DOE NE IRP
Transient Fuel Testing Benchmark
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Task 1.2.6: Computational and Experimental Benchmarking for Transient Fuel Testing

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Participants on Task 1.2.6

- Bill Martin (lead)
- Dr. Scott Wilderman (Research staff)
- Ethan Pacheck (PhD student)
- Assistance from Volkan Seker
- Ben Betzler (ORNL) has agreed to provide assistance to this project.
- And we have a local expert (Brian Kiedrowski) who worked with Ben Betzler at LANL on this research.
Alternative time-dependent analysis using OpenMC

- An alternative transient methodology based on steady state Monte Carlo (OpenMC).
- OpenMC analyzes the state of the reactor and estimates quantities that allow the determination of the eigenvalue spectrum and associated forward and adjoint eigenfunctions.
- Takes advantage of the capability of Monte Carlo to model arbitrarily complex geometries with continuous energy cross sections.
- This is a research project due to the relatively recent development of the methodology and the fact it has yet to be applied to transient applications with reactivity feedback.
Description of the TRM Method - 1

- Based on PhD work of Ben Betzler at the University of Michigan who graduated in 2014.
- The forward and adjoint $\alpha$-eigenvalue equations with delayed neutron precursors are the starting point for the method.
- A transition rate matrix (TRM) formulation of the adjoint system is obtained by using OpenMC [4] to estimate the adjoint TRM elements. This is possible even though OpenMC is a steady-state forward Monte Carlo code and is not aware of delayed neutrons.
- The forward TRM is then determined by taking the transpose of the adjoint TRM.
- A standard linear algebra package (LAPACK) is then used to determine all of the forward and adjoint eigenfunctions and eigenvalues for this system.
The evolution of the system response to a specified source is obtained by standard eigenfunction expansion using bi-orthogonality of the forward and adjoint eigenfunctions:

\[
\psi(r, E, \hat{\Omega}, t) = \sum_{n=1}^{\infty} A_n(t) \psi_n(r, E, \hat{\Omega})
\]

\[
A_n(t) = A_n(0) e^{\alpha_n t}
\]

\[
A_n(0) = \frac{\langle \psi_n, S_0 \rangle}{\langle \psi_n, \nu^{-1} \psi_n \rangle + \sum_m \langle C_m^{\dagger}, C_{m,n} \rangle}
\]
Example: five-region loosely coupled system

- For this five-region problem, the right fuel region thickness is either 1 (symmetric) or 1.1 (asymmetric)
- The fuel is varied to make subcritical, near critical, and supercritical configurations
- All configurations have only two real eigenvalues
The estimated detector response for critical symmetric problem for a detector in the right fuel region

- Shows the ability of the TRMM to accurately predict the response in a given region of the problem
- The higher modes are still present throughout a large portion of the response, due to the proximity of the first two eigenvalues
Betzler used this method to analyze the transient response of the Fort St. Vrain high temperature gas reactor to a 14 MeV pulsed neutron source.

Also used to analyze Caliban.

It can be used for subcritical, critical, or supercritical systems.

Primary impediment is the size of the phase space that is being evolved.

In essence, OpenMC is being used to analyze a time-dependent transient with delayed neutrons even though it never follows neutrons in time and never sees a delayed neutron.
Recent progress on Task 1.2.6 (1)

- Have adapted OpenMC to use OTF capability currently in MCNP6. This will account for Doppler broadening during the transient, which will be important for LEU.
- Using dummy isotope approach suggested by Volkan (and used in BATMAN), have shown that we can model a mixture of graphitized and non-graphitized carbon with OpenMC.
- This dummy isotope approach has also been shown to account for thermal spectrum feedback due to temperature. This works because the $S(\alpha, \beta)$ cross sections are generated at a specific temperature so dummy isotopes can be set up with appropriate bracketing temperatures and then mixed accordingly.
Recent progress (2)

- Completed specification of a simple benchmark configuration to allow comparison of alternative transient methodology with true time-dependent Monte Carlo. This benchmark configuration has the following features:
  - 3x3 homogenized assemblies
  - Includes axial reflectors
  - No air gaps or other features
  - Will allow time-dependent Monte Carlo simulation with OpenMC for comparison to the alternative methodology developed by Ben Betzler for his PhD thesis.
- Preliminary results of test cases are in reasonable agreement with MIT and UM results for the heterogeneous configuration.
Test problem geometry

