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STABILIZING THE K-ALPHA ITERATION ALGORITHM IN VERY SUBCRITICAL REGIMES

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ABSTRACT

In the normal k–α iteration method, there are two possible sources of instability for subcritical analysis. The first involves the time source, in which the weight of the particle is increased due to an effective (n, 2n) reaction. For large negative α, the weight of the particle can grow without bounds. The remedy for this involves combining both fission source and time source iteration into one algorithm. The time source particles are added to the source bank and normalized, preventing infinite growth. The second issue involves the α updater. In some circumstances, the updater can become oscillatory or diverge. Using a technique from stochastic optimization, the updater is modified in such a way that oscillations will eventually converge. The combination of these two techniques allows one to compute α for k close to zero.

KEYWORDS: Monte Carlo, alpha eigenvalue, subcritical

1. INTRODUCTION

The α-eigenvalue form of the transport equation is obtained by taking a separation of variables of the flux between a spatially constant term and a temporally exponential term:

$$\psi(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t) = \psi(\vec{r}, E, \hat{\mathbf{\Omega}})e^{\alpha t}, \qquad \frac{d}{dt}\psi(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t) = \alpha\psi(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t)$$

Substituting this separation of variables into the transport equation (and ignoring delayed neutrons) results in the addition of an $(\alpha/v)\phi$ term. How this term is handled depends on the algorithm.

One of the algorithms used to compute α is known as the k–α algorithm [1]. A normal fission source iteration is performed with an additional $(\alpha/v)\phi$ loss term. The effect of the $(\alpha/v)\phi$ term depends on the sign of α. If it is positive, it can be treated as an absorption term with $\Sigma_\alpha = \alpha/v$ ("time absorption"). If α is negative, it can be treated as an (n, $(1 + \eta)/\eta$ n) reaction with $\Sigma_\alpha = \eta|\alpha|/v$ ("time source") [2]. $\eta = 1$ was used in this work, resulting in an (n, 2n) reaction. At the end of each iteration, k is computed and used to update α in some way such that $k \to 1$, reducing the transport equation back to the α-eigenvalue form.

There are two drawbacks to this technique. The first involves the time source reaction, and the second involves chaos theory on the α updater. These issues, as well as their solution will be discussed in the following section. Then, these solutions will be tested on a reduced density Godiva sphere which exhibits both of these issues.

2. ISSUES AND SOLUTIONS

2.1. Time Source

The time source reaction itself poses an issue with regard to the stability of the α-eigenvalue calculation. It is common to handle the (n, $(1+\eta)/\eta$ n) reaction by increasing the weight of the currently-in-flight particle, as the resulting particles have the same angle and energy as the initial particle. However, if the expected weight of the particle after a collision is larger than before, then the growth rate can be infinite. This occurs whenever the expected value of neutrons after a collision,

$$E[n] = \text{neutrons from time source} \times \text{probability of time source}$$
$$E[n] = \frac{1+\eta}{\eta} \times \frac{\Sigma_\alpha}{\Sigma_t + \Sigma_\alpha} = \frac{\eta+1}{\eta + \frac{\Sigma_t}{|\alpha|/v}},$$

exceeds 1, which occurs whenever $|\alpha|/v > \Sigma_t$.

One remedy for this is the same that prevents the fission source in k-eigenvalue problems from diverging. Some of the particles emitted in the time source reaction can be banked alongside the fission source for the next iteration. As the source bank is normalized, it cannot grow without bounds. For $\eta = 1$, banking at least one of the two particles prevents the infinite growth of the current particle's weight.

The number of banked particles results in a convergence / performance tradeoff. Banking all particles reduces the current batch run time as the particle is terminated. However, convergence is slowed as more computation is performed in future iterations. Banking a fraction of the particles converges quicker at an increased simulation cost. Preliminary testing indicated that banking one particle had superior performance as compared to banking two, and so was used for testing.

One disadvantage here is that current techniques to tally k are effectively incorrect, as fission to fission is no longer guaranteed to occur over one iteration. In effect, the ratio of current source to next source corresponds to a different eigenvalue than k, in which the multiplication factor scales both the fission and either the partial or full time source. This issue was avoided by updating α using the technique in [3], which does not rely on any eigenvalue, k or otherwise, directly.

