Progress of Thermal Scattering Law Development and Evaluations at North Carolina State University

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Nuclear Reactor Program
Department of Nuclear Engineering
North Carolina State University
Raleigh, North Carolina, USA
Acknowledgement

- The many graduate students, postdocs, and research staff at North Carolina State University

- Collaboration with LLNL and Bettis labs
  - David Heinrichs, Michael Zerkle, Jesse Holmes

- Funding
  - US NNSA Nuclear Criticality Safety program
  - US Naval Nuclear Propulsion Program
FY 2018/2019

- 4 new TSL evaluations
  - 3 first-of-a-kind evaluations

- Modern predictive methods for thermal neutron cross section calculations based on the use of atomistic simulations
  - Ab initio lattice dynamics
  - Molecular dynamics (ab initio and classical)
    - New materials
    - All states of matter (solid, liquid, gas)
    - Imperfect structure

- Expanding the FLASSH thermal scattering analysis platform
  - Removed approximations such as incoherent approximation, cubic approximation, atom site approximation and SCT approximation

- Initiated the integration of the Generalized Nuclear Data Structure (GNDS) format into FLASSH
Objectives

<table>
<thead>
<tr>
<th>Priority Needs */ Additional Needs</th>
<th>Thermal scattering (Paraffinic Oil, HF, Silicone Oil, UO₂F₂, PuH₂, UH₃, Paraffin, U₃O₈, U₃Si₂, UC, PuO₂, etc.), $^{239}$Pu, Fe, Cr, $^{237}$Np, Pb, $^{55}$Mn, Ti, $^{240}$Pu/$^{233}$U, Th, Be, $^{51}$V, Zr, F, K, Ca, Mo, Na, La</th>
</tr>
</thead>
<tbody>
<tr>
<td>Completed Evaluations (FY)</td>
<td>Minor Actinides (13), SiC (17), SiO₂ (17), C₅H₂O₈ (16), CH₂ (17), Be (17), BeO (17), Graphite (17), UO₂ (17), UN (17), $^{55}$Mn (12), $^{58,60}$Ni (14), $^{180,128,183,184,186}$W (14), Ca (16), $^{59}$Co (17), $^{63,65}$Cu (17)</td>
</tr>
</tbody>
</table>
Objectives

Completed light water (H₂O)

Finalizing molten salt FLiBe
Neutron Thermalization

Using first Born approximation combined with Fermi pseudopotential, it can be shown that the double differential scattering cross section has the form

\[
\frac{d^2 \sigma}{d\Omega dE'} = \frac{1}{4\pi} \sqrt{\frac{E'}{E}} \left\{ \sigma_{coh} S(\vec{k}, \omega) + \sigma_{incoh} S_s (\vec{k}, \omega) \right\}
\]

The scattering law \( S(\vec{k}, \omega) \) is composed of two parts

\[
S(\vec{k}, \omega) = S_s (\vec{k}, \omega) + S_d (\vec{k}, \omega)
\]

Van Hove’s space-time formulation

\[
I(\vec{k}, t) = \int G(\vec{r}, t) \exp(i\vec{k} \cdot \vec{r}) d\vec{r}
\]

\[
S(\vec{k}, \omega) = \frac{1}{2\pi \hbar} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G(\vec{r}, t) e^{i(\vec{k} \cdot \vec{r} - \omega t)} d\vec{r} dt
\]

where \( G(\vec{r}, t) \) is the dynamic pair correlation function and can be expressed in terms of time dependent atomic positions.
\[ S_s(\alpha, \beta) = k_B T \cdot S_s(\bar{\kappa}, \omega) \]

\[ \frac{d^2 \sigma}{d\Omega dE'} \bigg|_{\text{inelastic}} = \frac{\sigma}{2k_B T} \sqrt{\frac{E'}{E}} S_s(\alpha, \beta) \]

\[ \beta = \frac{E - E'}{k_B T} \quad \text{Energy transfer} \quad \alpha = \frac{(E + E' - 2\sqrt{EE'} \cos \theta)}{k_B T} \quad \text{Momentum transfer} \]

The scattering law (TSL) is the Fourier transform of a Gaussian correlation function

\[ S_s(\alpha, \beta) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\beta t} e^{-\gamma(t)} dt \]

\[ \gamma(t) = \frac{\alpha}{2} \int_{-\infty}^{\infty} \frac{\rho(\beta)}{\beta \sinh(\beta / 2)} \left[ 1 - e^{-i\beta t} \right] e^{\beta / 2} d\beta \]

\[ \rho(\beta) \text{ – density of states (e.g., phonon frequency distribution)} \]
Thermal Scattering Law Analysis

Key development in the last 20 years is the use of atomistic simulations methods to support the evaluation process.

