Verification of the Hexagonal Ray Tracing Module and the CMFD Acceleration in nTRACER

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Seongchan Kim, Changhyun Lim, Young Suk Ban and Han Gyu Joo*

Reactor Physics Laboratory
Department of Nuclear Engineering
Seoul National University

* joohan@snu.ac.kr
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☐ Conclusions
Introductions

- **Motivations**
  - Restricted Hexagonal core calculation applicability in nTRACER\(^a\)
    - Restricted to 2D calculation
    - Triangle based hexagonal CMFD kernel
  - Expanded hexagonal core calculation applicability

- **Purposes**
  - Verification of effectiveness of hexagonal CMFD acceleration
  - Verification of accuracy of hexagonal MOC calculation

- **Objectives**
  - Verify the hexagonal MOC calculation for various geometries
  - Asses the effectiveness of hexagonal CMFD acceleration
  - Asses the accuracy of hexagonal MOC calculation

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Sub-meshing in Hexagonal Assembly

- Elongated Boundary Pin Cell and Trapezoidal Gap Cell
  - Two types of boundary pin cells and gap cells
  - Azimuthal rotation
    - Number of boundary pin cell types: 12
    - Number of gap cell types: 12
    - Number of inner pin cell types: 1

- Source Meshes in Pin Cells

Assembly based modular ray tracing method
Explicit Geometry Treatment

Flexible Applicability

ex) ABR metallic benchmark\(^a\) (Fast reactor)
- Assemblies with various different pin pitches
- Multiple duct layers in assemblies

→ Applicable without any assumption or approximation

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Fuel Assembly     Reflector Assembly     Shield Assembly     Control Rod Assembly

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Hexagonal CMFD

Finite Difference Formula

\[
\sum_i \left( \tilde{D}_m^i - \hat{D}_m^i \right) S_{m+i} \phi_m - \sum_i \left( \tilde{D}_m^i + \hat{D}_m^i \right) S_{m+i} \phi_{m+i} + \Sigma_{t,m} \phi_m V_m = Q_m V_m
\]

\[
\tilde{D}_m = \frac{D_m D_{m+1}}{D_m l_{m+1} + D_{m+1} l_m}
\]

\[
\hat{D}_m = -\frac{-\hat{J}_m - \tilde{D}_m (\phi_{m+1} - \phi_m)}{\phi_{m+1} + \phi_m}
\]

Various types of CMFD meshes

Applicable for general geometries

---

C5G7 Hexagonal Variation Benchmark\textsuperscript{a})

\begin{itemize}
\item Cell and Assembly
\end{itemize}

\begin{itemize}
\item Core
\end{itemize}

\begin{itemize}
\item Number : Material in the Pellet
\item Residual Area : Moderator
\item 1/6 Symmetry
\item UA-1 vs. UA-2 : 3D cases
\end{itemize}

Three 3D Cases of C5G7 H Benchmark

- Control Rod Insertion Types

![Diagram of Control Rod Insertion Types]

- 3D Cases

<table>
<thead>
<tr>
<th>Problems / Assembly</th>
<th>UA-1</th>
<th>UA-2</th>
<th>MA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unrodded</td>
<td>TA</td>
<td>TA</td>
<td>TA</td>
</tr>
<tr>
<td>Rodded A</td>
<td>TB</td>
<td>TA</td>
<td>TA</td>
</tr>
<tr>
<td>Rodded B</td>
<td>TC</td>
<td>TB</td>
<td>TA</td>
</tr>
</tbody>
</table>
Calculation Conditions

- **nTRACER**
  - Number of azimuthal angles : 24 in $\pi$
  - Number of polar angles : 4 in $\pi/2$
  - Ray spacing : 0.05 cm
  - 1D $S_P^3$ SENM axial calculation
  - 4 sub-planes per plane

- **McCARD**
  - Number of inactive cycles (NI) : 500
  - Number of active cycles (NA) : 1000
  - Number of particles per cycle (NP) : 1,000,000

