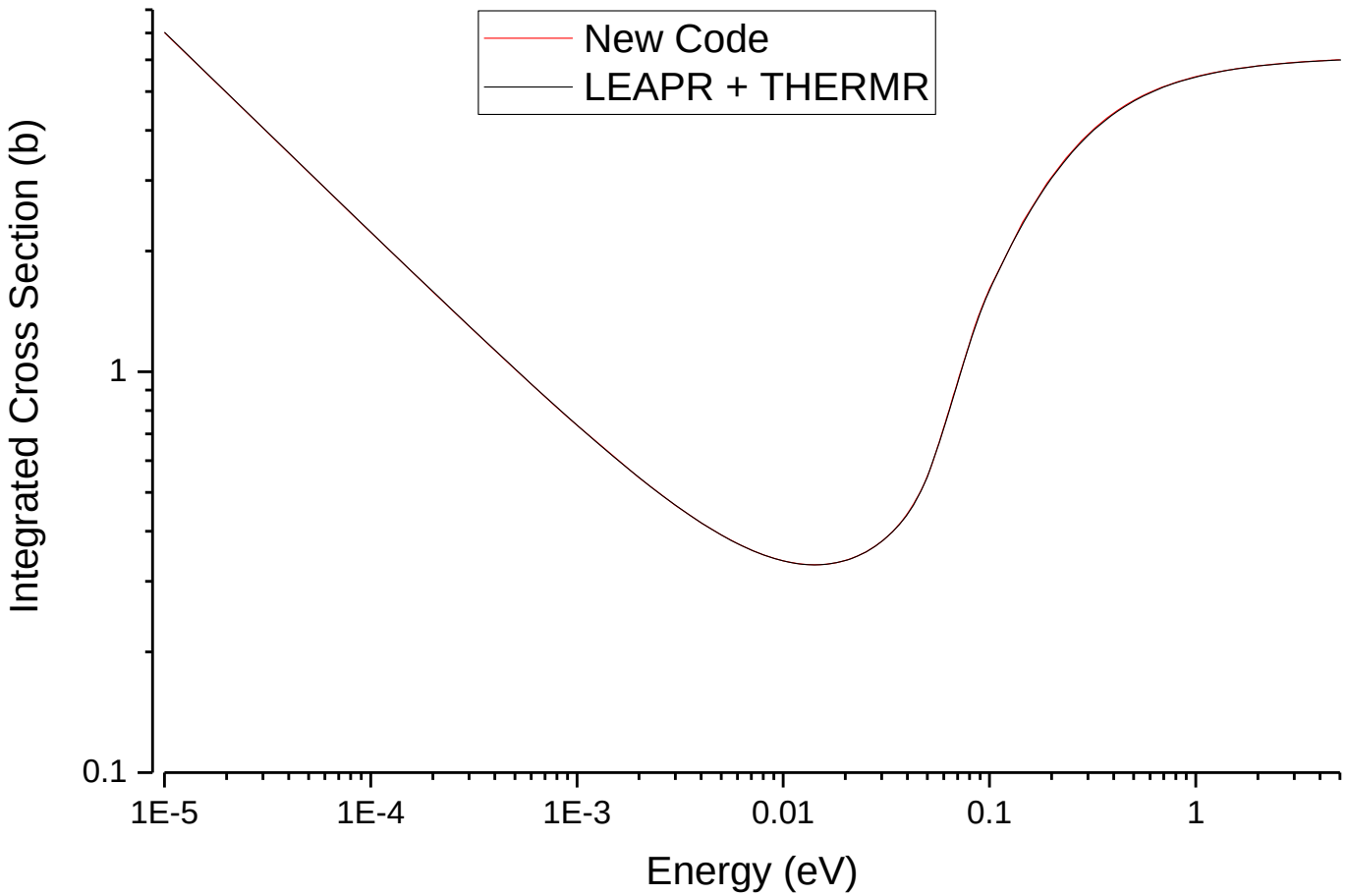


Differential Scattering Cross Section





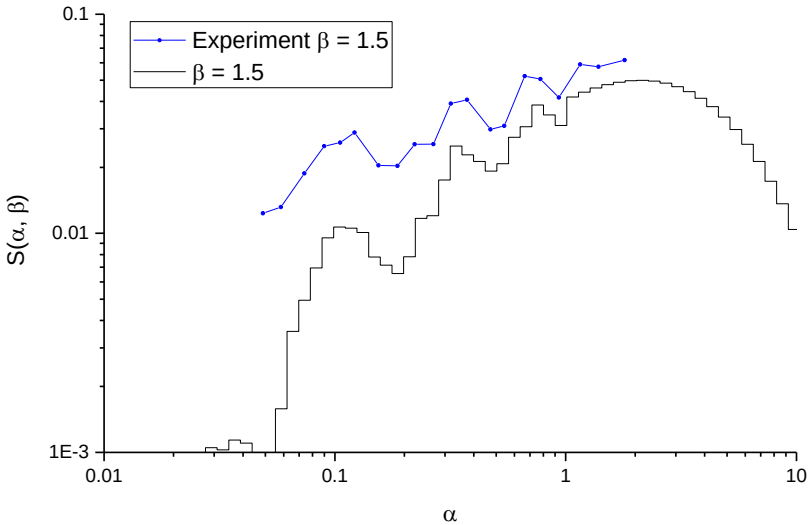
Integrated Cross Section

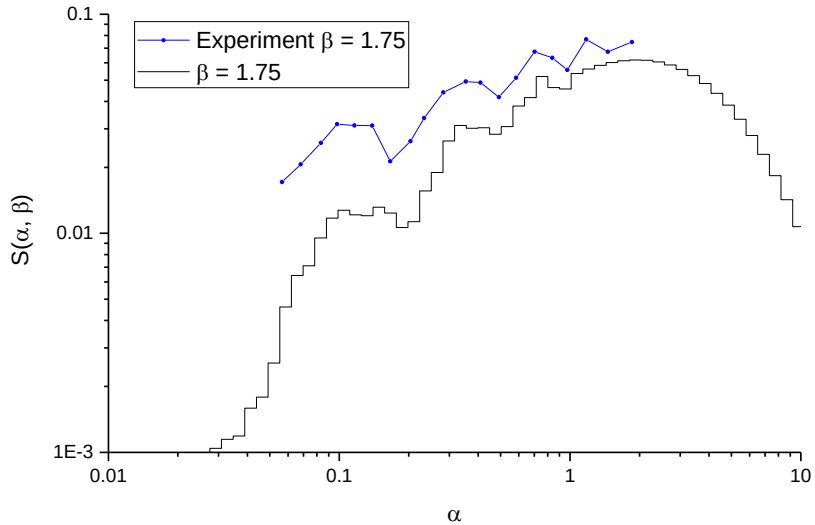


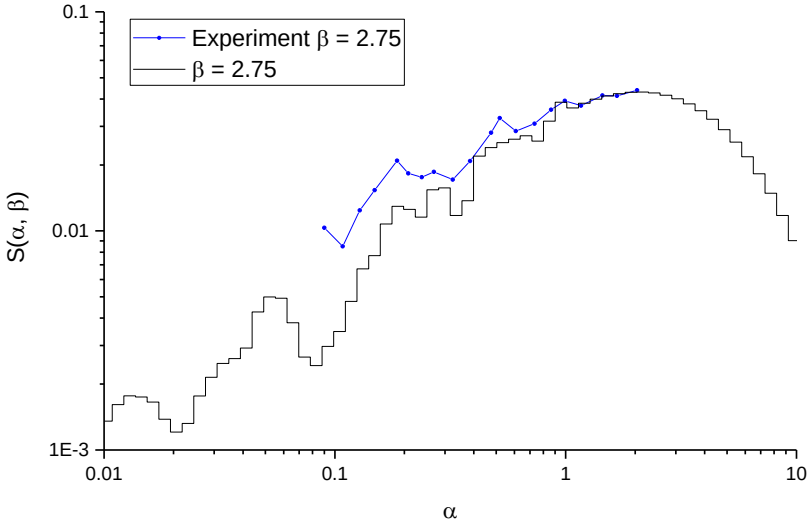
Coherent inelastic one-phonon correction routine

