LANL Criticality Data Testing using CIELO Candidate Evaluations

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Abstract

We review criticality data testing performed at Los Alamos with a combination of ENDF/B-VII.1 + potential CIELO nuclear data evaluations.
Outline

- CIELO Overview
- Data Testing
- Current and Continuing Work
- Summary
CIELO Overview

- CIELO = Coordinated International Evaluated Library Organization (WPEC Subgroup 40).

- Goal: To develop updated, best available evaluated nuclear data files for a select group of nuclides … \( ^1H, ^{16}O, ^{56}Fe, ^{235},^{238}U \) and \( ^{239}Pu \).

- Why: The major international evaluated nuclear data libraries don’t agree on the internal cross section details of these most important nuclides!
CIELO Overview

Recent status …

- $^1$H: Little done to date, will most likely take what comes from the latest IAEA “Standards” recommendation.
  
  - A new WPEC Subgroup, SG42 “Thermal Scattering Kernel $S(\alpha,\beta)$: Measurement, Evaluation and Application”, dealing with thermal scattering kernels will also contribute … a new H-H$_2$O scattering kernel is already available for testing.

- $^{16}$O: ORNL has contributed a resonance based evaluation; LANL (Hale) has a partial re-evaluation … differences in evaluated $(n,\alpha)$ cross sections are an open issue.

- $^{56}$Fe: ORNL produced a new RRR evaluation up to 2 MeV last year; BNL has recently released a new evaluation to cover higher energies.
CIELO Overview

Recent status …

- $^{235}\text{U}$: Work is being coordinated by France; a revised RRR evaluation has been contributed by ORNL that includes new LANL and RPI data and resolves the large capture cross section difference in the low keV region with Japan (“o4brc2”); a revised pfns will come from the recent IAEA PFNS Coordinated Research Project (“g6” and variants).

- $^{238}\text{U}$: New RR parameters are available for data testing. Also updated (n,2n) and more evaluations incorporating advanced reaction theory and new measured data (part of the IAEA’s new IRDFF library).

- $^{239}\text{Pu}$: Will build on the improvements developed in the recently completed SG34 that yielded improved PST calculated eigenvalues. Reaction theory refinements, particularly for capture and inelastic scattering, continues. Also a new LANL evaluation for the pfns and its uncertainty is nearing completion.
CIELO Overview

- Previously data files have been shared informally among the interested parties.
  - Not the most efficient system.

- More recently the IAEA Nuclear Data Section has created a web page ... https://www-nds.iaea.org/CIELO/ ... with links to candidate evaluated data files.
A suite of 45 HEU-SOL-THERM benchmark critical configurations has been used for many years.

- Accurate calculated eigenvalues, correlated against Above-Thermal Leakage Fraction (ATLF), have been obtained since ENDF/B-VI.3 in the early 1990s.
- Tests of revised data sets must answer the question … “are we still ok or did we break something?”.

Also use a subset of LEU-COMP-THERM benchmarks

- The variable rod pitch in LCT7 allows testing of undermoderated, optimally moderated and overmoderated conditions.
- As with HST, we’re in pretty good shape for this benchmark class, so “… if it isn’t broke, don’t fix it!”.
Near unity intercept and near zero slope confirm no bias in calculated eigenvalues with e71.

- CNEA h-h$_2$O kernel:
  - $b = 1.0003(33)$
  - $m = -0.0005(87)$

- Hale $^{16}$O:
  - $b = 1.0002(33)$
  - $m = -0.0037(86)$

- ORNL v4 $^{16}$O:
  - $b = 1.0006(32)$
  - $m = -0.0029(85)$
235U (& 1H, 16O) – HST Benchmarks

More CIELO combinations:

- IAEA “g6” 235U
  - \( b = 1.0010(32) \)
  - \( m = +0.0073(84) \)

- IAEA “g6” 235U & Hale 16O
  - \( b = 1.0004(32) \)
  - \( m = +0.0051(85) \)

- IAEA “g6jn4” 235U
  - \( b = 1.0010(32) \)
  - \( m = +0.0071(85) \)

- IAEA “g6jn4” 235U & Hale 16O
  - \( b = 1.0005(32) \)
  - \( m = +0.0045(86) \)

