$A^3\text{MCNP}$

(Automated Adjoint Accelerated MCNP)

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Overview - History

• $A^3$MCNP was developed by John Wagner* and Alireza Haghighat in 1997 (Wagner’s PhD dissertation)

• Since then we have used the code system for various important problems successfully

• The $A^3$ Patch is marketed through the HSW Technologies; five copies have been sold thus far

• In 2003, we implemented a new volumetric source distribution (sponsored by Mitsubishi Heavy Industries – MHI)

• We are planning to combine the neutral and charge particle algorithms
Contents

CADIS Methodology

$A^3$MCNP

Application of $A^3$MCNP
**CADIS – Consistent Adjoint Driven Importance Sampling**

**Description:**

*Uses a 3-D $S_N$ importance function distribution for source biasing and transport biasing in a consistent manner*, within the weight-window $(r, E)$ technique.

*their biasing formulations are derived based on importance sampling applied to the source integral and transport integral.*
**Source biasing**

**Detector (\(\sigma_d\)) response formulation**

\[
H \psi = s
\]

where \( p = (\vec{r}, E, \Omega) \)

\[
R = \int \sigma_d(p) \psi(p) dp
\]

\[
H^+ \psi^+ = \sigma_d
\]

\[
R = \int q(p) \psi^+(p) dp
\]


**CADIS**

**Source biasing**

**Biased source**

\[ \hat{q}(p) = \frac{\phi^+(p)q(p)}{\int_{p} \phi^+(p)q(p)dp} = \frac{\phi^+(p)q(p)}{R} \]

**Particle weight**

\[ W(p) = \frac{R}{\phi^+(p)} \]
CADIS – Consistent Adjoint Driven Importance Sampling

Transport biasing

Transport equation

\[
\phi(p) = \int_{p'} K(p' \rightarrow p)\phi(p')dp' + q(p)
\]

Transport equation for the biased source

\[
\hat{\phi}(p) = \int_{p'} \hat{K}(p' \rightarrow p)\hat{\phi}(p')dp' + \hat{q}(p)
\]

where

\[
\hat{\psi}(p) = \frac{\psi^+(p)\psi(p)}{R} \quad \hat{q}(p) = \frac{\psi^+(p)q(p)}{R}
\]

\[
\hat{K}(p' \rightarrow p) = K(p' \rightarrow p)\left[\frac{\phi^+(p)}{\phi^+(p')}\right]
\]
Transport biasing

\[ \hat{K}(p' \rightarrow p) = K(p' \rightarrow p) \left[ \frac{\phi^+(p)}{\phi^+(p')} \right] \]

- If \( \left( \frac{\psi^+(p)}{\psi^+(p')} \right) < 1 \), particles are processed through the Russian roulette,
- Otherwise, particles are split

- Particle statistical weight

\[ w(p) = \left( \frac{\psi^+(p')}{\psi^+(p)} \right) w(p') \]
**Note:**

The word "consistent" in CADIS refers to the transport biasing formulation is derived consistently based on the biased source.
A³MCNP – Automated Adjoint Accelerated MCNP

• CADIS methodology effective, but

• Automation tools are needed for determination of “importance” function

• Hence, we developed A³MCNP
A³MCNP Calculations

Step 1
- mesh distribution
- material composition
- input files

Step 2
- multi-group cross sections
- $S_N$ adjoint function

Step 3
- VR parameters
- non-analog MC Calculation
Application of $A^3$MCNP

• **PWR Cavity dosimetry**
  
  For determination of neutron interaction rates with dosimetry materials placed at the reactor cavity, and estimation of fluence at the reactor pressure vessel

• **BWR Core Shroud**
  
  Determination of neutron and gamma fields at the reactor pressure vessel

• **Storage cask**
  
  Determination of neutron and gamma fields at the cask’s outside surface
Application

