LA-UR-14-24367
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:	American Nuclear Society Annual Meeting 2014, 2014-06-15/2014-06-19 (Anaheim, California, United States)
Issued:	2014-06-13

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

Brian C. Kiedrowski

Los Alamos National Laboratory

June 17, 2014

Abstract

A standard approach in Monte Carlo and deterministic methods for computing the α (time absorption) eigenvalue involves solving a k eigenvalue problem, and then finding the what insertion of a fictitious α/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 α. 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 α 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 α/v absorber or source would make $k = 1$.
- This work explores using a collision c and leakage l eigenvalues instead.

α-Eigenvalue Equation

- Assume separability of time in the neutron flux:

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

- Substitute and find the prompt α-eigenvalue transport equation:

$$v\left(S + M - L - T\right)\psi = \alpha\psi.$$

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

$$\Psi(\mathbf{r}, \hat{\mathbf{\Omega}}, E, t) = \sum_{j=0}^{\infty} \psi_j(\mathbf{r}, \hat{\mathbf{\Omega}}, E)e^{\alpha_j t}.$$

A Classic Solution Technique

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

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

- Guess α, solve for k using standard iteration methods (e.g., power iteration).
- Find value of α that makes $k = 1$.
- Iterate until consistent value of k and α 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 α:

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

- where τ_x is the appropriate neutron lifetime given by

$$\tau_x = \frac{\left\langle \frac{1}{v}\psi \right\rangle}{\langle G_x \psi \rangle}.$$

- Iterate until α converged.

Collision and Leakage Eigenvalue Forms

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

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

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

- 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 Σ_t by adding current α/v.
  - 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 $\Sigma_t + \alpha/v$.
- Compute lifetime from fluxes, and iterate until α 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 Σ_t by adding current α/v.
  - 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 α converges, and then keep running iterations until uncertainty on α 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 α step is too large such that l does not exist, take smaller steps until it does.