IAEA “g6” is e71 but new pfns at thermal, 500 keV and 2 MeV; “g6mbc” (only new pfns at thermal) + Hale 16O has 
\( b=1.0005(32); m=+0.0047(86) \).
LCT7 Lattice Results - I

- LCT7.x, cases 1 through 4, vary the rod pitch ... undermoderated to overmoderated.
- CNEA h-h\textsubscript{2}O kernel increases the calculated eigenvalue by \~30 to 50 pcm.
- Hale \textsuperscript{16}O decreases the calculated eigenvalue by \~90 to \~120 pcm.
- IAEA “g6” \textsuperscript{235}U increases the calculated eigenvalue by \~120 to \~220 pcm.
- Combined impact of “g6” \textsuperscript{235}U, Hale \textsuperscript{16}O and “ibxx” \textsuperscript{238}U on calculated eigenvalue is \~50 to \~130 pcm.
- Specific results shown on next page ...
LCT7 Lattice Results - II

- On average the LCT benchmark class eigenvalues are near unity with ENDF/B-VII.1 cross sections – see Sub-Group 22’s final report.
- Therefore it is good to see little change when applying these new evaluated data sets.

<table>
<thead>
<tr>
<th>Benchmark</th>
<th>ENDF/B-VII.1</th>
<th>ENDF/B-VII.1 + CNEA h-h_2o</th>
<th>ENDF/B-VII.1 + Hale _16O</th>
<th>ENDF/B-VII.1 + IAEA _235U &quot;g6&quot; (.06c) + Hale _16O (.02c)</th>
<th>ENDF/B-VII.1 + IAEA _235U &quot;g6&quot; (.06c) + Hale _16O (.02c) + _238U ib36 (.02c)</th>
<th>ENDF/B-VII.1 + IAEA _235U &quot;g6&quot; (.06c) + Hale _16O (.02c) + _238U ib42 (.03c)</th>
<th>ENDF/B-VII.1 + IAEA _235U &quot;g6mbc&quot; (.09c) + Hale _16O (.02c)</th>
<th>( k_{\text{calc}} ) C/E</th>
</tr>
</thead>
<tbody>
<tr>
<td>LCT7.1</td>
<td>0.99750</td>
<td>0.99807</td>
<td>0.99632</td>
<td>0.99926</td>
<td>0.99768</td>
<td>0.99812</td>
<td>0.99812</td>
<td>0.99918</td>
</tr>
<tr>
<td>LCT7.2</td>
<td>0.99876</td>
<td>0.99921</td>
<td>0.99769</td>
<td>1.00094</td>
<td>0.99991</td>
<td>0.99987</td>
<td>1.00013</td>
<td>1.00109</td>
</tr>
<tr>
<td>LCT7.3</td>
<td>0.99763</td>
<td>0.99793</td>
<td>0.99660</td>
<td>0.99956</td>
<td>0.99833</td>
<td>0.99837</td>
<td>0.99850</td>
<td>0.99935</td>
</tr>
<tr>
<td>LCT7.4</td>
<td>0.99800</td>
<td>0.99856</td>
<td>0.99710</td>
<td>0.99919</td>
<td>0.99851</td>
<td>0.99853</td>
<td>0.99851</td>
<td>0.99931</td>
</tr>
</tbody>
</table>
239Pu (& 1H, 16O) – PST Benchmarks

- The average calculated eigenvalue for the Pu-SOL-THERM benchmark class has been biased high by about 500 pcm for many years (ENDF/B-VII.1 results shown).

We use a small subset of the Pu-SOL-THERM benchmark population to assess candidate files.
- PST1.4 & PST12.13 span the ATLF space.
- PST12.10 & PST34.15 span the ATFF space.
- PST4.1 & PST18.6 span the 239Pu atom percent space.
- PST12.10 & PST34.4 span the g Pu per liter space.
**239Pu (& 1H, 16O) – PST Benchmarks**

- **k\textsubscript{eff} C/E results with various SG34 and CIELO candidate files ...**

