Adaptive-in-temperature method for fast on-the-fly sampling of thermal neutron scattering data in MCNP6

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➢ Collaborators
  o Forrest Brown (retired) – Los Alamos National Laboratory
  o Robert Little – Los Alamos National Laboratory
Acknowledgement

This work was supported by the Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the Department of Energy.
Project Objective and Motivation

- Develop thermal data libraries for selected isotopes in 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.
A General Random Walk Sampling in MCNP

Need x-sec data at $T_2$ to sample the collision distance

Thermal neutron scattering dominated by $S(\alpha, \beta)$ scattering law

$$\sigma(E \rightarrow E', \mu, T) = \frac{\sigma_b}{2kT} \sqrt{\frac{E'}{E}} e^{-\beta^2/2} S(\alpha, \beta, T)$$

$\alpha$: momentum transfer  $\beta$: energy transfer
Current Data Storage Format for MCNP6

- NJOY is used to create correlated energy-angle distributions for inelastic scattering.

- These consist of two parts.
  - A set of equally probable final energy bins for each incident energy.
  - A set of equally probable cosine bins for each incoming and outgoing energy pair.

- This is done for each temperature.
Current Data Storage Format for MCNP6

<table>
<thead>
<tr>
<th>$T_1$</th>
<th>$CDF_1$</th>
<th>...</th>
<th>$CDF_n$</th>
<th>...</th>
<th>$CDF_N$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_1$</td>
<td>$E'_{1,1}$</td>
<td>...</td>
<td>$E'_{1,n}$</td>
<td>...</td>
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<tr>
<td>...</td>
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<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>$E_m$</td>
<td>$E'_{m,1}$</td>
<td>...</td>
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</table>

<table>
<thead>
<tr>
<th>$T_1$</th>
<th>$E'_1$</th>
<th>...</th>
<th>$E'_n$</th>
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<tbody>
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<td>...</td>
<td></td>
<td></td>
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<tr>
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<table>
<thead>
<tr>
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<th>$CDF_k$</th>
<th>...</th>
<th>$CDF_K$</th>
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<tbody>
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<td>$\mu'^{1,1,k}$</td>
<td>...</td>
<td>$\mu'^{1,1,K}$</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>$(E_m,E'_n)$</td>
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<td>...</td>
<td>$\mu'^{m,n,k}$</td>
<td>...</td>
<td>$\mu'^{m,n,K}$</td>
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<tr>
<td>$(E_M,E'_N)$</td>
<td>$\mu'^{CDF,M,N}$</td>
<td>...</td>
<td>$\mu'^{M,N,k}$</td>
<td>...</td>
<td>$\mu'^{M,N,K}$</td>
</tr>
</tbody>
</table>
Current Sampling Procedure in MCNP6

1. Determination of target’s temperature (T).
2. Find data sets at nearest temperatures ($T_i < T < T_{i+1}$).
3. Sample outgoing energy based on $T_i$ and $T_{i+1}$ data sets, and then do interpolation to obtain outgoing energy at T.
4. Similar procedure to obtain outgoing angle at T.
Data Storage Requirements by MCNP6

To be able to **sample** thermal scattering, MCNP stores all the thermal data directly.

This leads to a large amount of data that is needed.

- For example, in the thermal energy range: 24 MB per temperature for graphite or H in water
- For a realistic reactor, 50-100 temperatures are needed

<table>
<thead>
<tr>
<th>Material</th>
<th>File Size (MB)</th>
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<tbody>
<tr>
<td>Al</td>
<td>25</td>
</tr>
<tr>
<td>Be (Metal)</td>
<td>28</td>
</tr>
<tr>
<td>H in Benzene</td>
<td>69.5</td>
</tr>
<tr>
<td>Be in BeO</td>
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</tr>
<tr>
<td>Fe</td>
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<td>H in H$_2$O</td>
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<td>O$_2$ in UO$_2$</td>
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<td>Si in SiO$_2$</td>
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<tr>
<td>U in UO$_2$</td>
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</tr>
<tr>
<td>Zr in ZrH</td>
<td>56.1</td>
</tr>
</tbody>
</table>
How to Decrease Data Storage for MCNP6?

- Any better way to improve the storage requirement (and associated sampling procedures)?

\[ \beta = \frac{E' - E}{kT}, \quad \alpha = \frac{E + E' - 2\mu\sqrt{EE'}}{AkT} \]

\( \beta \): energy transfer
\( \alpha \): momentum transfer

\( E \rightarrow E' \), then \((E, E') \rightarrow \mu \)

\( E \rightarrow \beta \), then \( \beta \rightarrow \alpha \)
Sample momentum ($\alpha$) and energy ($\beta$) transfer directly.

