Title: Comparison of Iterative Time-Eigenvalue Methods with Discrete Ordinates and Monte Carlo

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Comparison of Iterative Time-Eigenvalue Methods with Discrete Ordinates and Monte Carlo

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Abstract

A standard approach in Monte Carlo and deterministic methods for computing the $\alpha$ (time absorption) eigenvalue involves solving a $k$ eigenvalue problem, and then finding the what insertion of a fictitious $\alpha/v$ absorber or source would make $k = 1$. This talk looks at using alternative multiplicative eigenvalues, the collision $c$ and leakage $l$ eigenvalues, as the basis to compute $\alpha$. Results suggest that in some cases, the use of the $c$ eigenvalue may be more efficient than using the $k$ eigenvalue.
Introduction

- Methodology
- Implementation (SN and Monte Carlo)
- Results
Motivation

- The asymptotic, logarithmic time rate of change of the neutron population (assuming no feedback) may be obtained with the $\alpha$ eigenvalue.
- Useful in subcritical measurements and analysis of prompt supercritical excursions in simple systems.
- A classic approach uses a $k$ eigenvalue calculation and finds what insertion of a fictitious $\alpha/\nu$ absorber or source would make $k = 1$.
- This work explores using a collision $c$ and leakage $l$ eigenvalues instead.
**$\alpha$-Eigenvalue Equation**

- Assume separability of time in the neutron flux:

  \[ \Psi(r, \hat{\Omega}, E, t) = n(t)\psi(r, \hat{\Omega}, E). \]

- Substitute and find the prompt $\alpha$-eigenvalue transport equation:

  \[ v(S + M - L - T)\psi = \alpha\psi. \]

- The time-dependent solution is a sum of eigenfunctions and exponentials:

  \[ \Psi(r, \hat{\Omega}, E, t) = \sum_{j=0}^{\infty} \psi_j(r, \hat{\Omega}, E) e^{\alpha_j t}. \]
A Classic Solution Technique

- Stiffness of the problem makes the $\alpha$-eigenvalue equation difficult to solve with standard iteration methods.
- Classic approach involves constructing a hybrid $k-\alpha$ equation:

$$\left(\frac{\alpha}{V} + L + T - S\right)\psi = \frac{1}{k}M\psi.$$ 

- Guess $\alpha$, solve for $k$ using standard iteration methods (e.g., power iteration).
- Find value of $\alpha$ that makes $k = 1$.
- Iterate until consistent value of $k$ and $\alpha$ are found.
Generalized Multiplicative Eigenvalue Formulation

- The $k$ eigenvalue is one of many possible multiplicative eigenvalues.
- Define the generalized multiplicative eigenvalue $x$:

\[
\left( \frac{\alpha}{v} + H_x \right) \psi = \frac{1}{x} G_x \psi.
\]

- Here $H_x$ and $G_x$ are operators for the left- and right-hand sides of the transport equation, depending upon the choice of $x$.
- E.g., for $x = k$, $H_x = L + T - X$ and $G_x = M$.
- Criticality condition is $x = 1$, regardless of choice of $x$.
- Question: Are some choices of $x$ more computationally efficient than others?
Hybrid Solution Technique

- Inner iteration $i$, solve for eigenvalue $x$:
  \[ x_{i+1} = \frac{N_{i+1}}{N_i} x_i. \]

- Once $x$ is converged, perform outer iteration $j$, solve for $\alpha$:
  \[ \alpha_{j+1} = \alpha_j + \frac{x_j - 1}{\tau_{x,j}}, \]

  where $\tau_x$ is the appropriate neutron lifetime given by
  \[ \tau_x = \frac{\langle \frac{1}{v} \psi \rangle}{\langle G_x \psi \rangle}. \]

- Iterate until $\alpha$ converged.
Collision and Leakage Eigenvalue Forms

- Two forms involve a collision $c$ and leakage $l$ eigenvalue:

$$\left(\frac{\alpha}{v} + L + T\right) \psi = \frac{1}{c} (S + M) \psi,$$

$$\left(\frac{\alpha}{v} + L\right) \psi = \frac{1}{l} (S + M - T) \psi.$$

- Eigenvalue $c$ uniformly adjusts multiplication of all collisions to achieve balance.
- Eigenvalue $l$ uniformly adjusts material atomic densities to achieve balance.
- $k = c = l = 1$ are equivalent.
Discrete Ordinates (SN) Implementation

- Uses standard 1-D diamond difference transport sweep.
- $k$ eigenvalue solution has standard power iteration on transport and fission source.
- $c$ and $l$ only iterate on transport source.
- In all cases, modify $\Sigma_t$ by adding current $\alpha/\nu$.
  - $k$ scales the fission source $M\psi$.
  - $c$ scales the collision source $(S + M)\psi$.
  - $l$ scales the collision source and modified total cross section $\Sigma_t + \alpha/\nu$.
- Compute lifetime from fluxes, and iterate until $\alpha$ converges.
Monte Carlo (MC) Implementation