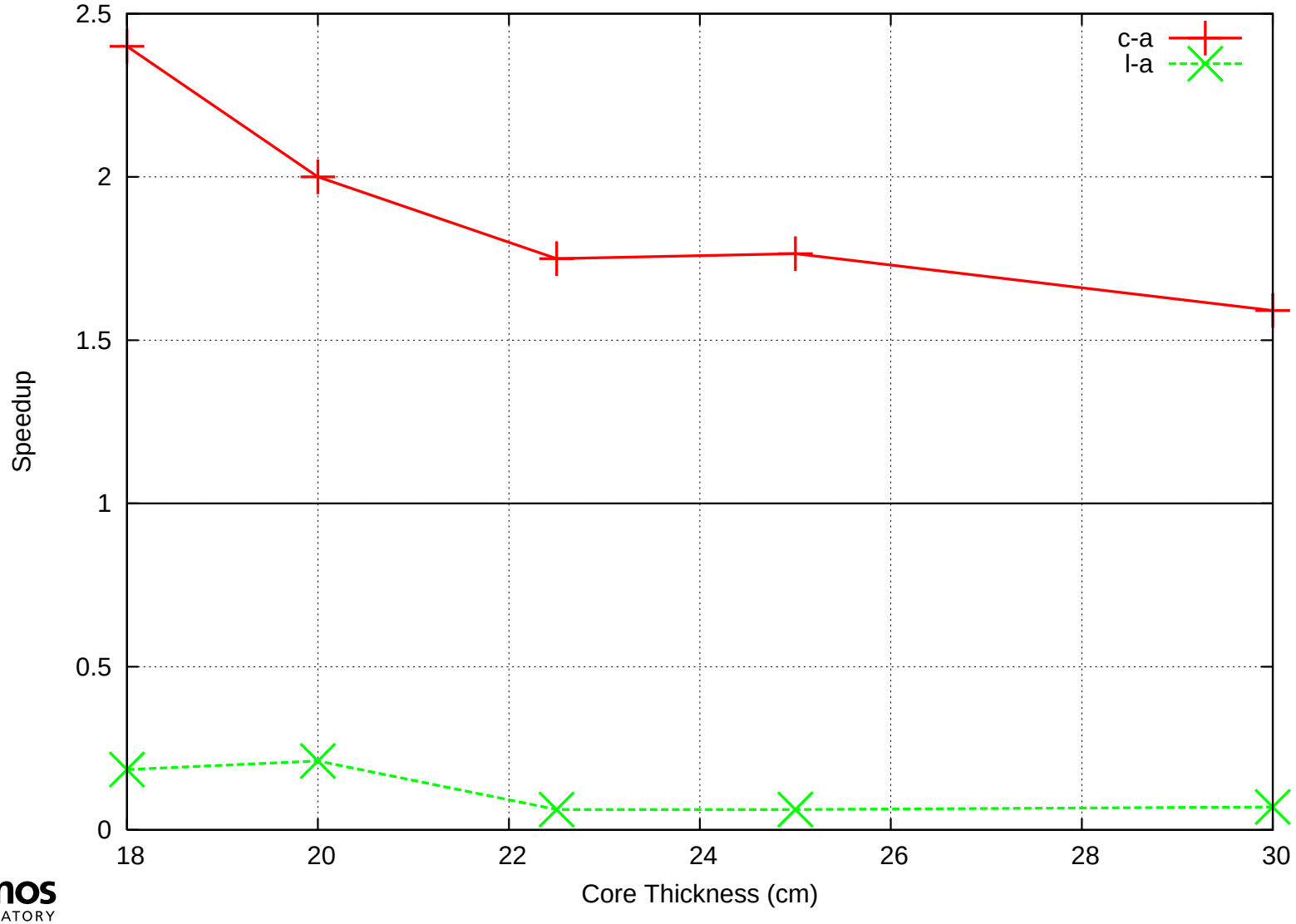
- Empirically, the l eigenvalue can exhibit oscillatory and very slow convergence (possibly a complex dominance ratio?).
- Simple acceleration is to take midpoint of oscillation (improves convergence rate by factor of 2 or more).
- α will also oscillate, and midpoint technique improves convergence there as well.

