A Spectral Verification of the HELIOS-2 Lattice Physics Code

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A Spectral Verification of the HELIOS-2 Lattice Physics Code

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INTRODUCTION

Core modeling of the Advanced Test Reactor (ATR) at INL is currently undergoing a significant update through the Core Modeling Update Project¹. The intent of the project is to bring ATR core modeling in line with today’s standard of computational efficiency and verification and validation practices. The HELIOS-2 lattice physics code² is the lead code of several reactor physics codes to be dedicated to modernize ATR core analysis. This presentation is concerned with an independent verification of the HELIOS-2 spectral representation including the slowing down and thermalization algorithm and its data dependency. Here, we will describe and demonstrate a recently developed simple cross section generation algorithm based entirely on analytical multigroup parameters for both the slowing down and thermal spectrum. The new capability features fine group detail to assess the flux and multiplication factor dependencies on cross section data sets using the fundamental infinite medium as an example.

FROM FISSION TO THERMALIZATION

In a typical thermal reactor, after neutron birth at high energy (about 1 Mev), neutrons lose energy on collision (slow down) until they reach energies near the temperatures of the surrounding material. At this point, neutrons become thermalized after surviving the resonance regions, and are available to produce fission to restart the cycle. The following slowing down equation describes the self-sustaining neutron cycle in an infinite medium:

\[
\Sigma(E)\phi(E) = \int_0^{E_0} dE' \Sigma_s(E' \to E') \phi(E') + \frac{\Sigma(E)}{k} \int_0^{E_0} dE' \nu(E') \Sigma_f(E') \phi(E').
\]

(1)

\(\Sigma\)s represent macroscopic cross sections, \(\nu\) is the number of neutrons per fission appearing at energy \(E\) with distribution \(\chi\) and \(\phi\) is the neutron flux distribution at energy \(E\). The highest neutron energy is assumed to be \(E_0\) at 20 Mev. We introduce the multiplication factor \(k\) to maintain a sustained neutron population, therefore defining an eigenvalue problem.

Elastic Scattering

Neutron elastic scattering is assumed for a homogeneous mixture while slowing down. Thermal scattering is considered subsequently. In multigroup form, Eq(1) becomes

\[
\sum_{g'g} \phi_{g'} = \sum_{g'=1}^{N_g} \sum_{g'g} \phi_{g'} + \frac{\Sigma_{g}}{k} \sum_{g'=1}^{N_g} \nu \Sigma_{fg} \phi_{g'}.
\]

(2a)

where \(\sum_{g'g}\) is the isotropic scattering transfer cross section from group \(g'\) to \(g\),

\[
\phi_{g'g} \equiv \int_{\Delta E_{g'}} dE' \int_{\Delta E_{g}} dE \Sigma_s(E' \to E) \phi(E')
\]

\(\Sigma_g\) is the group \(g\) cross section

\[
\phi_{g} \equiv \int_{\Delta E_{g}} dE \Sigma_i(E) \phi(E)
\]

\(i = \text{total, scattering or fission}\) and \(\phi_{g}\) is the group flux

\[
\phi_{g} = \int_{\Delta E_{g}} dE \phi(E).
\]

(2b)

The multigroup form assumes \(N_g\) subintervals \(\Delta E_g\) and the decomposition of the scattering integral (by element \(j\))

\[
\int_0^{E_0} dE \Sigma_g(E' \to E) \phi(E') = \sum_{g'=1}^{N_g} \int_0^{E_0} dE \Sigma_{fg'}(E' \to E) \phi(E').
\]

Based on the experimental nature of cross section data, i.e., interval measurement uncertainty, the group partition is made practical by assuming a flux weighting of an average flux across each interval (measurement uncertainty)

\[
\phi(E) = f_g(E) \phi_g
\]
requiring $f_g$ be normalized to unity. If one assumes piecewise constant cross sections in an interval $\Delta E_g$ and a weighting function of $1/E$,

$$f_g(E) \equiv \frac{\alpha_{0g}}{E}, \quad \alpha_{0g} \equiv \left[ \ln \left( \frac{E_{g-1}}{E_g} \right) \right]^{-1},$$

then, for elastic scattering from the $j^{th}$ material with scattering parameter $\alpha_j$, the group to group transfer cross section becomes

$$\Sigma_{gjg} \equiv \frac{\alpha_{0g}}{1-\alpha_j} \left[ \Theta \left( E_{g-1} - \alpha_j E_g \right) T_{\alpha_j} \left( \frac{E_{g-1}}{E_g} \right) + \Theta \left( E_{g+1} - \alpha_j E_g \right) T_{\alpha_j} \left( \frac{E_g}{E_{g+1}} \right) - \Theta \left( E_{g-1} - \alpha_j E_g \right) T_{\alpha_j} \left( \frac{E_g}{E_{g-1}} \right) + \Theta \left( E_{g+1} - \alpha_j E_g \right) T_{\alpha_j} \left( \frac{E_{g+1}}{E_g} \right) \right]$$

with

$$T_k(x,y) = \beta_{jk} \left[ \frac{1}{x} - \frac{1}{y} \right] - \gamma_{jk} \ln \left( \frac{y}{x} \right).$$

Table 1 gives the appropriate constants for $T_j(x,y)$.

<table>
<thead>
<tr>
<th>$k$</th>
<th>$\beta_{jk}$</th>
<th>$\gamma_{jk}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$E_{g-1}$</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>$E_g$</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>$E_{g-1}$</td>
<td>$\alpha_j$</td>
</tr>
<tr>
<td>4</td>
<td>$E_g$</td>
<td>$\alpha_j$</td>
</tr>
</tbody>
</table>

It should be emphasized that the particular advantage of Eq(2c) is that it represents multigroup slowing down entirely analytically.