- $\alpha$ and $\beta$ can then be converted into $E'$ and $\mu$

\[
E' = E + \beta kT \\
\mu = \frac{2E + kT(\beta - A\alpha)}{2\sqrt{E(E + \beta kT)}}
\]

MC21 implements this strategy.
Coupled $\alpha$ and $\beta$ distributions are created.

- A table of incident energies versus CDF values that contain $\beta$ values.
- A table of $\alpha$ versus $\beta$ mesh values that contain function values, which serve as a memory reduction technique where the function values are used to create $\alpha$ CDFs on-the-fly.

This is done for each temperature.
Data Storage in MC21

\[
\begin{array}{cccc}
T_1 & CDF_1 & \cdots & CDF_N \\
E_1 & \beta_{1,1} & \beta_{1,n} & \beta_{1,N} \\
\cdots \\
E_m & \beta_{m,1} & \beta_{m,n} & \beta_{m,N} \\
\cdots \\
E_M & \beta_{M,1} & \beta_{M,n} & \beta_{M,N} \\
\end{array}
\]

\[
F(\alpha_m, \beta_n) = \int_0^{\alpha_m} S(\alpha', \beta_n) e^{\beta_n/2} d\alpha'
\]

\[
\alpha_{CDF}(\alpha | \beta_n, E) = \frac{F(\alpha, \beta_n) - F(\alpha_{\text{min}}, \beta_n)}{F(\alpha_{\text{max}}, \beta_n) - F(\alpha_{\text{min}}, \beta_n)}
\]

\[
\alpha_{\text{max}} = \frac{\sqrt{E} + \sqrt{E - \beta kT}}{AkT}
\]

\[
\alpha_{\text{min}} = \frac{\sqrt{E} - \sqrt{E - \beta kT}}{AkT}
\]


Sampling Procedure in MC21

1. Determination of target’s temperature (T).
2. Find data sets at nearest temperatures (\(T_i < T < T_{i+1}\)).
3. Sample \(\beta\) based on \(T_i\) and \(T_{i+1}\) data sets, and then do interpolation to obtain \(\beta\) at \(T\).
4. Similar procedure to obtain \(\alpha\) at \(T\).
5. Convert \(\alpha\) and \(\beta\) to outgoing energy and scattering angle at \(T\).

<table>
<thead>
<tr>
<th>(T_i)</th>
<th>(CDF_1)</th>
<th>(CDF_n)</th>
<th>(CDF_{n+1})</th>
<th>(CDF_N)</th>
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</thead>
<tbody>
<tr>
<td>(E_1)</td>
<td>(\beta_{1,1})</td>
<td>(\beta_{1,n})</td>
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<td>(\beta_{1,N})</td>
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<tr>
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<td>(\beta_{m+1,n})</td>
<td>(\beta_{m+1,n+1})</td>
<td>(\beta_{m+1,N})</td>
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<tr>
<td>(E_M)</td>
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<td>(\beta_{M,n})</td>
<td>(\beta_{M,n+1})</td>
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</table>

<table>
<thead>
<tr>
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<th>(CDF_1)</th>
<th>(CDF_n)</th>
<th>(CDF_{n+1})</th>
<th>(CDF_N)</th>
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<tr>
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<td>(\beta_{1,N})</td>
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<tr>
<td>(E_M)</td>
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<td>(\beta_{M,n})</td>
<td>(\beta_{M,n+1})</td>
<td>(\beta_{M,N})</td>
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</table>
A Little Recap