- Produce data necessary to calculate the TSL including:
  - DOS for evaluation of TSL
  - Direct access to TSL using correlation analysis
## ENDF/B-VIII TSL Evaluations

<table>
<thead>
<tr>
<th>Material</th>
<th>ENDF Library Name</th>
<th>Evaluation Basis</th>
<th>Institution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beryllium metal</td>
<td>tsl-Be-metal.endf</td>
<td>DFT/LD</td>
<td>NCSU</td>
</tr>
<tr>
<td>Beryllium oxide (beryllium)</td>
<td>tsl-BeinBeO.endf</td>
<td>DFT/LD</td>
<td>NCSU</td>
</tr>
<tr>
<td>Beryllium oxide (oxygen)</td>
<td>tsl-OinBeO.endf</td>
<td>DFT/LD</td>
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</tr>
<tr>
<td>Light water (hydrogen)</td>
<td>tsl-HinH2O.endf</td>
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</tr>
<tr>
<td>Light water ice (hydrogen)</td>
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</tr>
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<tr>
<td>Polymethyl Methacrylate (Lucite)</td>
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<td>Polyethylene</td>
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<tr>
<td>Crystalline graphite</td>
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<tr>
<td>Reactor graphite (10% porosity)</td>
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Thermal Scattering Cross-Sections

**Evaluation DFT/LD**

- **VASP**
  - Optimize the system structure
  - Evaluate Hellmann–Feynman Forces

- **PHONON**
  - Generate displacements
  - Evaluate the Dynamical Matrix
  - Sample the Brillouin Zone

- **DFT**
  - Pseudo-potential
  - Quantum Mechanical model

- **LD**
  - Phonon model
  - Harmonic potential

**Thermal Scattering Law**: \( S(\alpha, \beta) \)

**Density of States**

**Thermal Scattering Cross Section**

**FLASH**: Phonon model

Cubic Approximation
Thermal Scattering Cross-Sections

Evaluation MD/QM

**LAMMPS**

- Equilibrate the system
- Generate particle trajectories
- Evaluate classical $G^{cl}(r, t) \text{ and } I^{cl}(k, t)$
- Quantum Correction

**FLASSH**

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

**MD**

- Pair potential
- Classical system

**Quantum mechanical model**

- No specific assumption
Computational Capabilities

- Hybrid mini cluster - 17 nodes
  - 324 CPU cores
  - 22 Nvidia GPUs
  - Expanding.....

- Parallel computations
  - Atomistic simulations
  - TSL analysis
  - Neutronic simulations
  - System design

- VASP, PHONON, LAMMPS
  PREPRO, NJOY, FUDGE,
  SAMMY, MCNP, Serpent,
  GEANT4, McStas, PARET,
  RELAP, COMSOL
Heavy Paraffinic Oil
Light Water

Flexible TIP4P/2005 potential

\[ U^{\text{tot}} = U^{\text{inter}} + U^{\text{intra}} = \sum_{i \neq j} 4\varepsilon \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^{6} + \sum_{i \neq j} \frac{q_i q_j}{r_{ij}} + D_r \left\{ 1 - \exp \left[ -\beta(r_{OH} - r_{eq}) \right] \right\}^2 + \frac{1}{2} K_\theta (\theta - \theta_{eq})^2 \]
Light Water

File 7

Total XS (barns)

Energy (eV)

NCSU 473K/293K
ENDF8 473K/293K
ENDF7 450K/293K
Dritsa [EXFOR #22613] (473 K / 293 K)

S(\alpha,\beta)

Energy (eV)

NCSU 473K/293K
ENDF8 473K/293K
ENDF7 450K/293K
Dritsa [EXFOR #22613] (473 K / 293 K)

S(\alpha,\beta)

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S(\alpha,\beta)

Energy (eV)

NCSU 473K/293K
ENDF8 473K/293K
ENDF7 450K/293K
Dritsa [EXFOR #22613] (473 K / 293 K)
Liquid FLiBe – FY 2019

- Eutectic with a mixture of 2:1 ratio of LiF and BeF₂
- Melting Point: 732K Boiling Point: 1703K
- DFT and MD analysis (with QM corrections)
- TSL evaluation between 750K and 1500K

Born-Mayer potential

\[ U_{i,j}(r_{i,j}) = U_1 + U_2 + U_3 + U_4 \]

\[ U_1 = \frac{Z_i Z_j e^2}{r_{i,j}}, U_2 = \frac{c_i c_j}{r_{i,j}^6}, U_3 = \frac{D}{r_{i,j}}, U_4 = b_{i,j} \left( 1 + \frac{Z_i}{N_i} + \frac{Z_j}{N_j} \right) \exp \left( \frac{r_i + r_j - r_{i,j}}{\rho} \right) \]
Hydrofluoric Acid

