Using RAPID for solving VT$^3$G-SNFP benchmark

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For presentation at the OECD Workshops on Benchmarks and Uncertainty Quantification, May 18-22, 2015, Universidad Politecnica de Madrid (UPM), Madrid, Spain
Criticality Calculation

• Standard approach - Full Monte Carlo calculations face difficulties in this area
  • Convergence is difficult due to low coupling between regions (due to absorbers)
    • Convergence can also be difficult to detect
  • Computation times are very long, especially to get detailed information
  • Changing pool configuration requires complete recalculation

• Developed a Multi-stage Response-function Transport approach using the Fission Matrix (FM) technique
Derivation of Fission Matrix (FM) Formulation

• Eigenvalue formulation in operator form is expressed by

\[ H\psi = \frac{1}{k} F\psi \]

Where,

\[ H = \frac{\Omega}{\mu} \cdot \nabla + \sigma_t(\vec{r}, E) - \int_0^\infty dE' \int_{4\pi} d\Omega' \sigma_s(\vec{r}, E' \rightarrow E, \mu_0) \]

\[ F = \frac{\chi(E)}{4\pi} \int_0^\infty dE' \int_{4\pi} d\Omega' v \sigma_f(\vec{r}, E') \]
FM Derivation (cont)

• We may write above equation as

\[ H \psi = \frac{1}{k} \chi \tilde{F} \psi \]

Where,

\[ \tilde{F} = \frac{1}{4\pi} \int_0^\infty dE' \int_{4\pi} d\Omega' \nu \sigma_f(\vec{r}, E') \]

• Then, solve for

\[ \psi = \frac{1}{k} H^{-1} \chi \tilde{F} \psi \]

• Then, we obtain fission density by operating \( \tilde{F} \) onto the above equation to obtain

\[ S = \frac{1}{k} AS \]

Where,

\[ S = \tilde{F} \psi \]

\[ A = \tilde{F} H^{-1} \chi \]
FM Formulations

• **Eigenvalue** formulation

\[ AS(\overline{P}) = \int d\overline{P}'a(\overline{P}' \rightarrow \overline{P})S(\overline{P}') \]

- \( k \) is eigenvalue
- is fission source, is fixed source in cell \( j \)
- is the number of fission neutrons produced in cell due to a fission neutron born in cell.

• **Subcritical multiplication** formulation

- is the number of fission neutrons produced in cell due to a source neutron born in cell.
Developed a Multi-stage methodology for determination of FM coefficients

- As the computational cell size, use a single pin
  - $N = 9 \times 9 \times 336 = 27,216$ total fuel pins/ fission matrix cells
  - Considering 24 axial segments per rod, then
  - $N = 653,184$
  - Allows for good accuracy and pin-resolved fission rates

- Standard FM would require $N = 653,184$ separate fixed-source calculations to determine the coefficient matrix
  - One calculation for each pin
  - A matrix of size $N \times N = 4.26649E+11$ total coefficients (6 GB of memory is needed)

- The standard approach is clearly NOT feasible

- We have developed a multi-stage approach to obtain detailed FM coefficients (in the process of filing for a patent)
Remarks on the multi-stage methodology

• **Coefficients are calculated at different stages including:**
  - Pin-wise (axially dependent) for one assembly for different burnups, cooling times, lattice structures, and enrichments
  - For assemblies in the pool (pin-wise or regional)

• **Reduction in computation time and memory**
  - **Computation time**
    - Geometric similarity
    - Geometric symmetry
    - Degree of coupling
    - Sensitivity of the coefficients to different parameters
  - **Memory by indexing**
Solution method - FM approach for eigenvalue problems

• After determination of $FM$ coefficients, then we solve a system of equations based on the power iteration to obtain $k$ and fission density (fundamental eigenfuction)

\[ F_i^{(0)} = \frac{1}{N} \quad \& \quad k^{(0)} = 1 \]

\[ F_i^{(m+1)} = \frac{1}{k^{(m)}} \sum_{j=1}^{N} a_{i,j} F_j^{(m)} \]

Where, \( k^{(m)} = \sum_{i=1}^{N} F_i^{(m)} \)
RAPID tool

• Developed the RAPID (Real-time Analysis for spent fuel Pool In situ Detection) tool for determination of
  • Eigenvalue
  • Subcritical multiplication
  • Pin-wise, axial fission density

• With application to
  • Criticality safety
  • Safeguards
  • Nonproliferation and materials accountability
RAPID code system - Structure

Pre-Calculation (one time):
  1. Burnup Calculation – to obtain material composition
  2. Fission Matrix Coefficient Generation

Real-time Analysis:
  1. Run Fission Matrix Code
  2. Process Results
Pre-calculation

1. SCALE* burnup calculation
2. SCALE output processing
3. MCNP input generation & calculation
4. MCNP tally processing

Pre-calculation – Step 1

• At each desired burnup, run a quarter assembly SCALE (t-dep1 module) model
  • Reflected on -x and -y
  • Octal symmetry
  • 49 fuel materials (each pin within octant is unique)
Pre-calculation – Step 2

• SCALE outputs:
  • neutron/gamma spectra
  • actinide/fission product concentrations
  • Fission Spectrum \((\chi)\)
    • Fit to Watt fission spectrum (nonlinear regression)

• Process SCALE outputs
  • `getdat.sh` - prepares material and source information for MCNP input file
  • `fitChi.R` - prepare continuous energy fission spectrum (Watt’s spectrum format) from multigroup SCALE generated spectrum for MCNP input file
Pre-calculation – Step 3

- Automatic input file generation for MCNP
  - `calcMat.f90` – generates necessary input block segments as a function of burnup and cooling time (source definition and material composition)
  - `makeMCNP.sh` – concocts input block segments to generate a full MCNP input file
  - `mkzmcnp.sh` – generate 55 unique input files for each $a$ & $b$ calculation

- Run MCNP for each coefficient as a function of burnup and cooling times
Pre-calculation – Step 4

• Processing MCNP output files to generate database
  • `getFMco.sh` - extract fission density tally from each MCNP output file
  • `rdmc.f90` – generates FM coefficient database file
Pre-processing—Estimated Time Requirements

- For a single coefficient calculation and processing.