<table>
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<th>$T_1$</th>
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</thead>
<tbody>
<tr>
<td>$E_1$</td>
<td>$E'_{1,1}$</td>
<td>$\ldots$</td>
<td>$E'_{1,n}$</td>
<td>$E'_{1,N}$</td>
</tr>
<tr>
<td>$E_m$</td>
<td>$E'_m,1$</td>
<td>$\ldots$</td>
<td>$E'_m,n$</td>
<td>$E'_m,N$</td>
</tr>
<tr>
<td>$E_M$</td>
<td>$E'_M,1$</td>
<td>$\ldots$</td>
<td>$E'_M,n$</td>
<td>$E'_M,N$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$T_1$</th>
<th>$E'_1$</th>
<th>$\ldots$</th>
<th>$E'_n$</th>
<th>$E'_N$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_1$</td>
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<td>$\ldots$</td>
<td>$\mu'_{CDF,1,n}$</td>
<td>$\mu'_{CDF,1,N}$</td>
</tr>
<tr>
<td>$E_m$</td>
<td>$\mu'_{CDF,m,1}$</td>
<td>$\ldots$</td>
<td>$\mu'_{CDF,m,n}$</td>
<td>$\mu'_{CDF,m,N}$</td>
</tr>
<tr>
<td>$E_M$</td>
<td>$\mu'_{CDF,M,1}$</td>
<td>$\ldots$</td>
<td>$\mu'_{CDF,M,n}$</td>
<td>$\mu'_{CDF,M,N}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$T_1$</th>
<th>$CDF_{1}$</th>
<th>$\ldots$</th>
<th>$CDF_k$</th>
<th>$\ldots$</th>
<th>$CDF_K$</th>
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</thead>
<tbody>
<tr>
<td>$(E_1,E'_1)$</td>
<td>$\mu'_{CDF,1,1}$</td>
<td>$\mu'_{1,1,k}$</td>
<td>$\mu'_{1,1,K}$</td>
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<td></td>
</tr>
<tr>
<td>$(E_m,E'_m)$</td>
<td>$\mu'_{CDF,m,n}$</td>
<td>$\mu'_{m,n,k}$</td>
<td>$\mu'_{m,n,K}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$(E_M,E'_M)$</td>
<td>$\mu'_{CDF,M,N}$</td>
<td>$\mu'_{M,N,k}$</td>
<td>$\mu'_{M,N,K}$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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\[ F(\alpha, \beta_n) = \int_0^{\alpha_m} S(\alpha', \beta_n) e^{\beta_n/2} d\alpha' \]
Current Data Storage Techniques

Key Points:
- Both MCNP6 and MC21 interpolate scattering data in order to account for temperature effects.
- Therein, a large amount of data is needed to ensure accuracy.

Any further improvement to decrease data storage?
- We (RPI) have (or had*) a solution!

From \((E, E', \mu')\) Space to \((\alpha, \beta)\) Space

\[
\begin{array}{cccc}
T_1 & CDF_1 & \ldots & CDF_N \\
E_1 & E'_{1,1} & \ldots & E'_{1,N} \\
\vdots & \vdots & \ddots & \vdots \\
E_m & E'_{m,1} & \ldots & E'_{m,N} \\
E_M & E'_{M,1} & \ldots & E'_{M,N} \\
\end{array}
\quad
\begin{array}{cccc}
T_1 & E'_1 & \ldots & E'_N \\
E_1 & \mu'_{CDF,1,1} & \ldots & \mu'_{CDF,1,N} \\
\vdots & \vdots & \ddots & \vdots \\
E_i & \mu'_{CDF,m,1} & \ldots & \mu'_{CDF,m,N} \\
E_M & \mu'_{CDF,M,1} & \ldots & \mu'_{CDF,M,N} \\
\end{array}
\]

\[
\begin{array}{cccc}
T_1 & CDF_1 & \ldots & CDF_K \\
(E_1,E'_1) & \mu'_{CDF,1,1} & \mu'_{1,1,1} & \mu'_{1,1,K} \\
\vdots & \vdots & \ddots & \vdots \\
(E_m,E'_m) & \mu'_{CDF,m,n} & \mu'_{m,n,1} & \mu'_{m,n,K} \\
(E_M,E'_M) & \mu'_{CDF,M,N} & \mu'_{M,N,1} & \mu'_{M,N,K} \\
\end{array}
\]

\[
\begin{array}{cccc}
T_1 & CDF_1 & \ldots & CDF_N \\
E_1 & \beta_{1,1} & \beta_{1,n} & \beta_{1,N} \\
\vdots & \vdots & \ddots & \vdots \\
E_m & \beta_{m,1} & \beta_{m,n} & \beta_{m,N} \\
E_M & \beta_{M,1} & \beta_{M,n} & \beta_{M,N} \\
\end{array}
\quad
\begin{array}{cccc}
T_1 & \beta_1 & \ldots & \beta_N \\
\alpha_1 & F(\alpha_1,\beta_1) & F(\alpha_1,\beta_N) \\
\vdots & \vdots & \ddots & \vdots \\
\alpha_m & F(\alpha_m,\beta_1) & F(\alpha_m,\beta_N) \\
\alpha_M & F(\alpha_M,\beta_1) & F(\alpha_M,\beta_N) \\
\end{array}
\]

\[
F(\alpha_m,\beta_n) = \int_{0}^{\alpha_m} S(\alpha',\beta_n) e^{\beta_n/2} d\alpha'
\]
A Better Strategy Than MCNP6 & MC21
These $\beta(T)_{m,n}$ and $\alpha(T)_{m,n}$ enable "on-the-fly" treatment of temperature-dependence (vs. interpolation between temperatures).