<table>
<thead>
<tr>
<th>Benchmark</th>
<th>E71 (w/ fixed 239Pu, 94239.62c)</th>
<th>E71 + SG34 239Pu (TK1a = 94239.02c)</th>
<th>E71 + SG34 239Pu (TK1a = 94239.02c) + CAB00 h-h\textsubscript{2}O</th>
<th>E71 + TK1a 239Pu + Hale 16O (8016.02c)</th>
<th>E71 + TK1a 239Pu with hybrid Romano+e71+DN3 pfns (94239.07c)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PMF1 (Jezebel, rev3)</td>
<td>1.00061</td>
<td>1.00083</td>
<td>---</td>
<td>---</td>
<td>1.00069</td>
</tr>
<tr>
<td>PMF6 (Flattop-Pu)</td>
<td>1.00111</td>
<td>1.00109</td>
<td>---</td>
<td>---</td>
<td>1.00098</td>
</tr>
<tr>
<td>PST1.4</td>
<td>1.00451</td>
<td>1.00209</td>
<td>1.00323</td>
<td>1.00021</td>
<td>1.00089</td>
</tr>
<tr>
<td>PST4.1</td>
<td>1.00411</td>
<td>1.00052</td>
<td>1.00045</td>
<td>0.99926</td>
<td>0.99918</td>
</tr>
<tr>
<td>PST9</td>
<td>1.01934</td>
<td>1.01547</td>
<td>1.01469</td>
<td>1.01517</td>
<td>1.01517</td>
</tr>
<tr>
<td>PST12.10</td>
<td>1.00417</td>
<td>1.00078</td>
<td>1.00067</td>
<td>0.99946</td>
<td>1.00011</td>
</tr>
<tr>
<td>PST12.13</td>
<td>1.00974</td>
<td>1.00623</td>
<td>1.00598</td>
<td>1.00528</td>
<td>1.00591</td>
</tr>
<tr>
<td>PST18.6</td>
<td>1.00484</td>
<td>1.00195</td>
<td>1.00239</td>
<td>1.00095</td>
<td>1.00152</td>
</tr>
<tr>
<td>PST34.4</td>
<td>1.00248</td>
<td>0.99933</td>
<td>0.99874</td>
<td>0.99810</td>
<td>0.99845</td>
</tr>
<tr>
<td>PST34.15</td>
<td>0.99733</td>
<td>0.99719</td>
<td>0.99551</td>
<td>0.99580</td>
<td>0.99669</td>
</tr>
<tr>
<td><strong>PST average:</strong></td>
<td><strong>1.00582</strong></td>
<td><strong>1.00295</strong></td>
<td><strong>1.00100</strong></td>
<td><strong>1.00172</strong></td>
<td><strong>1.00224</strong></td>
</tr>
<tr>
<td><strong>PST average (w/o PST9):</strong></td>
<td><strong>1.00388</strong></td>
<td><strong>1.00116</strong></td>
<td><strong>1.00100</strong></td>
<td><strong>0.99987</strong></td>
<td><strong>1.00039</strong></td>
</tr>
</tbody>
</table>

Essentially no eigenvalue bias with SG34 improvements to endf/b-vii.1 239Pu and Hale 16O.

Not shown, but “DN17” file is similar to, but slightly worse than the original E71 result, 😞.
### 235,238U – LANL Fast Crits

- "g6" is ok.
- "o4brc2 Big-10 is very bad.
- "g6jn4" Godiva is bad.