SN Results

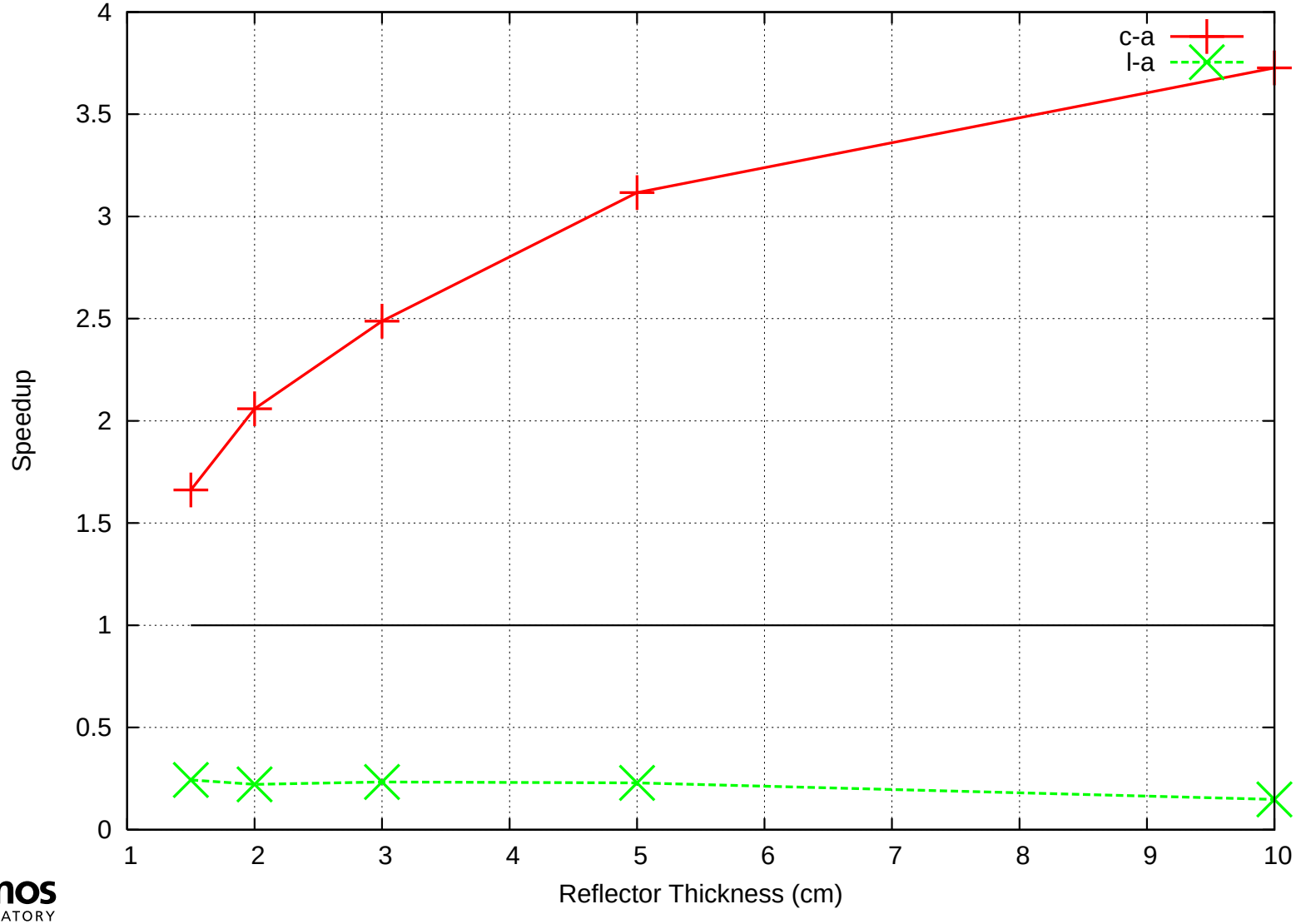
- Three multigroup slab test problems:
  - Bare, fast (4-group), vary slab thickness
  - Reflected, fast (4-group), vary reflector thickness
  - Reflected, thermal (8-group), vary fuel/moderator ratio.
- Use S_{64} Gauss-Legendre quadature, 1000 total spatial elements.
- Speedup (wall-clock time ratio)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