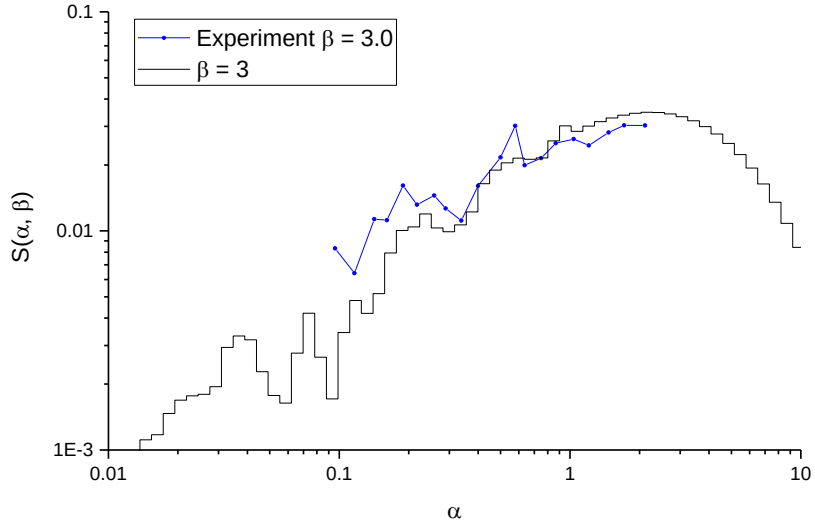
	New Code
Supported structure	Any crystal structure
Supported material	Any material
Compound material	Yes
Debye-Waller Factor	Exact
Polarization vector	Exact
Sampling of the full reciprocal space	Yes
Structure Factor	Exact