  - Both code utilized 1/6 symmetry

---

## Effectiveness of the Hexagonal CMFD Acceleration

### 2D Core Calculation

<table>
<thead>
<tr>
<th>Case</th>
<th># of outer MOC iterations</th>
<th>Computation Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sole MOC</td>
<td>222</td>
<td>569 x 1/20</td>
</tr>
<tr>
<td>CMFD Accelerated</td>
<td>11</td>
<td>34</td>
</tr>
</tbody>
</table>

**CMFD inner iterations = 521**

---

Convergence criteria = $10^{-6}$

- ⋯⋯⋯⋯⋯ k-eff Error
- – – – Fission Source Error
- — — — Residual Error

---

*a) Intel® Xeon E5- 2640 2.60 GHz, 128 GB of memory, 16 thread per node*
## 2D Core Calculation

### Comparison between nTRACER and McCARD

<table>
<thead>
<tr>
<th>K-eff</th>
<th>McCARD (σ, pcm)</th>
<th>nTRACER (Δρ, pcm)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1.16243 (2)</td>
<td>1.16231 (-9)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Absolute Pin power error(^a), %</th>
<th>Max.</th>
<th>RMS</th>
</tr>
</thead>
<tbody>
<tr>
<td>McCARD</td>
<td>1.94</td>
<td>0.50</td>
</tr>
<tr>
<td>nTRACER</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Relative Pin power error(^a), %</th>
<th>Max.</th>
<th>RMS</th>
</tr>
</thead>
<tbody>
<tr>
<td>McCARD</td>
<td>2.47</td>
<td>0.70</td>
</tr>
<tr>
<td>nTRACER</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\(^a\) Pin Power σ < 0.69%

**Diagram:**
- **McCARD pin by pin power**
- **nTRACER Absolute Pin Power Error**
- **nTRACER Relative Pin Power Error**

**Observations:**
- 
  - **Absolute Pin Power Error**
    - McCARD: MAX: 1.94%, RMS: 0.51%
    - nTRACER: MAX: 2.47%, RMS: 0.70%

  - **Relative Pin Power Error**
    - McCARD: MAX: 2.47%, RMS: 0.70%

  - **K-eff**
    - McCARD: 1.16243 (2)
    - nTRACER: 1.16231 (-9)
Comparison between nTRACER and DeCART\(^a\)

- **Calculation Conditions of DeCART**
  - Number of azimuthal angles: 12 in \(\pi\)
  - Number of polar angles: 2 in \(\pi/2\)
  - Ray spacing: 0.05 cm
  - 1D NEM-SP\(_3\) axial calculation

- **2D Core Calculation**

<table>
<thead>
<tr>
<th></th>
<th>nTRACER</th>
<th>DeCART</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\Delta \rho), pcm</td>
<td>-9</td>
<td>9</td>
</tr>
<tr>
<td>Max. Relative Error</td>
<td>2.47</td>
<td>1.83</td>
</tr>
<tr>
<td>RMS Relative Error</td>
<td>0.70</td>
<td>0.50</td>
</tr>
</tbody>
</table>

# 3D Core Calculations

<table>
<thead>
<tr>
<th></th>
<th>Unrodded</th>
<th>Rodded A</th>
<th>Rodded B</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>McCARD</strong>&lt;sup&gt;a,b&lt;/sup&gt;</td>
<td>k-eff (σ, pcm)</td>
<td>1.12273 (1)</td>
<td>1.11886 (1)</td>
</tr>
<tr>
<td><strong>nTRACER</strong></td>
<td>k-eff (Δρ, pcm)</td>
<td>1.12280 (6)</td>
<td>1.11890 (3)</td>
</tr>
<tr>
<td>Slice 1 Pin Power Error, %</td>
<td>Max.</td>
<td>2.73</td>
<td>2.66</td>
</tr>
<tr>
<td></td>
<td>RMS</td>
<td>0.67</td>
<td>0.68</td>
</tr>
<tr>
<td>Slice 2 Pin Power Error, %</td>
<td>Max.</td>
<td>2.74</td>
<td>2.61</td>
</tr>
<tr>
<td></td>
<td>RMS</td>
<td>0.69</td>
<td>0.67</td>
</tr>
<tr>
<td>Slice 3 Pin Power Error, %</td>
<td>Max.</td>
<td>2.58</td>
<td>2.33</td>
</tr>
<tr>
<td></td>
<td>RMS</td>
<td>0.66</td>
<td>0.66</td>
</tr>
<tr>
<td>2D Integrated Pin Power Error, %</td>
<td>Max.</td>
<td>2.56</td>
<td>2.29</td>
</tr>
<tr>
<td></td>
<td>RMS</td>
<td>0.64</td>
<td>0.63</td>
</tr>
</tbody>
</table>