$$\text{Speedup} = \frac{\text{WallTime}_x}{\text{WallTime}_k}.$$

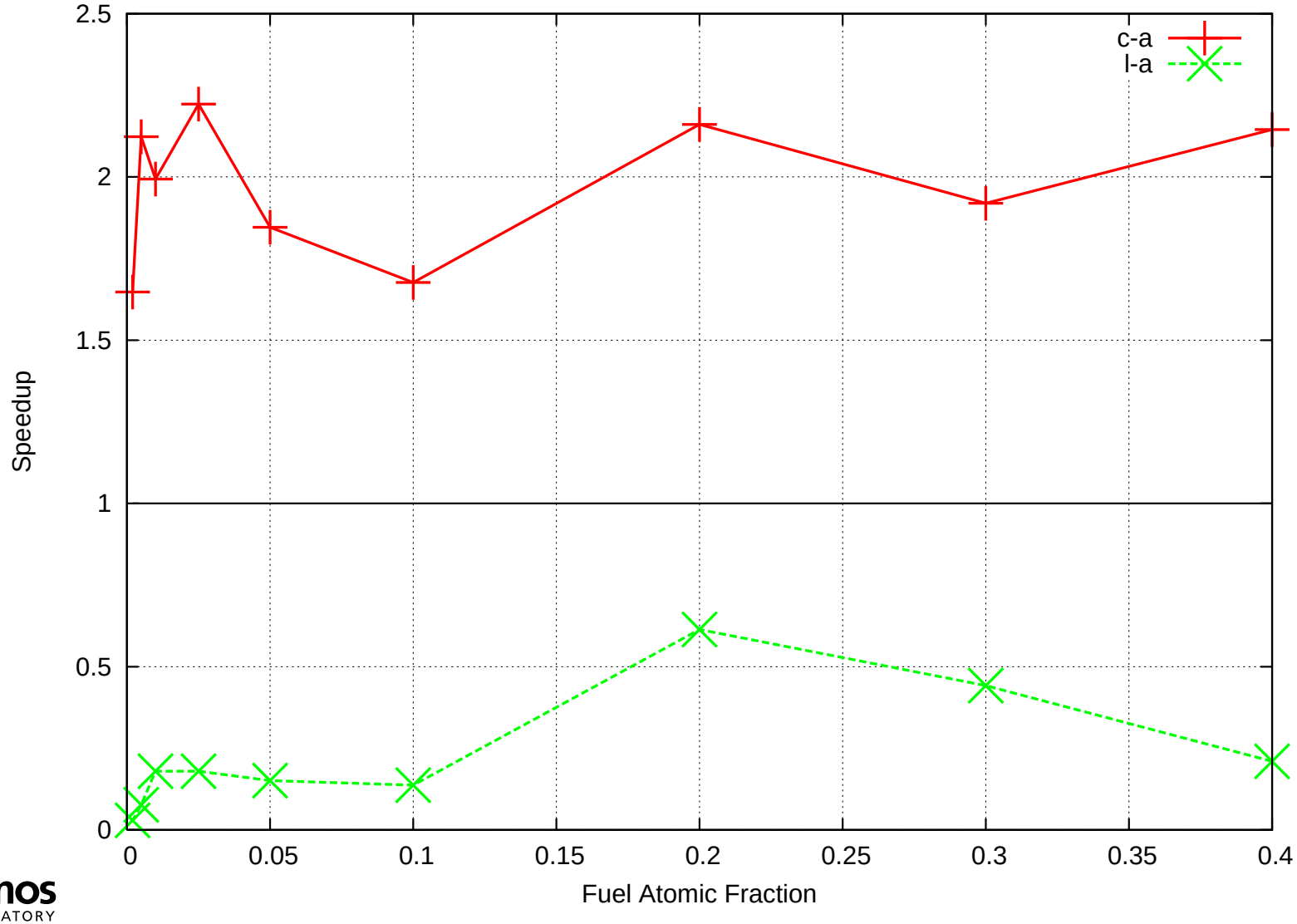
SN, Bare-Fast Case



SN, Reflected-Fast Case



SN, Reflected-Thermal Case

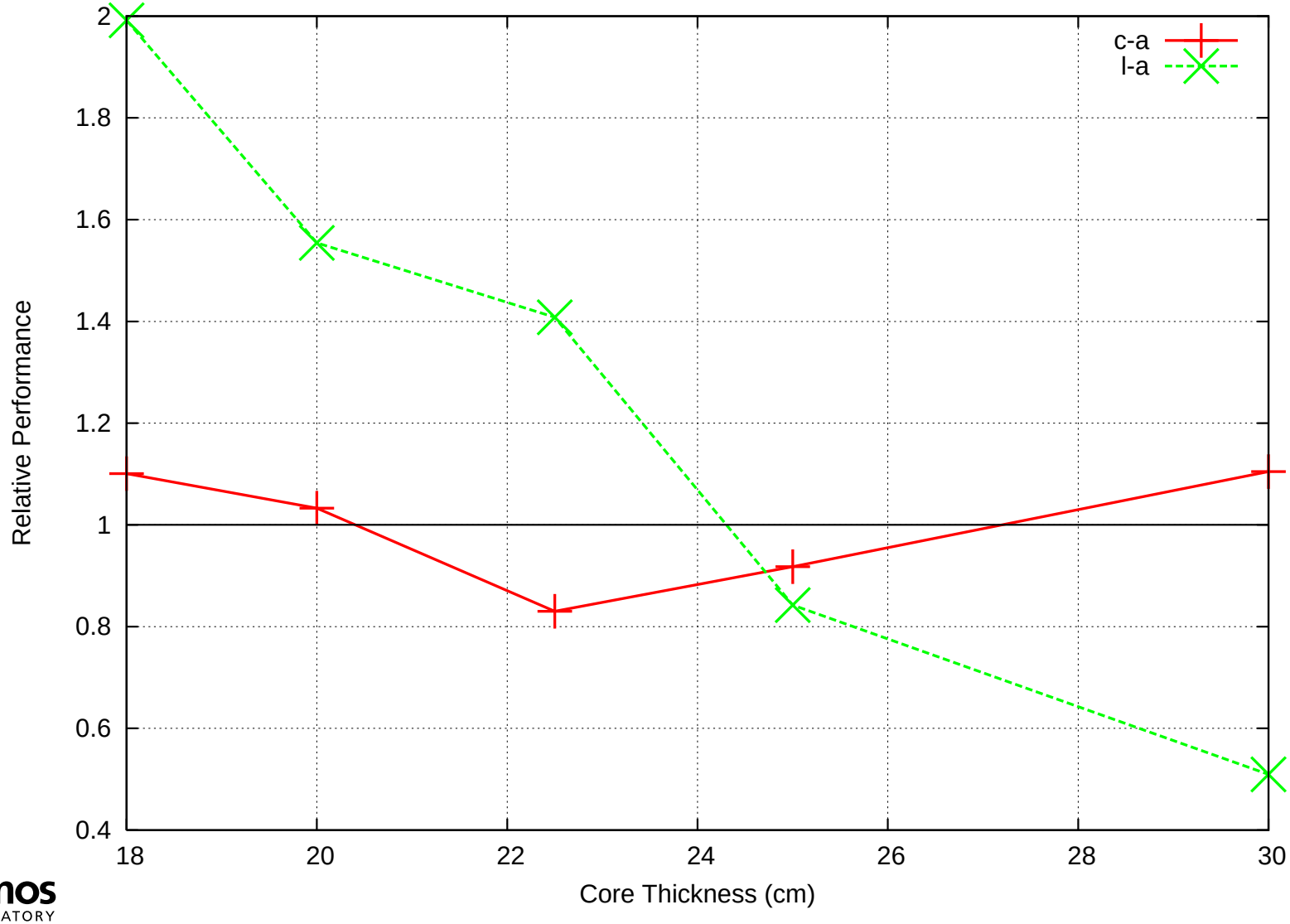