PWR cavity dosimetry

- Objective: Estimation of neutron reaction rates at the cavity dosimeter for benchmarking of the PV fluence.
- Problem size: $R=350$ cm, $\theta=45^\circ$, $z=400$ cm
- Deep penetration
- Detector size (radius of $\sim2$ cm, $\sim$height of the model)
- $R-\theta$, Sn DORT calculation: 8500 meshes, S8, 47-group/P3; CPU time = 15 min
Application

PWP cavity dosimetry (continued)

\[
\frac{FOM(CADIS)}{FOM(MCNP)} \cong 50,000
\]

Relatively speaking, DORT CPU time is negligible, hence

\[
\frac{CPU(CADIS)}{CPU(MCNP)} \cong 50,000
\]
Application

BWR Core Shroud

Determination of neutron and gamma DPA at the core shroud
Application

Different A³MCNP meshing for the core shroud problem was developed to examine the performance of the code, e.g.

<table>
<thead>
<tr>
<th>Case</th>
<th>Total # of meshes (# axial meshes)</th>
<th>Mesh size (x, y, z) (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>86400 (24)</td>
<td>5, 5, 15.875</td>
</tr>
<tr>
<td>2</td>
<td>43200 (12)</td>
<td>5, 5, 31.75</td>
</tr>
<tr>
<td>3</td>
<td>38400 (24)</td>
<td>7.5, 7.5, 15.875</td>
</tr>
<tr>
<td>4</td>
<td>10800 (12)</td>
<td>10, 10, 31.75</td>
</tr>
<tr>
<td>5</td>
<td>2700 (12)</td>
<td>20, 20, 31.75</td>
</tr>
<tr>
<td>6</td>
<td>1200 (12)</td>
<td>30, 30, 31.75</td>
</tr>
<tr>
<td>7</td>
<td>300 (12)</td>
<td>60, 60, 31.75</td>
</tr>
</tbody>
</table>

Table 2 - Different back-thinned cases.

<table>
<thead>
<tr>
<th>Case</th>
<th>No. of Meshes (axial mesh)</th>
<th>Max. mesh size (cm) in Fuel, moderator, steel</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Ref. Back-thinned</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>86400(24) 65067(24)</td>
<td>5.0, 10.0, 5.0</td>
</tr>
<tr>
<td>9</td>
<td>43200(12) 32557(12)</td>
<td>5.0, 10.0, 5.0</td>
</tr>
<tr>
<td>10</td>
<td>38400(24) 18525(24)</td>
<td>15.0, 15.0, 7.5</td>
</tr>
</tbody>
</table>
Application

BWR Core-Shroud (continued)

- 3-D Sn TORT calculations: different # of meshes, S8, 47-group/P3, different CPUs
- Detector size (?)

- Sample:

Importance function distributions for different fixed mesh cases
Application

BWR Core-shroud (continued)

Results:

Table 3 - Estimated DPA and associated statistics after 100 CPU minutes for the unbiased case and cases 1 to 10.

