Fast on-the-fly Monte Carlo sampling of temperature dependent thermal scattering

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Team Members and Collaborators

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Acknowledgement

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Project Objective and Motivation

- Develop thermal data libraries for MCNP6 to support on-the-fly S(\alpha, \beta) sampling for temperature ranges applicable to nuclear criticality safety

Enhance the physics treatment in MCNP6 so that it can perform fast on-the-fly sampling of S(\alpha, \beta) data at arbitrary temperature
### Current Data Storage Format for MCNP6

<table>
<thead>
<tr>
<th>Material</th>
<th>Temperature Range [K]</th>
<th># Files</th>
<th>Total Size [MB]</th>
</tr>
</thead>
<tbody>
<tr>
<td>be-beo</td>
<td>293.6 - 1200</td>
<td>8</td>
<td>339.34</td>
</tr>
<tr>
<td>o-beo</td>
<td>293.6 - 1200</td>
<td>8</td>
<td>280.24</td>
</tr>
<tr>
<td>grph</td>
<td>296 - 2000</td>
<td>10</td>
<td>393.99</td>
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<tr>
<td>grph10</td>
<td>296 - 2000</td>
<td>10</td>
<td>328.88</td>
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<td>grph30</td>
<td>296 - 2000</td>
<td>10</td>
<td>312.08</td>
</tr>
<tr>
<td>h-h2o</td>
<td>283.6 - 800</td>
<td>18</td>
<td>536.1</td>
</tr>
</tbody>
</table>

- Current MCNP ACE file thermal library is large
- Unwieldy for HPC simulations
On-The-Fly (OTF) Data Storage Format

- Small thermal library for select materials
- Adaptive in temperature
- Retains accuracy
- Maintains computational complexity

Single file for a material
Works for any temperature
Only 20-30 MB
From Current Library to On-The-Fly Library

Current library: Each book represents the data for a single temperature for a specific material.

OTF library: Each book represents the date for a specific material for any temperature.
Approaches to Produce OTF Libraries

1. Generate material specific Thermal Scattering Law (TSL) data - $S(\alpha, \beta, T)$.

2. Calculate sampling probability distributions (PDFs and CDFS) on a fine temperature mesh over the applicable range.

3. Apply a regression model to remove temperature dependence from the data.

4. Validation of the regression model
Approaches – Start

- Sample leapr inputs from ENDF/B-VIII.0
- Contains information to evaluate TSL data
  - Phonon spectrum
  - Material parameters
Approaches – Stage 1

- Generate high fidelity TSL data.
  - Utilize NJOY to evaluate TSL on fine grids
  - Alpha, beta, and temperature must be chosen for each material
  - These grids must capture material behavior
Approaches – Stage 1

$S(\alpha, \beta)$ values for graph at 1036 K

Start | Stage 1 | Stage 2 | Stage 3 | Stage 4 | End
Approaches – Stage 1

- Example input grids for graphite
  - Alpha grid: 1E-3 to 38.6 with 1000 points
  - Beta grid: 0 to 80 eV with 2500 points
  - Temperature grid: 296 to 2000 K (every 5 K)
Approaches – Stage 2

- This alone is not enough for sampling. Sampling PDFs and CDFS need to be created.

\[
g(\beta|E, T) = \exp \left( -\frac{\beta}{2} \right) \frac{\int_{\alpha_-}^{\alpha_+} S(\alpha, \beta, T) d\alpha}{\int_{\beta_-}^{\beta_+} \int_{\alpha_-}^{\alpha_+} \exp \left( -\frac{\beta}{2} \right) S(\alpha, \beta, T) d\alpha d\beta}
\]

\[
\hat{h}(\alpha|\beta, T) = \frac{S(\alpha, \beta, T)}{\int_0^{\infty} S(\alpha, \beta, T) d\alpha}
\]

\[
G(\beta|E, T) = \int_{\beta_-}^{\beta} g(\beta'|E, T) d\beta'
\]

\[
\tilde{H}(\alpha|\beta, T) = \int_0^{\alpha} \hat{h}(\alpha|\beta, T) d\alpha'
\]
Approaches – Stage 2

Graph CDFs for Beta at 296 K

Graph CDFs for Alpha at 296 K

Start | Stage 1 | Stage 2 | Stage 3 | Stage 4 | End
Approaches – Stage 3

- Store a single data set for any temperature!

<table>
<thead>
<tr>
<th></th>
<th>$CDF_1$</th>
<th></th>
<th>$CDF_n$</th>
<th></th>
<th>$CDF_N$</th>
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<tbody>
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<td>$E_1$</td>
<td>$\beta(T)_{1,1}$</td>
<td></td>
<td>$\beta(T)_{1,n}$</td>
<td></td>
<td>$\beta(T)_{1,N}$</td>
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<tr>
<td>$\vdots$</td>
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<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>$E_m$</td>
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<td></td>
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<td>$\beta(T)_{m,N}$</td>
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<tr>
<td>$\vdots$</td>
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<td></td>
</tr>
<tr>
<td>$E_M$</td>
<td>$\beta(T)_{M,1}$</td>
<td></td>
<td>$\beta(T)_{M,n}$</td>
<td></td>
<td>$\beta(T)_{M,N}$</td>
</tr>
</tbody>
</table>

- How to define $\beta(T)$ and $\alpha(T)$?

Start | Stage 1 | Stage 2 | Stage 3 | Stage 4 | End
Approaches – Stage 3

- Current technique uses polynomial curve fitting.

- This creates coefficients that can be used to reevaluate the alpha and beta values OTF.

- With simple polynomials, OTF evaluation only adds 10~20% (currently) to the sampling time.
Approaches – Stage 4

- Validation efforts center around randomly sampling the data.
  - Recreate MCNP’s thermal sampling procedure to compare accuracy and computation time.
- More advanced comparisons are planned.
Approaches – Stage 4

Histograms for BeinBeO at 700 K: 1e-01 eV, 1e+06 samples.
Approaches – End

- Final product
  - Single file for each material
  - Small size
  - Used for any temperature
  - Maintains accuracy
  - Not computationally expensive

\[
\beta = \sum_{l} B_i \cdot X_{\beta}(T)
\]

\[
\alpha = \sum_{l} A_i \cdot X_{\alpha}(T)
\]
Current and Future

- Advanced on-the-fly (OTF) strategy driven libraries have been developed for six materials based on ENDF/B-VIII.0.
- Validation of the OTF libraries are being conducted.
- Investigation of the application for neural networks to be used to directly sample scattering data.