MC Results

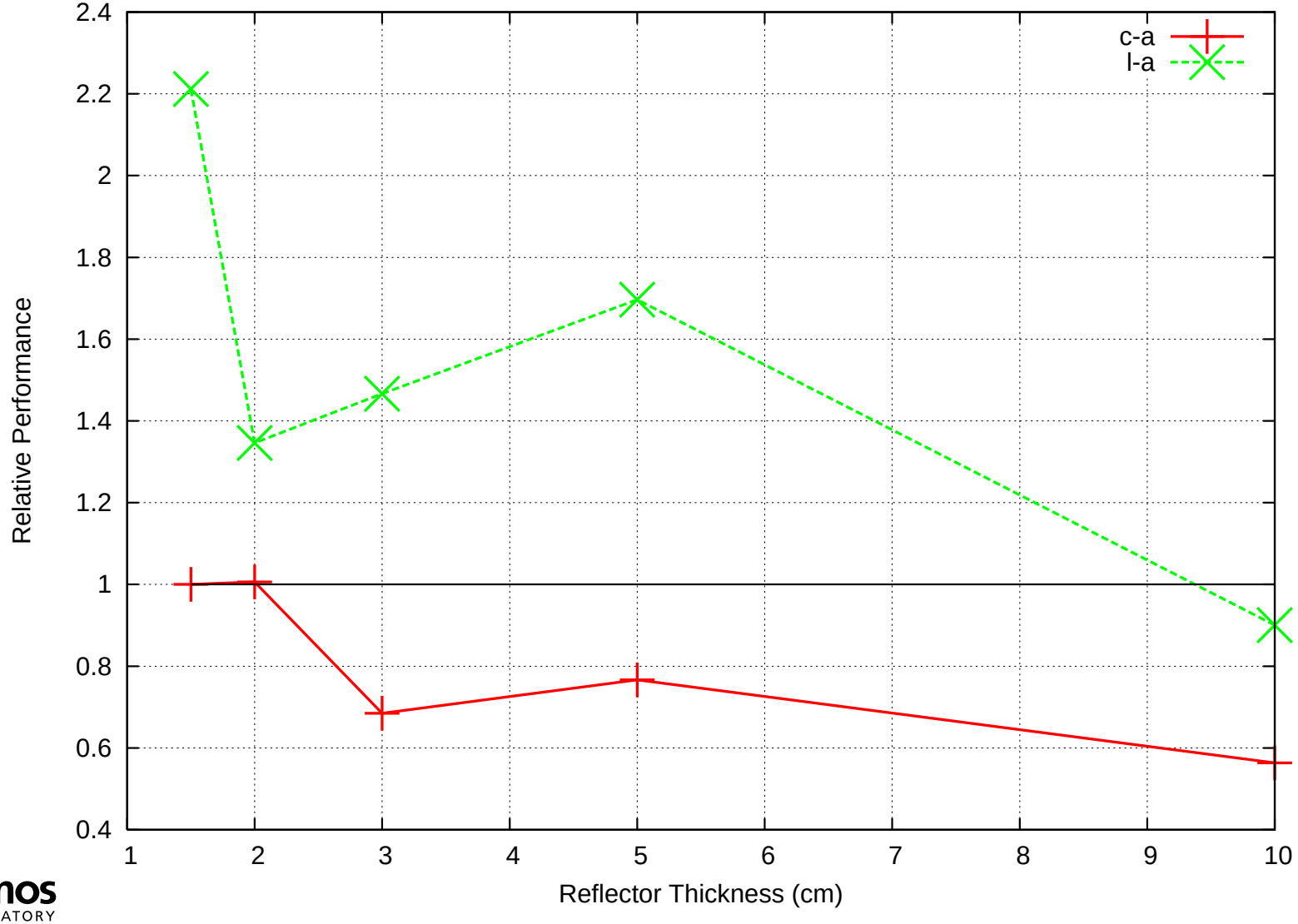
- Same three multigroup problems:
  - Bare, fast (4-group), vary slab thickness
  - Reflected, fast (4-group), vary reflector thickness
  - Reflected, thermal (8-group), vary fuel/moderator ratio.
- Use 10,000 neutron histories per inner iteration, 50 skip, 500 active inner iterations per outer iteration.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