<table>
<thead>
<tr>
<th>Case No.</th>
<th># of meshes (# of axial meshes)</th>
<th>DPA [dpa/sec]</th>
<th>Relative Error [%]</th>
<th>FOM</th>
<th>MCNP Speedup FOM_{biased}/FOM_{unbiased}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unbiased</td>
<td>N/A</td>
<td>3.877E-10</td>
<td>14.97*</td>
<td>0.022*</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>86400 (24)</td>
<td>3.571E-10</td>
<td>1.05</td>
<td>90.7</td>
<td>4123</td>
</tr>
<tr>
<td>2</td>
<td>65067 (24)</td>
<td>3.504E-10</td>
<td>1.19</td>
<td>70.6</td>
<td>3209</td>
</tr>
<tr>
<td>3</td>
<td>43200 (12)</td>
<td>3.452E-10</td>
<td>1.26</td>
<td>63.1</td>
<td>2868</td>
</tr>
<tr>
<td>4</td>
<td>10800 (12)</td>
<td>3.440E-10</td>
<td>1.35</td>
<td>54.9</td>
<td>2945</td>
</tr>
<tr>
<td>5</td>
<td>2700 (12)</td>
<td>3.513E-10</td>
<td>2.46</td>
<td>16.5</td>
<td>750</td>
</tr>
<tr>
<td>6</td>
<td>1200 (12)</td>
<td>3.512E-10</td>
<td>2.56</td>
<td>15.3</td>
<td>696</td>
</tr>
<tr>
<td>7</td>
<td>300 (12)</td>
<td>3.470E-10</td>
<td>5.88</td>
<td>2.89</td>
<td>131</td>
</tr>
<tr>
<td>8</td>
<td>38400 (24)</td>
<td>3.517E-10</td>
<td>1.25</td>
<td>64.0</td>
<td>2909</td>
</tr>
<tr>
<td>9</td>
<td>32557 (12)</td>
<td>3.469E-10</td>
<td>1.57</td>
<td>40.6</td>
<td>1845</td>
</tr>
<tr>
<td>10</td>
<td>18525 (24)</td>
<td>3.593E-10</td>
<td>1.52</td>
<td>43.3</td>
<td>1968</td>
</tr>
</tbody>
</table>

* result after 2000 CPU minutes
Application

BWR core-shroud (continued)

Results:

Table 4 - Comparison of total CPU time \((TORT+A^3MCNP^{TM})\) to achieve 1.0\% \((1\sigma)\) statistical uncertainty for the unbiased case and cases 1 to 10.

<table>
<thead>
<tr>
<th>Case No.</th>
<th>No. of meshes (# of axial meshes)</th>
<th>TORT [minutes]</th>
<th>(A^3MCNP) [minutes]</th>
<th>Total [minutes]</th>
<th>Overall Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unbiased</td>
<td>N/A</td>
<td>N/A</td>
<td>448,201</td>
<td>448,201</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>86400 (24)</td>
<td>424.6</td>
<td>110.3</td>
<td>534.9</td>
<td>838</td>
</tr>
<tr>
<td>2</td>
<td>65067 (24)</td>
<td>309.0</td>
<td>141.6</td>
<td>450.6</td>
<td>995</td>
</tr>
<tr>
<td>3</td>
<td>43200 (12)</td>
<td>257.2</td>
<td>158.8</td>
<td>416.0</td>
<td>1077</td>
</tr>
<tr>
<td>4</td>
<td>10800(12)</td>
<td>40.8</td>
<td>182.7</td>
<td>223.5</td>
<td>2005</td>
</tr>
<tr>
<td>5</td>
<td>2700 (12)</td>
<td>10.2</td>
<td>604.8</td>
<td>615.0</td>
<td>729</td>
</tr>
<tr>
<td>6</td>
<td>1200 (12)</td>
<td>5.0</td>
<td>655.2</td>
<td>660.2</td>
<td>679</td>
</tr>
<tr>
<td>7</td>
<td>300 (12)</td>
<td>1.3</td>
<td>3461.4</td>
<td>3462.7</td>
<td>129</td>
</tr>
<tr>
<td>8</td>
<td>38400 (24)</td>
<td>256.7</td>
<td>156.3</td>
<td>413.0</td>
<td>1085</td>
</tr>
<tr>
<td>9</td>
<td>32557 (12)</td>
<td>205.5</td>
<td>246.5</td>
<td>452.0</td>
<td>992</td>
</tr>
<tr>
<td>10</td>
<td>18525 (24)</td>
<td>128.7</td>
<td>231.0</td>
<td>359.7</td>
<td>1246</td>
</tr>
</tbody>
</table>
Application

Shipping cask

• Objective: Estimation of Neutron and gamma dose on the cask surface
• Problem Size: 180 x 180 x 840 cm³
• A Deep penetration problem
Application

Shipping cask (continued)