a) NI = 500, NA = 1000, NP = 2,000,000  
b) Pin Power σ < 0.50%  

* Normalized to unity for 3D core  
* Relative pin power error
Case: Rodded B

Slice 1
- MAX: 3.15%
- RMS: 0.79%

Slice 2
- MAX: 2.99%
- RMS: 0.71%

Slice 3
- MAX: 2.56%
- RMS: 0.75%

2D Integrated
- MAX: 2.70%
- RMS: 0.67%
Radially Integrated Pin Power Error

- **McCARD Results**
  - Each sub-plane: 3.57 cm
  - Increased control rod insertion → Increased axial power slope

- **nTRACER Errors**
  - Maximum: 1.01%
# 12 Azimuthal Divisions in Pin Cells

## 2D Core Calculation

<table>
<thead>
<tr>
<th>K-eff</th>
<th>McCARD (σ, pcm)</th>
<th>1.16243 (2)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>nTRACER (Δρ, pcm)</td>
<td>1.16257 (10)</td>
</tr>
<tr>
<td>Relative Pin power error$^a$</td>
<td>Max.</td>
<td>1.56</td>
</tr>
<tr>
<td></td>
<td>RMS</td>
<td>0.39</td>
</tr>
</tbody>
</table>

## 3D Core Calculations

<table>
<thead>
<tr>
<th>McCARD$^a$)$^b$</th>
<th>k-eff (σ, pcm)</th>
<th>Unrodded</th>
<th>Rodded A</th>
<th>Rodded B</th>
</tr>
</thead>
<tbody>
<tr>
<td>nTRACER</td>
<td>k-eff (Δρ, pcm)</td>
<td>1.12273 (1)</td>
<td>1.11886 (1)</td>
<td>1.10264 (1)</td>
</tr>
<tr>
<td>Slice 1 Pin Power Error, %</td>
<td>Max.</td>
<td>1.51</td>
<td>1.69</td>
<td>2.25</td>
</tr>
<tr>
<td></td>
<td>RMS</td>
<td>0.36</td>
<td>0.37</td>
<td>0.50</td>
</tr>
<tr>
<td>Slice 2 Pin Power Error, %</td>
<td>Max.</td>
<td>1.69</td>
<td>1.65</td>
<td>2.13</td>
</tr>
<tr>
<td></td>
<td>RMS</td>
<td>0.39</td>
<td>0.38</td>
<td>0.45</td>
</tr>
<tr>
<td>Slice 3 Pin Power Error, %</td>
<td>Max.</td>
<td>1.88</td>
<td>2.12</td>
<td>2.53</td>
</tr>
<tr>
<td></td>
<td>RMS</td>
<td>0.44</td>
<td>0.43</td>
<td>0.57</td>
</tr>
<tr>
<td>2D Integrated Pin Power Error, %</td>
<td>Max.</td>
<td>1.46</td>
<td>1.43</td>
<td>1.85</td>
</tr>
<tr>
<td></td>
<td>RMS</td>
<td>0.33</td>
<td>0.32</td>
<td>0.38</td>
</tr>
</tbody>
</table>

---

*a) NI = 500, NA = 1000, NP = 2,000,000 * Normalized to unity for 3D core  
*b) Pin Power σ < 0.50%  
* Relative pin power error
2D ABR C5G7 Variation Benchmark

- **ABR Metallic Benchmark**
  - ABR (Advanced Burner Reactor)
  - Designed for the study of future fast reactor designs
  - Fuel Assembly pitch: 16.2471 cm
  - Fuel Pin Pitch: 0.8966 / 1.5528 / 4.8578 / 3.3603 cm
  - Selected to verify hexagonal calculations for various geometries