$$\text{Performance} = \frac{\text{FOM}_x}{\text{FOM}_k}.$$

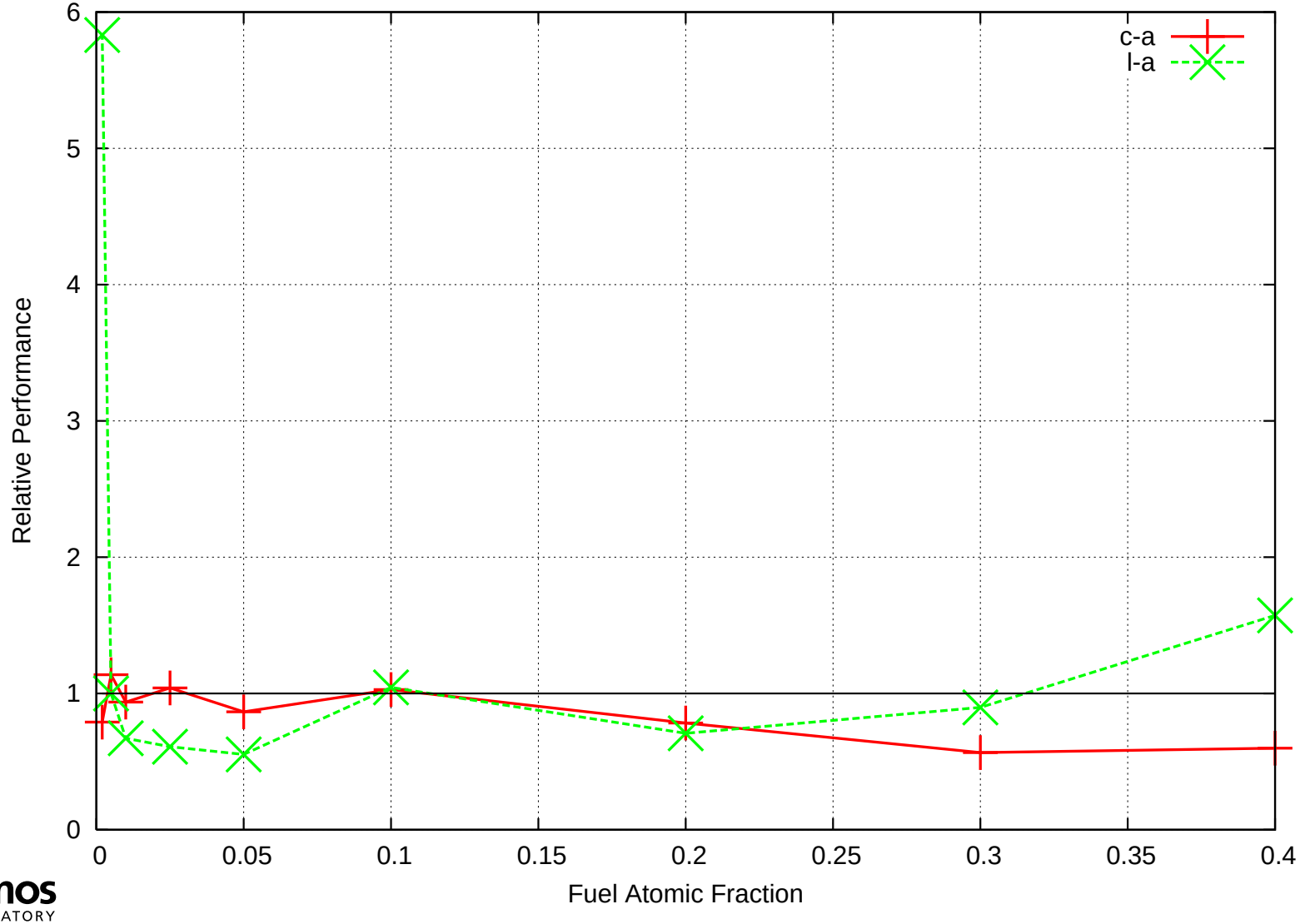
MC, Bare-Fast Case



MC, Reflected-Fast Case



MC, Reflected-Thermal Case



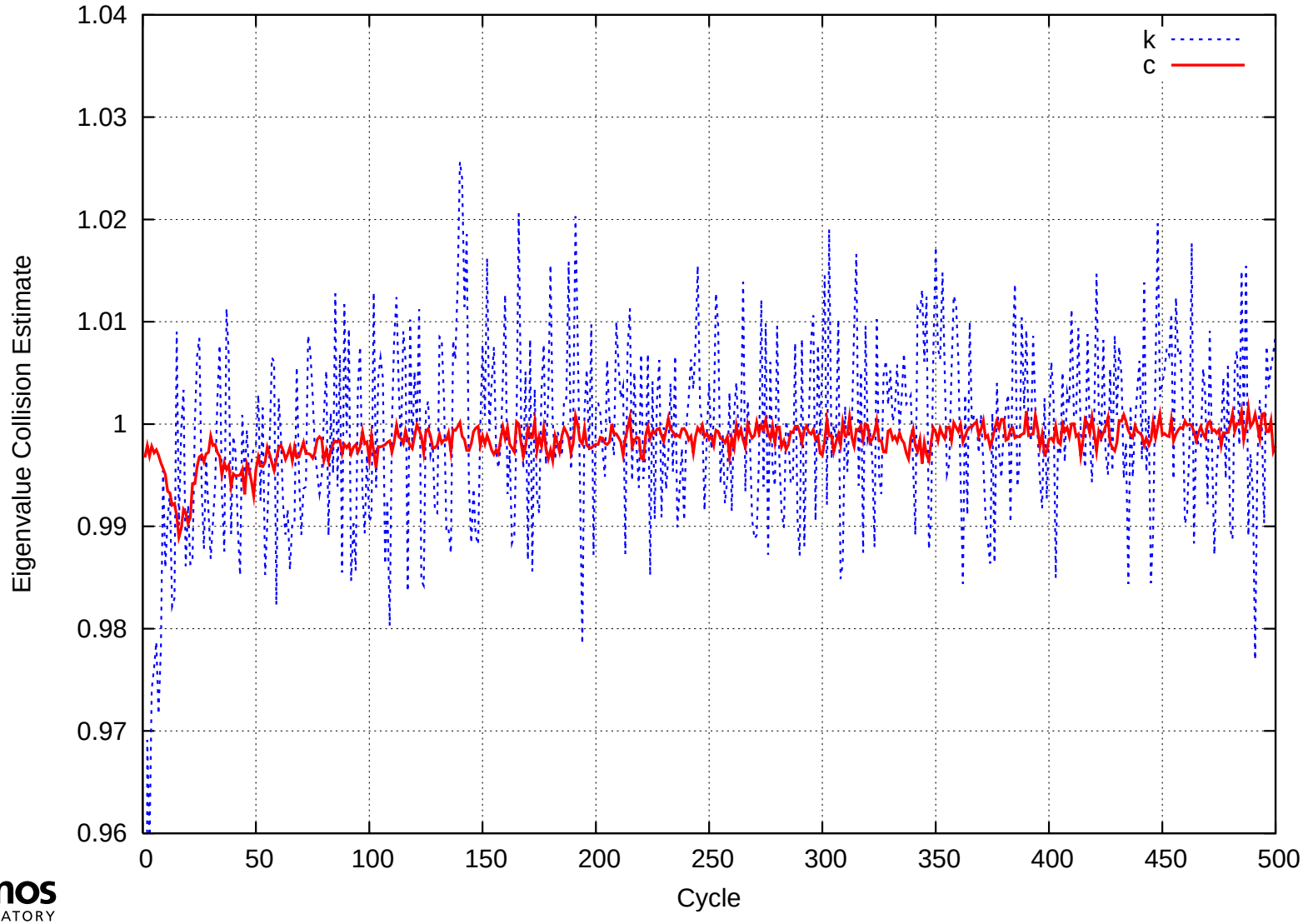
Discussion

- SN results suggest greater efficiency gains.
  - Need to compare against state-of-the-art SN methods for computing α.
- Unfortunately, multigroup MC results show lower efficiency at worst and margin gains at best.
  - How does this compare in continuous energy?

MCNP Continuous-Energy Results

- About two years ago, implemented prototype for c-α methods in research version of MCNP6.
- Since all histories are a single track, may use Newton-Rhapson to compute α that makes $c = 1$ after α source is converged.
- Significant improvements observed over MCNP's internal k-α 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

	k-α		c-α	
Case	α	FOM	α	FOM
1	0.176	9.2×10^3	0.176	2.0×10^4
2	1.468	5.9×10^4	1.474	5.4×10^5
3	Failed	—	-3.181×10^{-4}	260
4	2.425×10^{-5}	19	1.944×10^{-5}	44

Summary & Future Work

- α 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

- Funding provided by the U.S. DOE/NNSA Advanced Scientific Computing Program and Nuclear Criticality Safety Program.

Questions?