LA-UR-13-29477
Approved for public release; distribution is unlimited.

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

Author(s): Kiedrowski, Brian C.

Intended for: 2014 American Nuclear Society Annual Meeting, 2014-06-15/2014-06-19 (Reno, Nevada, United States)

Issued: 2013-12-17

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

Brian C. Kiedrowski

X-Computational Physics Division, Los Alamos National Laboratory, P.O. Box 1663, Los Alamos, NM 87545, bckiedro@lanl.gov

INTRODUCTION

The inverse prompt period α is of interest to analyzing the behavior of fast-burst reactors such as Godiva-IV or pulses in research reactors. The time-dependent problem is often posed as an static α-eigenvalue problem, which gives the time constant for the asymptotic rise or fall of prompt neutrons in a system. The properties of the α-eigenvalue, being the mathematical equivalent of an additive insertion of a fictitious $1/v$ (v is the neutron speed) absorber, makes the problem difficult to solve numerically. One common approach to solving the α-eigenvalue problem is to first solve a static k-eigenvalue problem, and then use that solution to find the α/v absorber that would make $k = 1$[1]. Two similar approaches are investigated here. Rather than using the k eigenvalue, which is based on multiplication, the collision or c-eigenvalue or leakage or l-eigenvalue equations[2] can be solved instead, and the α/v absorber that makes $c = l = 1$ is found.

These methods for solving α were implemented into research multigroup discrete ordinates (S_N) and Monte Carlo (MC) codes. The results show that using either the k-, c-, or l-eigenvalue equation will yield the same α. For many cases, it appears that for S_N the c-eigenvalue may offer significant efficiency gains toward computing α over the traditional k-eigenvalue approach. For MC, there appears to be little consistent trend as to which approach may be more efficient.

THEORY

The asymptotic inverse prompt period α for quasi-static analysis may be found using the α-eigenvalue form of the neutron transport equation by assuming separability of time from the rest of phase space. If only prompt neutrons are of interest, this equation may be written as

$$(S + M - L - T)\,\psi_\alpha = \frac{\alpha}{v}\psi_\alpha. \tag{1}$$

Here S is the operator for scattering, M is the operator for prompt fission, L is the operator for streaming, and T is the total interaction operator. ψ_α is the eigenfunction or shape function for the asymptotically changing neutron population during late times.

Since the α/v is an additive term, the α-eigenvalue equation cannot be solved directly with standard iterative methods used for the k eigenvalues; however, an indirect solution by these means is possible by solving for α iteratively using a hybrid eigenvalue equation:

$$\left(L + T - S + \frac{\alpha}{v}\right)\psi = \frac{1}{k}M\psi. \tag{2}$$

In this formulation, α is a parameter and the eigenvalue k is a function of this parameter. For the choice of $\alpha = 0$, this hybrid equation becomes the standard k-eigenvalue problem seen in reactor analysis. Solving for α is done iteratively. A guess for α is made, and k is solved. If the solution for k is greater than one, the guess for α is increased, and if k is less than one, the guess for α is decreased. This process continues until the α is found where $k = 1$, at which point the hybrid equation is the α-eigenvalue equation, and therefore the α-eigenvalue equation has been solved.

The choice of solving the k-eigenvalue equation iteratively is convenient because many transport codes already support methods for solving that problem. Alternative hybrid equations can be written based upon different eigenvalues, the collision or c-eigenvalue, or leakage or l-eigenvalue. These equations are

$$\left(L + T + \frac{\alpha}{v}\right)\psi = \frac{1}{c}\left(S + M\right)\psi, \tag{3}$$

$$\left(L + \frac{\alpha}{v}\right)\psi = \frac{1}{l}\left(S + M - T\right)\psi. \tag{4}$$

The c eigenvalue balances the sources from all collisions with the losses, and the l eigenvalue balances all interactions with streaming and can be thought of as a factor to uniformly increase the density to achieve criticality, effectively changing the neutron mean-free-path. Like before, α's can be guessed, c or l values found, and new guesses of α made until $c = l = 1$. At this point, all three hybrid equations reduce to the α-eigenvalue equation, and therefore the α found for each should be identical.

COMPUTATIONAL METHODS

Iterative approaches for solving α using the k, c, or l eigenvalues, hereafter called the k-α, c-α, and l-α methods, are implemented in both S_N and MC. The simplest case of multigroup, 1-D slab geometry is used, as it is illustrates the merits and disadvantages of each iterative scheme without unnecessary complications arising from higher dimensionality, curvilinear coordinates, continuous-energy cross sections, etc. There is every reason, however, that these

iteration schemes can be implemented into more sophisticated S_N or MC packages without any difficulties beyond those for the simplest case.