- **Core Configuration**

- **C5G7 Variation**

<table>
<thead>
<tr>
<th>Metallic</th>
<th>C5G7 Variation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inner Fuel</td>
<td>UO₂-Clad</td>
</tr>
<tr>
<td>Outer Fuel</td>
<td>4.3% MOX</td>
</tr>
<tr>
<td>Na</td>
<td>Moderator</td>
</tr>
<tr>
<td>HT-9</td>
<td>Guide Tube</td>
</tr>
<tr>
<td>Natural B₄C</td>
<td>Control Rod</td>
</tr>
</tbody>
</table>
2D ABR C5G7 Variation Benchmark Calculation

- **Effectiveness of Hexagonal CMFD Acceleration**

  Convergence criteria = $10^{-6}$

<table>
<thead>
<tr>
<th>Case</th>
<th># of outer MOC iterations</th>
<th>Computation Time (s)</th>
<th>Relative Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sole MOC</td>
<td>735</td>
<td>35,101</td>
<td>$x \frac{1}{105}$</td>
</tr>
<tr>
<td>CMFD Accelerated</td>
<td>7</td>
<td>344</td>
<td>$x \frac{1}{102}$</td>
</tr>
</tbody>
</table>

- **Comparison between nTRACER and McCARD**

<table>
<thead>
<tr>
<th>K-eff</th>
<th>McCARD&lt;sup&gt;b,c&lt;/sup&gt; ($\sigma$, pcm)</th>
<th>nTRACER ($\Delta\rho$, pcm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>K-eff</td>
<td>1.19693 (3)</td>
<td>1.19773 (56)</td>
</tr>
</tbody>
</table>

  b) $N_I = 500$, $N_A = 1000$, $N_P = 2,000,000$
  
  c) Pin Power $\sigma < 0.27\%$

  1. Underestimation of radial leakage
  2. Error along control rod assemblies
     - Relatively large source mesh area

  a) Intel® Xeon E5- 2640 2.60 GHz, 128 GB of memory, 16 thread per node
‘Full-Core’ VVER-440 Benchmark

Details of ‘Full-Core’ Benchmark

- 2D & vacuum boundary condition on the radial outer boundary
- Explicit radial reflector description
  - ‘Vygorodka’ : Internal edged metal sheet
  - Core basket (neglected), core barrel, and pressure vessel
- Fuel Pin Pitch : 1.23 cm
- Fuel Assembly (FA) pitch : 14.7 cm
- Pressure vessel outer radius : 191.1 cm
- Temperature of all materials : 543.15 K
- Selected to verify hexagonal calculations based on 47 group XS

Radial Reflectors

‘Vygorodka’

Core Barrel and Pressure Vessel
Effectiveness of the Hexagonal CMFD Acceleration

2D Core Calculation with $P_0$ Condition

Convergence criteria = $5 \times 10^{-5}$

<table>
<thead>
<tr>
<th>CASE</th>
<th>$P_0$</th>
<th>$P_1$</th>
<th>$P_2$</th>
<th>$P_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sole MOC</td>
<td>537</td>
<td>537</td>
<td>537</td>
<td>537</td>
</tr>
<tr>
<td>CMFD accelerated</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td>4</td>
</tr>
</tbody>
</table>

Computation Time (min.)

<table>
<thead>
<tr>
<th>CASE</th>
<th>$P_0$</th>
<th>$P_1$</th>
<th>$P_2$</th>
<th>$P_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sole MOC</td>
<td>4,777</td>
<td>5,356</td>
<td>6,009</td>
<td>9,211</td>
</tr>
<tr>
<td>CMFD accelerated</td>
<td>112</td>
<td>122</td>
<td>130</td>
<td>137</td>
</tr>
</tbody>
</table>