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





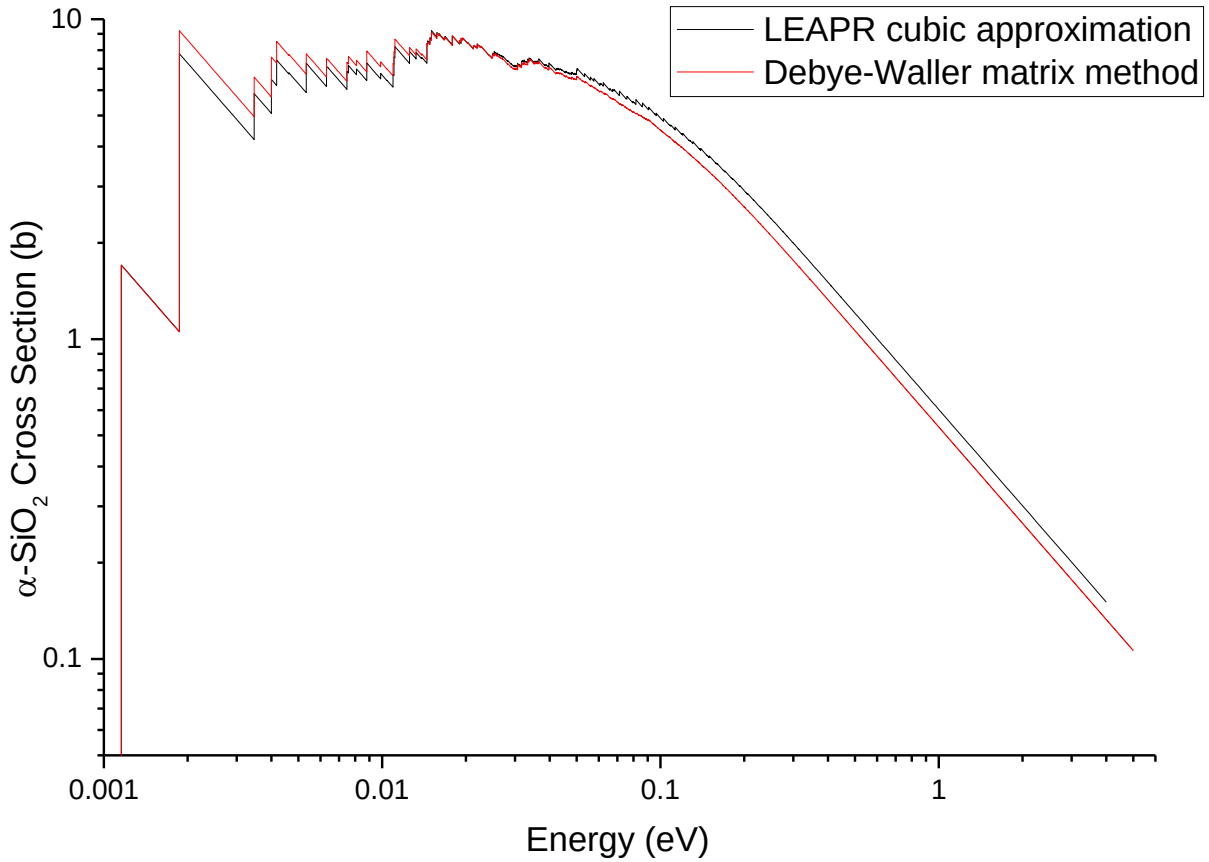




Coherent Elastic Routine

	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	No
Atom sites approximation	Yes	No
Coherent Elastic Scattering Cross Section	Over Ewald Sphere	On every reciprocal lattice point
Need to modify source code if calculating other materials	Yes	No

Coherent Elastic Cross Section of α-SiO_2



- The calculation shows around 15% divergence at low and high energies between the two methods in the cross sections of α-SiO_2.

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.