<table>
<thead>
<tr>
<th>$E_1$</th>
<th>$CDF_1$</th>
<th>$\beta(T)_{1,1}$</th>
<th>$\beta(T)_{1,n}$</th>
<th>$\beta(T)_{1,n+1}$</th>
<th>$\beta(T)_{1,N}$</th>
</tr>
</thead>
<tbody>
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<td>$\beta(T)_{2,n}$</td>
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<tr>
<td>$E_m$</td>
<td>$CDF_m$</td>
<td>$\beta(T)_{m,1}$</td>
<td>$\beta(T)_{m,n}$</td>
<td>$\beta(T)_{m,n+1}$</td>
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<td>$CDF_{m+1}$</td>
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<tr>
<td>$E_M$</td>
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<td>$\beta(T)_{M,n}$</td>
<td>$\beta(T)_{M,n+1}$</td>
<td>$\beta(T)_{M,N}$</td>
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</tbody>
</table>
A Better Strategy Than MCNP6 & MC21

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

- How do we define these \( \beta(T)_{m\,n} \) and \( \alpha(T)_{m\,n} \)?
- This is where new research direction can jump in.
  - Data Analytics Methods?
  - Machine Learning Methods?
On-The-Fly Strategy Data Storage Format

\[
\begin{align*}
| & \quad CDF_1 & \quad \ldots & \quad CDF_N \\
E_1 & [b_{1,1,1} \ldots b_{1,1,K}] & [b_{1,N,1} \ldots b_{1,N,J}] \\
\ldots & \ldots & \ldots \\
E_m & [b_{m,1,1} \ldots b_{m,1,K}] & [b_{m,N,1} \ldots b_{m,N,K}] \\
\ldots & \ldots & \ldots \\
E_M & [b_{M,1,1} \ldots b_{M,1,K}] & [b_{M,N,1} \ldots b_{M,N,K}] \\
\end{align*}
\]

\[
\begin{align*}
| & \quad CDF_1 & \quad \ldots & \quad CDF_N \\
\beta_1 & [a_{1,1,1} \ldots a_{1,1,L}] & [a_{1,N,1} \ldots a_{1,N,L}] \\
\ldots & \ldots & \ldots \\
\beta_m & [a_{m,1,1} \ldots a_{m,1,L}] & [a_{m,N,1} \ldots a_{m,N,L}] \\
\ldots & \ldots & \ldots \\
\beta_M & [a_{M,1,1} \ldots a_{M,1,L}] & [a_{M,N,1} \ldots a_{M,N,L}] \\
\end{align*}
\]

\[
\beta(T)_{m,n} = \sum_{k=1}^{K} b_{m,n,k} X^k(T) + \text{const.}
\]

\[
\alpha(T)_{m,n} = \sum_{l=1}^{L} a_{m,n,l} X^l(T) + \text{const.}
\]

Where K and L are the orders of the fits.

One typical example: \( \beta(T) \approx \sum_{n=0}^{N} b_{n} T^{-n} \), \( \alpha(T) \approx \sum_{m=0}^{M} a_{m} T^{-m} \)
On-The-Fly Strategy Data Generation

- Beta PDFs for graphite at 1.0 eV and various temperatures
- Beta CDFs for graphite at 1.0 eV and various temperatures

\[ \beta \text{ temperature fit meshes: } E, P_\beta \]
On-The-Fly Strategy Data Generation

Alpha PDFs for graphite at $\beta = 10$ and various temperatures

Alpha CDFs for graphite at $\beta = 10$ and various temperatures

$\alpha$ temperature fit meshes: $\beta$, $P_\alpha$
Current and Future ...

- Contract with LANL was finalized (delayed by a year) ...

- On-the-fly strategy driven libraries are being developed based on ENDF/B-VIII.0.

- Will report more details on the next review meeting.

- Any questions?
Rensselaer

why not change the world?