<table>
<thead>
<tr>
<th>Step</th>
<th>Time (serial)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1) SCALE Run</td>
<td>~158 min</td>
</tr>
<tr>
<td>1.2) SCALE Output Processing</td>
<td>n/a</td>
</tr>
<tr>
<td>3) MCNP Fixed-source Calculation:</td>
<td></td>
</tr>
<tr>
<td>3.1) Input Generation</td>
<td>n/a</td>
</tr>
<tr>
<td>3.2) Calculation</td>
<td>~28 min</td>
</tr>
<tr>
<td>4) Tally Processing/Consolidation</td>
<td>~1 min</td>
</tr>
<tr>
<td>Total</td>
<td>~187 min</td>
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</table>
Real-time Analysis

1. Inputs for pool setup
2. Examples
Input Files

- `pool.inp` – defines the pool structure and range of burnups and cooling times (driver file)
- `runName.burn` – defines assembly-wise axial burnup distribution
- `runName.cool` – defines assembly-wise cooling times
Test Problems (9x9 assemblies)

(a) Case 1  (b) Case 2  (c) Case 3  (d) Case 4

(e) Case 5  (f) Case 6  (g) Case 7  (h) Case 8

(i) Case 9  (j) Case 10  (k) Case 11  (l) Material Legend

<table>
<thead>
<tr>
<th>Case #</th>
<th>Number of Assemblies</th>
<th>Fuel Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1x1</td>
<td>4.95%</td>
</tr>
<tr>
<td>2</td>
<td>6x1</td>
<td>4.95%</td>
</tr>
<tr>
<td>3</td>
<td>3x3</td>
<td>4.95%</td>
</tr>
<tr>
<td>4</td>
<td>9x9</td>
<td>4.95%</td>
</tr>
<tr>
<td>5</td>
<td>1x1</td>
<td>4.45%</td>
</tr>
<tr>
<td>6</td>
<td>6x1</td>
<td>4.45%</td>
</tr>
<tr>
<td>7</td>
<td>3x3</td>
<td>4.45%</td>
</tr>
<tr>
<td>8</td>
<td>9x9</td>
<td>4.45%</td>
</tr>
<tr>
<td>9</td>
<td>2x1</td>
<td>Mixed</td>
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<tr>
<td>10</td>
<td>6x1</td>
<td>Mixed</td>
</tr>
<tr>
<td>11</td>
<td>3x3</td>
<td>Mixed</td>
</tr>
</tbody>
</table>
Case 3 Eigenfunction

Comparison of FM with MC

Reference Solution
Case 11 Eigenfunction

Reference Solution

Comparison with FM with MC

Fission Source

Assembly number

MCNP

FM
Case 4 Eigenfunction distribution

Comparison with FM with MC

Reference Solution
## Comparison of calculated M - FM vs. MCNP

<table>
<thead>
<tr>
<th>Case</th>
<th>FM</th>
<th>MCNP</th>
<th>Error in M (FM vs MCNP)</th>
<th>Speedup (FM vs MCNP)</th>
</tr>
</thead>
<tbody>
<tr>
<td>M</td>
<td>Time (min)</td>
<td>M</td>
<td>Time (min)</td>
<td>1-σ Uncertainty</td>
</tr>
<tr>
<td>1x1</td>
<td>3.343353</td>
<td>0.092</td>
<td>3.33155</td>
<td>925</td>
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<tr>
<td>6x1</td>
<td>4.328244</td>
<td>0.213</td>
<td>4.31336</td>
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<td>5.428051</td>
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<td>9x9</td>
<td>6.697940</td>
<td>8.17</td>
<td>6.67674</td>
<td>1928</td>
</tr>
</tbody>
</table>

*Note that the FM technique also provide pin-wise, axial-dependent fission source or power.*
Reference Spent Fuel Pool

- Being developed for I2S-LWR reactor design
- 19x19 $U_3Si_2$ fuel assemblies
- 4.45 and 4.95 w/o U-235
- Metamic® absorbers (Al-B4C) used between assemblies
- Burnup up to 55 GWd/MTU

One 19x19 Assembly

9x9 segment of spent fuel pool

Whole pool made up of 8 9x9 segments
Fission density plots

- Axial fission density for entire assembly (x-y integrated)
Fission density plots

- x-fission density for entire assembly (y-z integrated)
Fission density plots

- Axial fission density for a single pin (x=10, y=11)
Fission density plots

• $x$-fission density for a single $z$-level ($y=10$, $z=72$)
Post Processing: 1x1 Pool Layout

• 3-D Fission Density
  Y-LEVEL ANIMATION

Z-LEVEL ANIMATION
RAPID tool

• The current version of the RAPID can quickly and accurately calculate the eigenvalue and eigenfunction for a spent fuel pool

• By pre-calculating a database of FM coefficients for different conditions, pool simulation can be performed in real-time allowing for changes in configurations (assembly shuffling, removal and addition) for various burnup, cooling times, lattice structure, and enrichments