• TORT 3-D Sn calculation: 32256 meshes S8, 18-group/P3, CPU = 20.7 min

• Detector region: a shell over the whole surface of the cask

Adjoint source placed on the surface, thin (10 cm) air region, and axial height of [30.5 – 592.5 cm]
A$^3$MCNP SHIPPING CASK MESHING FOR TORT
A\textsuperscript{3}MCNP SHIPPING CASK MESHING FOR TORT (continued)
Shipping cask (continued)

Sample: Importance function distribution for group 1 gamma rays
Source Distribution

Unbiased

Biased
A³MCNP Performance

Behavior of FOM for estimation of axial dose

Axial mid-points of tally cells on the surface of the CASK, located between 30.48 and 592.5 cm.
A$^3$MCNP was used to examine determination of localized regions by performing different calculations.
Neutron Source

10  5.00E-05
9   4.09E-03
8   3.31E-02
7   1.63E-01
6   2.29E-01
5   2.57E-01
4   2.33E-01
3   7.03E-02
2   9.61E-03
1   5.00E-05

Importance Function
Distributions for different adjoint sources

Biased Sources
## Determination of surface dose, axial mid-plane (only)

*(1-\( \sigma \) Relative Error = 1%)*

<table>
<thead>
<tr>
<th>Model</th>
<th># CPU</th>
<th>Dose Ratio</th>
<th>FOM</th>
<th>Run Time (hrs)</th>
<th>Speedup</th>
<th>Values/ Hour</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unbiased Cont. Energy MCNP</td>
<td>8</td>
<td>1.00</td>
<td>0.78</td>
<td>214</td>
<td>1.0</td>
<td>19</td>
</tr>
<tr>
<td>Unbiased Multigroup MCNP</td>
<td>8</td>
<td>0.70</td>
<td>0.46</td>
<td>362</td>
<td>0.6</td>
<td>30</td>
</tr>
<tr>
<td>A³MCNP Cont. Energy</td>
<td>1</td>
<td>1.00</td>
<td>109</td>
<td>1.5</td>
<td>140</td>
<td>1,856</td>
</tr>
<tr>
<td>PENTRAN ‘Large’ Model</td>
<td>8</td>
<td>0.74</td>
<td>165</td>
<td>1.3</td>
<td>42,100</td>
<td></td>
</tr>
<tr>
<td>PENTRAN ‘Small’ Model</td>
<td>8</td>
<td>0.74</td>
<td>123</td>
<td>1.7</td>
<td>35,000</td>
<td></td>
</tr>
</tbody>
</table>
Tally locations: Four Annular Segments Near Top
(494 cm – 563 cm)

- No results for the unbiased MCNP case, after 220 hours on 8 processors

A³MCNP on 1 processor

<table>
<thead>
<tr>
<th>[(mRem/hr)/n/cm²/s]</th>
<th>FOM</th>
<th>PENTRAN/A³MCNP</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.14E-06 (2.73%)ᵃ</td>
<td>8.974</td>
<td>0.84</td>
</tr>
<tr>
<td>1.70E-06 (3.36%)ᵇ</td>
<td>1.843</td>
<td>0.82</td>
</tr>
<tr>
<td>9.97E-07 (5.08%)ᵇ</td>
<td>0.806</td>
<td>0.79</td>
</tr>
<tr>
<td>5.11E-07 (3.52%)ᵇ</td>
<td>1.682</td>
<td>0.80</td>
</tr>
</tbody>
</table>

ᵃ 2.5 hrs, 1 CPU
ᵇ 8 hrs, 1 CPU
Remarks

• To solve large/complex real-world problems in a reasonable amount of amount, we need to use hybrid methods

• Using deterministic importance function, A³MCNP can solve large complex problems faster (few orders of magnitudes) than the unbiased MCNP.

• Besides the computation speed, systems like PENTRAN & A³MCNP significantly reduce the engineer’s time and improve confidence in results.