- Strong hydrogen bonding
- Unique molecular structure dynamics

Example CMD Potential:

$$V(r) = A \left[ \left( \frac{B}{r} \right)^{12} - \left( \frac{B}{r} \right)^6 \right] + \ldots$$

$$V(r) = C \{ \exp[-D(r - r_0)] - 1 \}^2 + E_r$$
FLASSH Code
# FLASSH Code Features

<table>
<thead>
<tr>
<th>Feature</th>
<th>NJOY</th>
<th>FLASSH</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coherent Inelastic</td>
<td>☐</td>
<td>☑</td>
</tr>
<tr>
<td>Remove Incoherent Approximation</td>
<td>☐</td>
<td>☑</td>
</tr>
<tr>
<td>Remove Short Collision Time (SCT) Approximation</td>
<td>☐</td>
<td>☑</td>
</tr>
<tr>
<td>Integral against alpha differential cross section</td>
<td>Numerical</td>
<td>Default: Analytical</td>
</tr>
<tr>
<td>a, B Gridding</td>
<td>User input</td>
<td>Default: Automatic grid</td>
</tr>
<tr>
<td>Parallel Computing</td>
<td>☐</td>
<td>☑</td>
</tr>
<tr>
<td>Graphite User Interface</td>
<td>☐</td>
<td>☑</td>
</tr>
<tr>
<td>Syntax and Error Checking</td>
<td>☐</td>
<td>☑</td>
</tr>
</tbody>
</table>

## Coherent Elastic Calculation

<table>
<thead>
<tr>
<th>Feature</th>
<th>Hexagonal, FCC, BCC</th>
<th>Any crystal structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Supported Structure</td>
<td>Graphite, Beryllium, Beryllium Oxide, Aluminum, Lead, Iron</td>
<td>Any material</td>
</tr>
<tr>
<td>Compound Materials</td>
<td>2 elements with ratio 1:1</td>
<td>Any number of elements with any ratio</td>
</tr>
<tr>
<td>Remove Cubic Approximation</td>
<td>☐</td>
<td>☑</td>
</tr>
<tr>
<td>Remove Atom Site Approximation</td>
<td>☐</td>
<td>☑</td>
</tr>
<tr>
<td>Coherent Elastic Scattering Cross Section</td>
<td>Over Ewald Sphere</td>
<td>On every reciprocal lattice point</td>
</tr>
<tr>
<td>Need to modify source code if calculating other materials</td>
<td>Yes</td>
<td>No</td>
</tr>
</tbody>
</table>

Using OpenMP
Liquid Physics in **FLASHH**

- **Separation** of the diffusive DOS from the continuous (solid) DOS in LEAPR

- **Convolution** of the solid and liquid TSL components

\[
S_{\text{total}}(\alpha, \beta) = \left(S_{\text{diff.}}(\alpha, \beta) \ast S_{\text{cont.}}(\alpha, \beta)\right)(\beta)
\]
Liquid Physics in **FLASHH**

**Construct fine beta grid (for convolution):**
- Call `convolve_grid` subroutine to determine appropriate resolution and lower/upper beta limits

**Build liquid TSL model over the new beta grid:**
- Call liquid model function (e.g., `lang` for Langevin)
  - Call `besk1` (Bessel) function if necessary

**Interpolate solid TSL onto new beta grid:**
- Call `interp_grid` subroutine to interpolate values for every convolution ‘window’

**Convolve the liquid and solid components:**
- Call `convolve` subroutine to perform the convolution

**Construct total TSL:**
- Add in extra DW term

**Output results:**
- Write TSL components to various files
Doppler Broadening

- **Free Gas**
  - Assumes a Maxwellian velocity distribution

  \[
  \sigma^{FG}(E) = \int_{0}^{\infty} dE' \ S^{FG}(E',E) \sigma(E'), \quad S^{FG}(E',E) = \frac{1}{\Delta \sqrt{\pi}} \sqrt{\frac{E'}{E}} \exp \left[ -\frac{(E' - E)^2}{\Delta^2} \right]
  \]

- **Crystal Lattice**
  - Compound nucleus effects separated from lattice effects
  - Transition probability
  - Self Scattering Law
    - Identical to that used in thermal scattering
    - Describes the energy-momentum phase space of a material

  \[
  \sigma(E) = \frac{\sigma_0 \Gamma^2}{4} \int_{-\infty}^{\infty} d\beta \ \frac{S_s(\alpha, \beta)}{(E - E_0 - \beta k_B T)^2 + (\Gamma / 2)^2}
  \]
**Doppler Broadening**