The generic eigenvalue x (k, c, or l) is solved using a power iteration scheme, where x in iteration $i+1$ may be found by

$$x_{i+1} = \frac{N_{i+1}}{N_i} x_i, \tag{5}$$

where N_i is the number of neutrons produced in (inner) iteration i. For the k eigenvalue, this is the number of fission neutrons, and for the c and l eigenvalues, this is the number of collision neutrons.

Once x is converged, α is found iteratively via an outer loop. To find α based upon x for outer iteration j, the standard updating scheme for α used, and is based on a first-order Taylor series expansion:

$$\alpha_{j+1} = \alpha_j + \frac{x_j - 1}{\tau_{x,j}}, \tag{6}$$

where τ_x is the appropriate neutron lifetime given by

$$\tau_x = \frac{\left\langle \frac{1}{v}\psi \right\rangle}{\langle A_x \psi \rangle}. \tag{7}$$

Here A_x is a generic operator, which is M for the k-eigenvalue, $S+M$ for the c-eigenvalue, and $S+M-T$ for the l-eigenvalue cases.

The iterative approach tends to work well for supercritical systems, but can be problematic for those that are subcritical. This occurs because negative α/v is the mathematical equivalent of a source into the transport equation, which when it becomes larger than T makes the methods for solving the hybrid equation (either S_N or MC) numerically unstable. Therefore, the analysis done here is primarily for supercritical systems.

Discrete Ordinates Method

The S_N method involves an inner x-eigenvalue loop and an outer α-eigenvalue loop. Power iteration is used as the inner iteration where a guess for α from the outer loop is used to modify the total cross section. The eigenvalue calculation proceeds iteratively until a convergence tolerance for both the eigenvalue and eigenfunction are met. Once this is done, a convergence on the outer iteration for α is assessed. The convergence tolerance requires that both the eigenvalue be unity within, and the relative change in α from the previous iteration be less than some tolerance. For this work, this tolerance is 1×10^{-6}. If the tolerance is not met, the appropriate lifetime is computed and used to get a new guess for α and the inner loop is repeated. Once this tolerance is met, the α is considered found and the flux shape should correspond to ψ_α.

Monte Carlo Method

The MC method proceeds in a somewhat different manner than S_N because of the presence of inherent statistical noise in the calculation. The calculation still has the notion of an inner x-eigenvalue loop with an α-eigenvalue loop, except that there are skip cycles for both the outer and inner iterations. The calculation begins with an initial guess of α passed into the inner loop where the x eigenvalue is estimated (via a collision estimator) with its statistical uncertainty; estimates of the appropriate lifetime τ_x are made as well using collision estimators. A new guess of α is made, and another inner loop is executed. Loops of the outer iteration are done and discarded until the computed x is within 1σ of unity—a more sophisticated convergence test is probably needed for production, but works well for the simple problems tested—at which point a number of user-defined active outer iterations are run with the new guess for α being used as a score for an α tally. At the end of the outer iterations, the mean value of α is reported along with an estimate of its statistical uncertainty. In the future, α may be computed using some weighting average based upon how well the eigenvalue x matched unity.

Convergence of the l Eigenvalue

The l eigenvalue for some cases may have difficulties with convergence, likely related to its spectrum and the possible non-existence of a positive, real eigenvalue—there are many cases where no multiplicative factor on the density can make a configuration critical. One issue is that the convergence can be extremely slow and have oscillatory behavior. A simple acceleration that is used is when this is detected: the next guess is the midpoint between two previous iterations; this usually improves the convergence rate by factors of two or more.

Iterating on α can also exhibit the same kind of convergence behavior, and the acceleration to get reasonable convergence times is the same: taking a midpoint of two previous α guesses. Additionally, during iterating on α, it is possible to take a guess that is too large such that no value of l exists on the next iteration, as indicated by converging toward zero. In this case where $l < l_{\min} = 0.1$, the guess on α is decreased by 10% until one is found where l exists.

RESULTS

There are three test problems: a bare fast slab with 4-group cross sections and varied thickness, a low-Z reflected fast slab (both sides) with 4-group cross sections and varied reflector thickness, and a reflected thermal slab with 8-group cross sections and varied fuel to moderator concentration. The fast bare slab thickness was varied from 18 cm (slightly subcritical) to 30 cm; the reflector thickness

was varied from 1.5 cm to 10 cm with a fixed fast core slab thickness of 15 cm; the thermal reflected slab thickness is 10 cm in the core and 5 cm in the reflector on each side, with the fuel atomic fraction in the core varied from 0.2% where it is slightly subcritical, becomes supercritical, until 40% where it becomes slightly subcritical again.