**Thermal Scattering**

We now consider the simplest of thermal scattering models— the free hydrogen gas (H-gas) model. In this formulation, hydrogen is the primary scattering element doing so in its free gas molecular form. Hence, we create a thermal region with $N_T$ groups where the H-gas model applies, apart from the slowing down region. $E_T$ is the slowing down/thermal boundary.

The H-gas model assumes the following form:

$$f_g(E) \equiv f_{0g} e^{-\varepsilon}$$

where

$$F(\varepsilon) \equiv \text{erf} \left( \sqrt{\varepsilon} \right)$$

$$\varepsilon \equiv E / kT.$$
Then, detailed balance gives

\[
I_{fg} = \frac{1}{\sqrt{\pi}} (\sqrt{\varepsilon_{g-1}} e^{-\varepsilon_{g-1}} - \sqrt{\varepsilon_{g+1}} e^{-\varepsilon_{g+1}})
\]

\[
I_1 = \frac{1}{\sqrt{2}} (F(\sqrt{2\varepsilon_g}) - F(\sqrt{2\varepsilon_{g-1}}))
\]

Then, detailed balance gives

\[
\sum_{\chi \tau g'g} \frac{f_{0g} \sum_{\chi g}}{f_{0g} \sum_{\chi g'}} \sum_{\chi \tau g'g'}, \ g' \geq g + 1.
\]

Similarly, to the slowing down region, the thermal multigroup parameters have been found analytically, hence eliminating errors stemming from group parameter generation.

**NUMERICAL IMPLEMENTATION AND COMPARISON**

**Numerical Implementation**

The ENDF/B VII.1 library will be the source of the nuclear data\(^4\). The spectral coverage for the materials for this study will be \(10^{-4}\) ev \(\leq E \leq 20 Mev\). All that is required to determine the transfer cross sections is the total (integrated) scattering cross sections. The procedure to prepare this cross section in the multigroup setting begins by bringing the ENDF/B data local to be processed by a multigroup generation code called ENDFPR.f. The relevant ENDF data files are initially interrogated to determine the number of entries on each as well as the energy range which can vary across isotopes. The secondary function of ENDFPR.f is to assemble the cross section set. This is done by imposing the desired data set boundaries or specifying the widest possible available boundaries and then forming equal lethargy groups within the chosen boundaries. The final step in the cross section preparation is a Padé interpolation of degree 2 applied to all data to obtain values at the group boundaries now common to all materials.

In preparation for a demonstration, it was determined that neutron conservation for elastic scattering requires a “dump group” where scattered neutrons from elastic scattering initiated above the thermal cutoff can fall below the thermal cutoff. Hence, a last group extending from \(10^{-4}\) to \(10^{0}\) ev has been included to maintained neutron conservation.

One maintains neutron conservation for thermal scattering through a normalization of the differential scattering cross section to the total scattering cross section.

To complete the analysis, we assume the following fission spectrum:

\[
\chi(E) = \left(\frac{\pi b}{4a}\right)^{1/2} e^{-b/a} e^{-af} \sin(hbE)
\]

with \(a = 0.9, b = 1\) and \(E\) is in \(Mev\).

**Numerical Comparison to HELIOS-2**

The nuclear system for this demonstration will be a simple infinite medium U235/water mixture in the volume fraction ratio 0.001/0.999.

The most straightforward determination of the eigenvalue and eigenflux comes from writing Eq(1) as

\[
H \phi = \frac{1}{k} \chi f^T \phi
\]

Then, formally solving this equation gives the explicit representations

\[
k = f^T H^{-1} \chi
\]

\[
\phi = \frac{1}{k} H^{-1} \chi
\]

with \(F\) defined to be unity and the flux normalized to \(\phi_\tau / \phi_\tau\).

For the \(k\)-comparison, both the 49 and 177 group Helios sets are chosen. 7 and 14 groups are below the thermal cutoff of 0.1 ev respectively. Table 2 gives the multiplication factors for Helios and the simple model.

<table>
<thead>
<tr>
<th>Table II: (k)-Comparison</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simple(49)</td>
</tr>
<tr>
<td>Simple(177)</td>
</tr>
<tr>
<td>Helios(49)</td>
</tr>
<tr>
<td>Helios(177)</td>
</tr>
</tbody>
</table>

The agreement in \(k\) is rather remarkable given that the cross section data for the two calculations as well as the group structures are different and the thermal cutoff is a best guess. In addition, no attempt has been made to adjust the parameters to make the two calculations agree. If the simple model is run with the fast/thermal cutoff at 0.04 ev and only 3 groups of the 49 groups are below the cutoff, then \(k\) increases to 1.2203. For the corresponding
177 group case the $k$ increases to 1.2212. The sensitivity of $k$ indicates that the two calculations are probably within the first two digits and that most likely any additional digits are not correct. In addition, the value of $\nu$ in the simple model can be adjusted to give the Helios result exactly.

Even more remarkable, however, is the agreement between the group center flux shapes shown in Fig. 1—especially for the 177-group case. The shapes have been normalized to the peak flux in the fission spectrum energy region. Even for the 49-group case, the main spectral features are in reasonable agreement.

CONCLUSION
This initial comparison of the Helios code to a simple spectral model has produced surprisingly satisfying results. With no attempt to reconcile the two models, the flux shapes are in good agreement. This is true even with different ENDF/B cross section generations as well as for different group structures. The next step in the verification process will be to run the simple model with the same cross sections as Helios. In addition, the simple thermal scattering model will be upgraded to include other than Hydrogen scattering.

REFERENCES
3. NEUP Grant: CFP-09-807.