a) Intel® Xeon E5- 2640 2.60 GHz, 128 GB of memory, 16 thread per node

SNURPL
### ‘Full-Core’ VVER-440 Benchmark Calculation

#### Table:

<table>
<thead>
<tr>
<th>CASE</th>
<th>P_0</th>
<th>P_1</th>
<th>P_2</th>
<th>P_3</th>
</tr>
</thead>
<tbody>
<tr>
<td>K-eff</td>
<td>McCARDa)b</td>
<td>1.08857(2)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>nTRACER</td>
<td>1.08724</td>
<td>1.08665</td>
<td>1.08704</td>
</tr>
<tr>
<td></td>
<td>Δρ, pcm</td>
<td>-113</td>
<td>-163</td>
<td>-130</td>
</tr>
<tr>
<td>ΔPb)</td>
<td>Max, %</td>
<td>3.93</td>
<td>2.44</td>
<td>2.78</td>
</tr>
<tr>
<td></td>
<td>RMS, %</td>
<td>1.62</td>
<td>0.69</td>
<td>1.00</td>
</tr>
</tbody>
</table>

a) NI = 500, NA = 3000, NP = 500,000
b) Pin Power σ < 0.29%

#### Diagrams:

- **McCARD pin by pin power**
  - Bigger pin power at periphery
  - Smaller pin power at center

- **nTRACER pin power error : P_3**
  - MAX: 2.72%
  - RMS: 0.98%

**Power tilt**
- Bigger pin power at periphery
- Smaller pin power at center
# Renewal of nTRACER XS Library

## OLD

### P<sub>0</sub> – Inflow T.C.

<table>
<thead>
<tr>
<th></th>
<th>764s</th>
<th></th>
<th>800s</th>
</tr>
</thead>
<tbody>
<tr>
<td>P&lt;sub&gt;0&lt;/sub&gt;</td>
<td><img src="table1.png" alt="Table" /></td>
<td>P&lt;sub&gt;3&lt;/sub&gt;</td>
<td><img src="table2.png" alt="Table" /></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>k</td>
<td>1.00204</td>
<td>std : 2 pcm</td>
<td>k</td>
<td>1.0095</td>
<td>std : 2 pcm</td>
<td>k</td>
<td>1.00173</td>
<td>std : 2 pcm</td>
<td></td>
</tr>
<tr>
<td>Δρ</td>
<td>-86</td>
<td></td>
<td>Δρ</td>
<td>-109</td>
<td></td>
<td>Δρ</td>
<td>-31</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### SGFSP Time

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
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<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>764s</td>
<td>421s</td>
<td>435s</td>
<td></td>
</tr>
</tbody>
</table>

## NEW

### P<sub>0</sub>

<table>
<thead>
<tr>
<th></th>
<th>421s</th>
<th></th>
<th>435s</th>
</tr>
</thead>
<tbody>
<tr>
<td>P&lt;sub&gt;0&lt;/sub&gt;</td>
<td><img src="table3.png" alt="Table" /></td>
<td>P&lt;sub&gt;3&lt;/sub&gt;</td>
<td><img src="table4.png" alt="Table" /></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
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<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>k</td>
<td>1.00167</td>
<td>std : 2 pcm</td>
<td>k</td>
<td>1.00173</td>
<td>std : 2 pcm</td>
<td>k</td>
<td>1.00173</td>
<td>std : 2 pcm</td>
<td></td>
</tr>
<tr>
<td>Δρ</td>
<td>-37</td>
<td></td>
<td>Δρ</td>
<td>-31</td>
<td></td>
<td>Δρ</td>
<td>-31</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Conclusion

- **Hexagonal CMFD Acceleration**
  - 2D C5G7 H benchmark: factor of 20 in # of MOC, factor of 17 in time
  - 2D ABR C5G7 variation benchmark: 105 / 103
  - 2D ‘Full-Core’ VVER-440 benchmark: 134 / 67
  - Hexagonal CMFD kernel is confirmed to efficiently accelerate calculations

- **Hexagonal MOC Calculation**
  - -9 pcm reactivity error, 0.70 % RMS pin power error in for 2D C5G7 H
  - 6 pcm / 0.79 % for 3D C5G7 H benchmark
  - 56 pcm / 0.56 % for 2D ABR C5G7 variation benchmark
  - -132 pcm / 0.98 % for ‘Full-Core’ VVER-440 benchmark
  - Hexagonal MOC module is confirmed to accurately simulate the core

- **Future Work**
  - Simulate gap cells with high accuracy
  - Update nTRACER XS Library for hexagonal core calculation