For the S_N method, a S_{64} Gauss-Legendre quadrature set was used with 1000 spatial elements in both the core and the reflector when present; a reflecting boundary condition was used at the midplane for the reflected cases. For the MC method, 10,000 neutron histories per inner iteration with 50 skip and 500 active inner iterations per outer iteration, and 250 active outer iterations were used. The α values between the S_N and MC calculations agree between the methods for all three cases regardless of the eigenvalue x selected.

Discrete Ordinates

The speedup or slowdown is the ratio of the wall-clock times t it takes to compute the converged α given. Specifically, the speedup is relative to the k-α method, being the ratio of the t for k-α to the t for either the c-α or l-α methods. In other words, a speedup of unity means that the time to convergence is equal to that of the k-α method, greater if it is faster, and less if it is slower.

Figures 1-3 give the speedups for the methods for the bare-fast, reflected-fast, and reflected-thermal cases respectively. In this case, the c-α method always outperforms the k-α method, which significantly outperforms the l-α method. This is likely because the c-α method, doing an update every collision "generation" as opposed to fission generation, is using information more frequently. The one trend of note is that for the fast-reflected case, the c-α method tends to be more efficient as the reflector thickness increases.

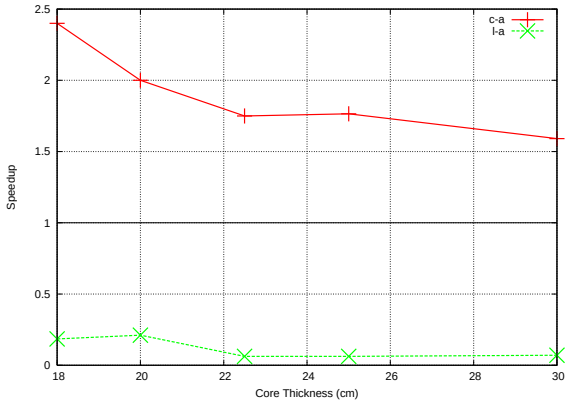

Fig. 1. Speedup of S_N methods for computing α on the bare-fast case.

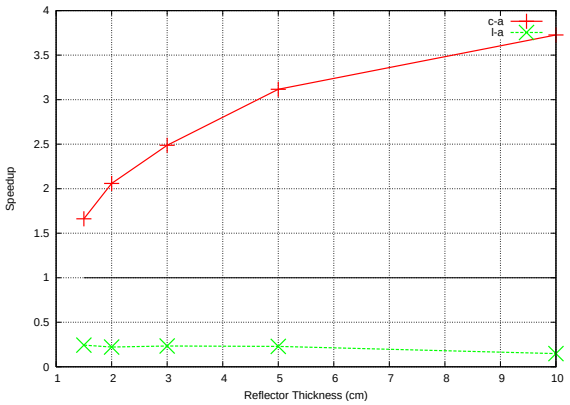

Fig. 2. Speedup of S_N methods for computing α on the reflected-fast case.

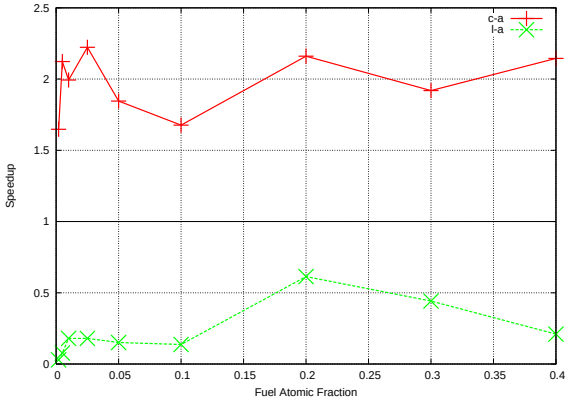

Fig. 3. Speedup of S_N methods for computing α on the reflected-thermal case.

Monte Carlo

Because of statistical fluctuations in a Monte Carlo calculation, assessing performance is not as simple of a matter as comparing wall-clock times. Performance of MC methods is typically assessed with the Figure-of-Merit,

$$\text{FOM} = \frac{1}{R^2 t}, \tag{8}$$

where R is the relative statistical uncertainty in α, and t is the wall-clock time of the active outer iterations. As with the comparisons with S_N, the value is relative to the k-α method. Since in this case a larger FOM means better, the ratio is inverse the S_N: the FOM for the method being compared to the FOM for the k-α method, which is called the "relative performance".