#### 238U files produce a small increase in fast and intermediate system calculated eigenvalues.

<table>
<thead>
<tr>
<th>Benchmark</th>
<th>ENDF/B-VII.1</th>
<th>ENDF/B-VII.1 + IAEA 235U &quot;g6&quot; (.06c)</th>
<th>ENDF/B-VII.1 + IAEA 235U &quot;o4brc2&quot; (.07c)</th>
<th>ENDF/B-VII.1 + IAEA 235U &quot;g6jn4&quot; (.08c)</th>
<th>ENDF/B-VII.1 + IAEA 235U ^235^U &quot;g6mbc&quot; (.09c)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HMF1 (Godiva)</td>
<td>0.99977</td>
<td>0.99951</td>
<td>0.99918</td>
<td>0.99509</td>
<td>0.99987</td>
</tr>
<tr>
<td>HMF28 (Flattop-25)</td>
<td>1.00270</td>
<td>1.00227</td>
<td>0.99942</td>
<td>0.99986</td>
<td>1.00296</td>
</tr>
<tr>
<td>IMF7 (Big-10)</td>
<td>0.99998</td>
<td>0.99742</td>
<td>0.98853</td>
<td>0.99728</td>
<td>0.99898</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Benchmark</th>
<th>ENDF/B-VII.1 + IAEA 235U &quot;g6&quot; (.06c)</th>
<th>ENDF/B-VII.1 + IAEA 235U &quot;g6&quot; (.06c) + 238U ib36 (.02c)</th>
<th>ENDF/B-VII.1 + IAEA 235U &quot;g6&quot; (.06c) + 238U ib42 (.03c)</th>
<th>ENDF/B-VII.1 + IAEA 235U &quot;g6&quot; (.06c) + 238U ib44 (.04c)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HMF1 (Godiva)</td>
<td>0.99951</td>
<td>0.99948</td>
<td>0.99965</td>
<td>0.99950</td>
</tr>
<tr>
<td>HMF28 (Flattop-25)</td>
<td>1.00227</td>
<td>1.00258</td>
<td>1.00350</td>
<td>1.00356</td>
</tr>
<tr>
<td>IMF7 (Big-10)</td>
<td>0.99742</td>
<td>0.99911</td>
<td>0.99875</td>
<td>0.99872</td>
</tr>
</tbody>
</table>
### 239Pu and 238U – LANL Fast Crits

<table>
<thead>
<tr>
<th>Benchmark</th>
<th>k&lt;sub&gt;calc&lt;/sub&gt; C/E</th>
<th>ENDF/B-VII.1 + TK1a&lt;sup&gt;239&lt;/sup&gt;Pu (DN17 pfns, .17c) + &lt;sup&gt;238&lt;/sup&gt;U ib36 (.02c)</th>
<th>ENDF/B-VII.1 + TK1a&lt;sup&gt;239&lt;/sup&gt;Pu (DN17 pfns, .17c) + &lt;sup&gt;238&lt;/sup&gt;U ib42 (.03c)</th>
<th>ENDF/B-VII.1 + TK1a&lt;sup&gt;239&lt;/sup&gt;Pu (DN17 pfns, .17c) + &lt;sup&gt;238&lt;/sup&gt;U ib44 (.04c)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PMF1 (Jezebel)</td>
<td>1.00061</td>
<td>0.99805</td>
<td>0.99926</td>
<td>0.99931</td>
</tr>
<tr>
<td>PMF6 (Flattop-Pu)</td>
<td>1.00111</td>
<td>0.99802</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- **C/E eigenvalue results for PMF1 (Jezebel) & PMF6 (Flattop-Pu) with various 239Pu and IAEA 238U files**
- “DN17” is latest Neudecker pfns.
Impact of pfns uncertainty on calculated eigenvalue and reaction rates …

- Use the LANL Pu-MET-FAST-001 (Jezebel) critical assembly
- ENDF/B-VII.1 cross sections plus the latest Neudecker $^{239}$Pu pfns yields a calculated eigenvalue of 0.99797(3).
- Generate a suite of 1000 pfns data sets, based upon evaluated uncertainty
  - Average $k_{\text{calc}}$ is 0.99798, population standard deviation is 0.00107.
  - The standard deviation in calculated spectral indices varies from a fraction of a percent to almost 10%, depending upon the reaction rate average energy …
    - e.g., $^{239}$Pu(n,f)/$^{235}$U(n,f) = 1.4203 ± 0.0017; $^{238}$U(n,f)/$^{235}$U(n,f) = 0.2031 ± 0.0022
    - e.g., $^{238}$U(n,2n)/$^{235}$U(n,f) = 0.0119 ± 0.0007; $^{169}$Tm(n,2n)/$^{235}$U(n,f) = 0.00307 ± 0.00029.
Summary

- Work to revise the evaluated data files for $^1\text{H}$, $^{16}\text{O}$, $^{56}\text{Fe}$, $^{235,238}\text{U}$, and $^{239}\text{Pu}$ continues …

- LANL testing to date has concentrated on ICSBEP benchmark eigenvalues. Reaction rate (spectral indices), pulsed spheres and Shielding (SINBAD) benchmarks are also important resources to be utilized in a comprehensive data testing regimen (and are being utilized by our international colleagues).

- The CIELO evaluated data files are expected to be an important component in the next ENDF/B release.