10.16 x 10.16 cm homogenized assemblies

63.57938 cm
homogenized end plug + reflector

120.9675 cm

59.45188 cm
homogenized end plug + reflector
Test problem

- 3x3 fully homogenized assemblies
- Center assembly for reactivity insertion
- Preserve standard assembly dimensions
- Preserve standard assembly materials
- Homogenized end plugs include graphite plus all structural materials
Effect of temperature and graphitization for 3x3 case

- All cases with 8M histories
- Approximately 40 pcm statistics
- Mixture of graphitized and non-graphitized carbon using dummy isotopes as suggested by Volkan and used in BATMAN

**Deviations from base case**

<table>
<thead>
<tr>
<th>Temp</th>
<th>Base 59%</th>
<th>0%</th>
<th>delta-k</th>
<th>100%</th>
<th>delta-k</th>
</tr>
</thead>
<tbody>
<tr>
<td>300K</td>
<td>1.45914</td>
<td>1.46433</td>
<td>519</td>
<td>1.45109</td>
<td>-805</td>
</tr>
<tr>
<td>600K</td>
<td>1.43179</td>
<td>1.43493</td>
<td>314</td>
<td>1.42972</td>
<td>-207</td>
</tr>
<tr>
<td>delta-k (T)</td>
<td>-2735</td>
<td>-2940</td>
<td>-2137</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
We still need to run OpenMC with different temperatures for $S(\alpha, \beta)$. Originally we were going to wait for Andrew Pavlou (RPI) and use his OTF $S(\alpha, \beta)$. Delays and complexity of this approach made us try to use the dummy isotope idea.

OpenMC was run with a 50-50 mixture of dummy carbon isotopes at 400K and 800K. Results were compared with an OpenMC run at 600K.

### Effect of 50-50 mixture of 400K and 800K isotopes of carbon

<table>
<thead>
<tr>
<th>Temperature</th>
<th>100% Graphitized Delta-k</th>
<th>59% Graphitized Delta-k</th>
</tr>
</thead>
<tbody>
<tr>
<td>600K</td>
<td>1.42972</td>
<td>1.43179</td>
</tr>
<tr>
<td>Mix</td>
<td>1.42749 -223</td>
<td>Mix 1.43112 -67</td>
</tr>
</tbody>
</table>
Late breaking results with 500K and 700K

- Using 400K and 800K dummy isotopes might be too large of a temperature range for accurate statistical interpolation.
- OpenMC runs were done with a 50-50 mixture of dummy isotopes at 500K and 700K. The results look very good:

<table>
<thead>
<tr>
<th></th>
<th>delta-k</th>
<th></th>
<th>delta-k</th>
</tr>
</thead>
<tbody>
<tr>
<td>100% graphitized</td>
<td>600K</td>
<td>1.42972</td>
<td>600K</td>
</tr>
<tr>
<td>Mix (500,700)</td>
<td>1.42904</td>
<td>-68</td>
<td>Mix</td>
</tr>
</tbody>
</table>
The current methodology has only been applied to the evolution of a reactor start without feedback. OTF Doppler has been incorporated into OpenMC using OTF with ACE files. Effect of graphitization can be accounted for using dummy isotopes. Effect of temperature on $S(\alpha, \beta)$ and free gas kernel can be accounted for using dummy isotopes. Additional analysis is needed to confirm the use of dummy isotopes but these results are promising.
The forward and adjoint $\alpha$-eigenvalue equations with delayed neutron precursors are the basis for the method. A transition rate matrix (TRM) formulation of the adjoint system is obtained. The continuous energy Monte Carlo code OpenMC [4] is used to estimate the adjoint TRM elements. This is possible even though OpenMC is a steady-state Monte Carlo code and is not aware of delayed neutrons. The forward TRM matrix elements are then determined by taking the transpose of the adjoint TRM. A standard linear algebra package (LAPACK) is then used to determine all of the forward and adjoint eigenfunctions and eigenvalues for this system. The evolution of the system response to a specified source is obtained by standard eigenfunction expansion using bi-orthogonality of the forward and adjoint eigenfunctions:
Is linear mixing in temperature reasonable?