- *Ab initio* lattice dynamics
  - Predictive density of states (DOS)
  - Current DOS implemented in the ENDF/B-VIII.0 cross section library for U in UO$_2$

![Doppler Broadening Graph](image)

![Fluorite Structure](image)

- Fluorite Structure
- 2x2x2 supercell
- GGA-PBE+U
Doppler Broadening

- *Ab initio* lattice dynamics
  - Predictive density of states (DOS)
  - Current DOS implemented in the ENDF/B-VIII.0 cross section library for U in UO₂

![Graph showing Doppler broadening and resonance cross section for ²³⁸U at 6.674 eV.](image)

- Fluorite Structure
- 2x2x2 supercell
- GGA-PBE+U
**FLASSH Generalized TSL**

\[ S_s(\bar{k}, \omega) = \frac{1}{2\pi\hbar} \int e^{-i\omega t} \left< U^2 \right> e^{-i\left<U\right> t} dt = e^{-2W} \sum_{n=0}^{\infty} \frac{(2W)^n}{n!} G_n \]

\[ \sum_s (\bar{k} \cdot \bar{e}_s)^2 = \frac{1}{3} k^2 \]

**Full Equation**

\[ G_1(\omega) = \frac{1}{\gamma(0)} \frac{1}{N} \frac{\hbar}{k_B T} \sum_s \frac{|\bar{e}_s|^2}{2\beta \sinh(\beta/2)} e^{-\beta/2} \]

\[ 2W = \frac{\hbar}{2MN} \sum_s \frac{|\bar{k} \cdot \bar{e}_s|^2}{\omega_s} \coth \left( \frac{\hbar \omega_s}{2k_B T} \right) \]

- Function of the polarization vector and dispersion relations

**Cubic Approximation**

\[ G_1(\omega) = \frac{1}{\lambda} \frac{\rho(\beta)}{2\beta \sinh(\beta/2)} e^{-\beta/2} \]

\[ 2W = \frac{\hbar k^2}{2M} \frac{\rho(\omega)}{\coth \left( \frac{\hbar \omega}{2k_B T} \right)} d\omega \]

- Function of the density of states \( \rho(\omega) \)
FLASH Generalized TSL

- Beryllium Metal
  - HCP (P63/mmc)
  - *Ab initio* lattice dynamics
  - 4x4x3 Supercell

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<thead>
<tr>
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Exact Debye-Waller Matrix (Å²)

\[
\beta = 1.58151407 \text{ cubic approximation}
\]

\[
S(\alpha, \beta)
\]

\[
\text{Density of State (arb.)}
\]

\[
\text{Energy (eV)}
\]
**FLASSH** Generalized TSL

- Beryllium Metal
  - HCP (P63/mmc)
  - *Ab initio* lattice dynamics
  - 4x4x3 Supercell

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Exact Debye-Waller Matrix (Å²)

- \( \beta = 1.58151407 \) exact non-cubic
- \( \beta = 1.58151407 \) cubic approximation

\( S(\alpha, \beta) \) vs. \( \alpha \)

\( E [\text{eV}] \) vs. wavevector

[20,21] AILD
Ongoing collaboration with LLNL

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**Background**

This library was produced by the Low Energy Interaction Physics (LEIP) group at North Carolina State University. The thermal scattering law data for hydrogen in H2O were developed using the molecular dynamics (MD) method [1]. There is no file MT = 3, i.e., coherent elastic cross sections. One temperature is available in this library: the LEAPR module from the NJOY 2016 code system was used to produce file MT = 4 data for H in H2O. By convention, MAT = 1 and ZA=1001 are used for H in H2O.

**References**

Summary

- **FY 2018**
  - 10 new TSL evaluations contributed to ENDF/B-VIII.0
  - 5 first-of-a-kind evaluations

- **FY 2019**
  - 4 new TSL evaluations
  - 3 first-of-a-kind evaluations

- Modern predictive methods for thermal neutron cross section calculations based on the use of atomistic simulations
  - Ab initio lattice dynamics
  - Molecular dynamics (ab initio and classical)
    - New materials
    - All states of matter (solid, liquid, gas)
    - Imperfect structure

- **FLASHH** is a new thermal scattering analysis platform that uses a generalized theoretical approach for TSL calculations
  - Removed approximations such as incoherent approximation, cubic approximation, atom site approximation and SCT approximation

- Progress on FY 2019 tasks