Figures 4-6 give the relative performance for the three cases. Unfortunately, the trends for the MC methods are much less clear than for S_N. The l eigenvalue sometimes appears to be superior in this case, but not always.

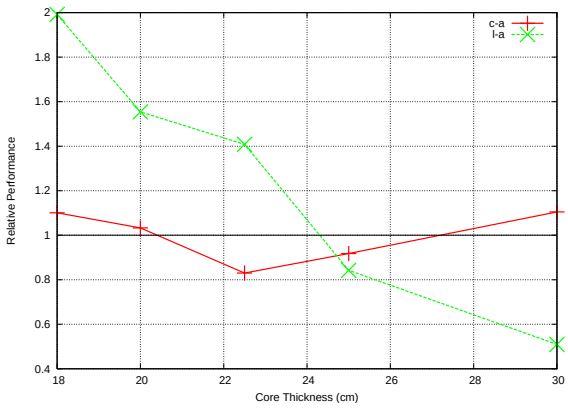

Fig. 4. Relative performance of MC methods for computing α on the bare-fast case.

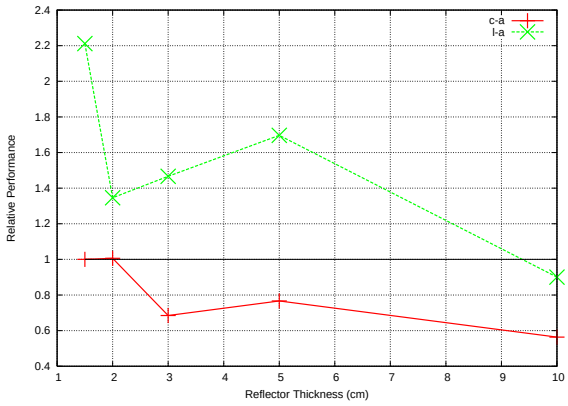

Fig. 5. Relative performance of MC methods for computing α on the reflected-fast case.

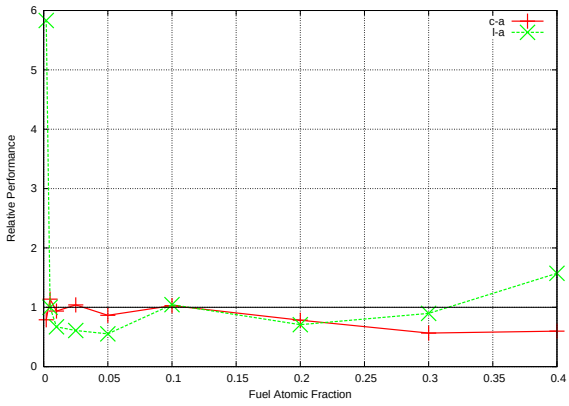

Fig. 6. Relative performance of MC methods for computing α on the reflected-thermal case.

Perhaps the metric used is not entirely fair as it looks at the *apparent* variance in α for the method and the *total* time spent in the active outer iterations. MC eigenvalue calculations tend to under predict the uncertainties of calculated values, i.e., the code states the result is more certain than it actually is. This is typically small for the k eigenvalue (a few tens of percent is typical), but this issue has not been yet investigated for the c and the l eigenvalues, let alone for α. Furthermore, the S_N method merely measured time to convergence, whereas the MC method used a fixed number of inactive cycles each execution of the inner loop regardless of how long it took to actually converge the eigenvalue—unlike S_N, automated convergence checks are problematic in MC because of statistical noise.

CONCLUSIONS & FUTURE WORK

The k-α, c-α, and l-α methods were developed in both S_N and MC, and compared using multigroup test problems. For S_N, the c-α method often had superior performance, but for MC, the trends are less clear for reasons discussed.

The current approach of inner and outer iterations is the simplest way, and more efficient approaches of updating α within the inner iterations needs to be investigated to see if it impacts conclusions. Furthermore, more effort needs to be done to have a more fair comparison of the MC methods, which could involve convergence detection so inactive iterations are not needlessly wasted, and a study of how poorly MC predicts uncertainties in α for the various methods.

ACKNOWLEDGMENTS

This work was funded by the DOE/NNSA Advanced Scientific Computing and Nuclear Criticality Safety Programs.

REFERENCES

1. D.V. BROCKWAY, P.D. SORAN, P.P. WHALEN, "Monte Carlo Alpha Calculation," LA-UR-85-1224, Los Alamos National Laboratory (1985).
2. Y. RONEN, D. SHVARTS, J.J. WAGSCHAL "A Comparison of Some Eigenvalues in Reactor Theory," *Nucl. Sci. Eng.*, **60**, 97-101 (1976).