- Using the keff results, linear interpolation in T vs linear interpolation in $T^{0.5}$ were compared. Results consistent with previous results. No clear winner (yet).

**OpenMC runs at 400K and 800K**

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Linear in T</th>
<th>Linear in $T^{0.5}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>400</td>
<td>1.45055</td>
<td>1.42975</td>
</tr>
<tr>
<td>800</td>
<td>1.41222</td>
<td>1.43139</td>
</tr>
</tbody>
</table>

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</tr>
</thead>
<tbody>
<tr>
<td>400</td>
<td>1.44182</td>
<td>1.43186</td>
</tr>
<tr>
<td>800</td>
<td>1.42189</td>
<td>1.43101</td>
</tr>
</tbody>
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Simple example – incident neutron pulse

- Simple multiple slab problem
- First analyze state of the reactor with OpenMC and estimate matrix elements of the transition matrix
- Send matrix to external library to get eigenvalue spectrum and associated forward and adjoint eigenfunctions
- Expand time-dependent response and calculate expansion coefficients
Results: Multi-Region Problem

- Alternating materials of equal thickness
- Material 1 is purely scattering and material 2 has a small absorption cross section
- The speed is effectively 10 so the continuum portion of the spectrum starts at -10
Eigenfunction expansion solution for incident pulse compared to time-dependent Monte Carlo
Second example – detector response

The forward and adjoint $\alpha$-eigenvalue equations with delayed neutron precursors are the basis for the method.

A transition rate matrix (TRM) formulation of the adjoint system is obtained.

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![Diagram of five-region loosely coupled system with regions labeled: vacuum, fuel, moderator, absorber, fuel, moderator, vacuum. The regions are connected with labels: Δ=1, Δ=1, Δ=5, Δ=1, Δ_5.]
The estimated detector response for critical symmetric problem for a detector in the right fuel region

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The fast-burst reactor CALIBAN

- **Measured data**
  - Fundamental eigenvalue
  - Inferred $\beta_{eff}$
  - Possible higher eigenvalues

- **With a coarse-interval TRM**
  - Track the behavior of the prompt and delayed fundamental eigenvalues
  - Show the change in criticality

- **With a large TRM**
  - Higher shape eigenfunctions
  - Demonstrate trend of higher eigenvalues
  - Apply to a system with a lower enrichment
Approach to critical and prompt critical

- Additional insertion of the BC3 (left) and BC2 (right) control rods
  - Critical (delayed supercritical) at 2.7 cm, prompt critical at 4 cm
- Fundamental $\alpha$ eigenvalue under predicts the measured by 10%
- Calculates a $\beta_{eff}$ 640 pcm compared to 633 pcm inferred
Fort St. Vrain pulsed neutron experiment

- General Atomics High Temperature Gas-Cooled Reactor
  - Graphite-moderated, prismatic core
  - Six stacked fuel blocks, 247 fuel columns distributed into 37 regions
  - Radially and axially asymmetric HEU-Th initial fuel loading
  - Multiple particle sized TRISO fuel formed in densely-packed compacts
  - Control rod pair runs axially through the center block (control block) of each fuel region
  - Pulsed neutron experiments on subcritical configurations during the startup physics tests
Fundamental eigenvalue and eigenfunction comparison

- The fundamental eigenvalue is 6% smaller than measured
  - Measured: $-164.6 \pm 4.9 \text{ s}^{-1}$ compared to TRMM: $-154.8 \text{ s}^{-1}$
  - Eigenfunction matches the GA calculation
A transition rate matrix (TRM) formulation of the adjoint system is obtained. The continuous energy Monte Carlo code OpenMC is used to estimate the adjoint TRM elements. This is possible even though OpenMC is a steady-state Monte Carlo code and is not aware of delayed neutrons. The forward TRM matrix elements are then determined by taking the transpose of the adjoint TRM. A standard linear algebra package (LAPACK) is then used to determine all of the forward and adjoint eigenfunctions and eigenvalues for this system. The evolution of the system response to a specified source is obtained by standard eigenfunction expansion using biorthogonality of the forward and adjoint eigenfunctions:

Questions?