- Simulate batches of particles in power iteration for fixed number of inner iterations satisfying convergence and statistical uncertainties.
- For $k$ eigenvalue, treat fission as absorption (bank neutrons for next iteration).
- For $c$ and $l$ eigenvalues, treat all collisions as absorption (banking neutrons).
- In all cases, modify $\Sigma_t$ by adding current $\alpha/\nu$.
  - $k$ scales the number of fission neutrons banked.
  - $c$ scales the number of collision neutrons banked.
  - $l$ scales the total cross section and number of collision neutrons banked.
- Lifetime estimate with collision tallies.
- Iterate until $\alpha$ converges, and then keep running iterations until uncertainty on $\alpha$ is sufficiently small.
Convergence of Leakage Eigenvalue

- The $l$ eigenvalue is not guaranteed to exist (i.e., no global density adjustment can make the transport equation balance).
- When $\alpha$ step is too large such that $l$ does not exist, take smaller steps until it does.
- Empirically, the $l$ eigenvalue can exhibit oscillatory and very slow convergence (possibly a complex dominance ratio?).
- Simple acceleration is to take midpoint of oscillation (improves convergence rate by factor of 2 or more).
- $\alpha$ will also oscillate, and midpoint technique improves convergence there as well.
SN Results

- Three multigroup slab test problems:
  - Bare, fast (4-group), vary slab thickness
  - Reflected, fast (4-group), vary reflector thickness
  - Reflected, thermal (8-group), vary fuel/moderator ratio.
- Use $S_{64}$ Gauss-Legendre quadature, 1000 total spatial elements.
- Speedup (wall-clock time ratio) to assess performance relative to $k$ eigenvalue:

\[
\text{Speedup} = \frac{\text{WallTime}_x}{\text{WallTime}_k}.
\]
SN, Bare-Fast Case
SN, Reflected-Fast Case

![Graph showing speedup vs. reflector thickness (cm)]
SN, Reflected-Thermal Case
MC Results

- Same three multigroup problems:
  - Bare, fast (4-group), vary slab thickness
  - Reflected, fast (4-group), vary reflector thickness
  - Reflected, thermal (8-group), vary fuel/moderator ratio.
- Use 10,000 neutron histories per inner iteration, 50 skip, 500 active inner iterations per outer iteration.
- 250 active outer iterations were used.
- Figure of merit \((1/R^2 T)\) ratio relative to \(k\) eigenvalue:

\[
\text{Performance} = \frac{\text{FOM}_x}{\text{FOM}_k}.
\]
### MC, Bare-Fast Case

The graph shows the relative performance of core thickness in centimeters. The X-axis represents the core thickness (in cm) ranging from 18 to 30, while the Y-axis represents the relative performance. Two lines are plotted: one in red labeled 'c-a' and one in green labeled 'l-a'.

- **Red Line ('c-a')**: Decreases as the core thickness increases.
- **Green Line ('l-a')**: Decreases initially but then increases as the core thickness increases.

The data points indicate a clear trend where the relative performance decreases with increasing core thickness for both 'c-a' and 'l-a'.
MC, Reflected-Fast Case
MC, Reflected-Thermal Case

![Graph showing relative performance vs. fuel atomic fraction. The graph plots the relationship between the two variables, with data points for different cases labeled as 'c-a' and 'l-a'.]
Discussion

- SN results suggest greater efficiency gains.
- Need to compare against state-of-the-art SN methods for computing $\alpha$.
- Unfortunately, multigroup MC results show lower efficiency at worst and margin gains at best.
- How does this compare in continuous energy?
About two years ago, implemented prototype for \( c-\alpha \) methods in research version of MCNP6.

Since all histories are a single track, may use Newton-Rhapson to compute \( \alpha \) that makes \( c = 1 \) after \( \alpha \) source is converged.

Significant improvements observed over MCNP’s internal \( k-\alpha \) method, but is an “apples to oranges” comparison of methods because:

- Different approaches used. Difficult to do Newton-Rhapson with multiple track histories.
- \( k \) eigenvalue routines in MCNP are inherently more complicated having more capabilities.
- Correlation effects of the \( c \) eigenvalue are not well understood (most likely a larger effect than \( k \)).
Noise in $c$ Versus $k$ (3D-PWR)
Continuous-Energy MC Test Problems

- Four test problems in order of complexity:

1. Supercritical, bare HEU sphere (Godiva with elevated density)
2. Supercritical, Be-reflected HEU sphere
3. Slightly subcritical can of Pu-Nitrate solution
4. Nearly critical 3-D Pressurized Water Reactor (Hoogenboom-Martin benchmark)
Continuous-Energy MC Results

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<th>Case</th>
<th>(k-\alpha)</th>
<th>(c-\alpha)</th>
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<tr>
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<td>1.468</td>
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</tbody>
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Summary & Future Work

- $\alpha$ eigenvalue iterations explored with multiplication $k$, collision $c$, and leakage $l$ eigenvalues.
- SN results show moderate improvement with using $c$ as opposed to $k$.
- MC results on equivalent multigroup problems shows general disadvantage to using other eigenvalues over $k$.
- MC results for CE problems are suggestive, but are not a fair comparison. More investigation needed.
Acknowledgments

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Questions?