2.2. Chaotic Updating

The second issue is that some updating algorithms for α lead to chaotic solutions [4]. As a result, the solution will oscillate between values or possibly diverge. One way to stabilize it involves the techniques used for stochastic approximation [5]. Assuming one has the following fixed point iteration algorithm:

$$x_{n+1} = x_n + f(x_n), \qquad \text{solve } f(x_n) = 0$$

stochastic approximation scales the $f(x_n)$ term by some coefficient s_n. To guarantee that all solutions are reachable, $\sum_{n=1}^{\infty} s_n = \infty$. To guarantee that the asymptotic solution converges,

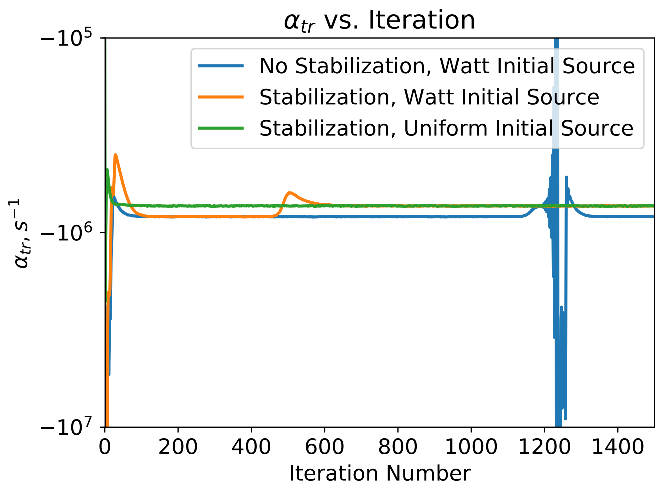

Figure 1: Track-length α as a Function of Iteration

$\sum_{n=1}^{\infty} s_n^2 < \infty$. A typical s_n that meets both of these requirements is:

$$s_n = \frac{a}{(n + n_0)^\beta}$$

The values a, n_0, and β (with $\beta \in (0.5, 1.0]$) control the convergence. While a meta-optimization process will eventually be warranted, $a = 1$, $n_0 = 15$, and $\beta = 0.75$ were chosen for testing.

3. TESTING

For this test problem, the Godiva benchmark (HEU-MET-FAST-001 of the ICSBEP benchmarks [6]) was run with the density reduced to 0.3 times the original value. Unless otherwise mentioned, this model was run with 5 million particles per batch with 500 inactive batches. This geometry has an approximate α eigenvalue as computed via a dynamic simulation of $-7.45 \times 10^5\,\mathrm{s}^{-1}$.

When run normally (no stabilization, initial $\alpha = 0$, Watt source), the simulation promptly crashed due to the infinite growth of particle weight. Adding the time source particles to the source iteration then allowed the simulation to run. The convergence of α as a function of iteration is shown as the blue line in Fig. 1. The simulation initially converged to $-8.3 \times 10^5\,\mathrm{s}^{-1}$. After 1150 iterations, the mode suddenly shifted to $-7.3 \times 10^5\,\mathrm{s}^{-1}$, after which the solution becomes chaotic. Once the algorithm resets (due to going above $\alpha = 0$), it eventually converged to $-8.3 \times 10^5\,\mathrm{s}^{-1}$ again.

Enabling stabilization yields the orange line in Fig. 1. Initially, the algorithm also converged to $-8.3 \times 10^5\,\mathrm{s}^{-1}$. At iteration 450, it too transitioned to $-7.3 \times 10^5\,\mathrm{s}^{-1}$, at which point the algorithm remained stable. The initial convergence is notably slower than the unstabilized case.

The final remaining issue is that convergence is probabilistic. The transition from the $-8.3 \times 10^5\,\mathrm{s}^{-1}$ mode to the $-7.3 \times 10^5\,\mathrm{s}^{-1}$ mode is unlikely. These modes correspond to spectra with flux peaks at $3.0\,\mathrm{eV}$ and $1.5\,\mathrm{eV}$, respectively. With the heavy atomic mass, the mostly absorbing resonance at

$2.03\,\mathrm{eV}$ in $^{235}\mathrm{U}$, and the large time source reaction cross section, the probability of a particle making the jump is small. Even with 5 million particles per iteration, this transition is still uncertain. Results can be further improved by adjusting the initial condition.

The green line in Fig. 1 is the convergence when the Watt spectrum is replaced with a uniform in lethargy source from $0.1\,\mathrm{eV}$ to $2\,\mathrm{MeV}$ and the initial α is set to $-1 \times 10^6\,\mathrm{s}^{-1}$. The simulation almost immediately converges to the $-7.3 \times 10^5\,\mathrm{s}^{-1}$ mode. The final result is $-7.292\,07(50) \times 10^5\,\mathrm{s}^{-1}$, which closely corresponds to the dynamic value. However, these benefits are not just limited to large numbers of particles per batch. Running with 10 thousand particles results in $-7.46(7) \times 10^5\,\mathrm{s}^{-1}$.

4. CONCLUSIONS

Overall, the two modifications ot the k–α algorithm improve stability for negative αs significantly. The modified source iteration eliminates the possibility of infinite particle generation within a batch. For models for which the algorithm becomes chaotic, the addition of the stochastic approximation-like stabilization also eliminates that issue. These two modifications combine to ensure that the α-eigenvalue for essentially all models can be computed in a stable fashion.

However, these improvements do not completely eliminate the need for the careful choice of initial conditions. Notable improvement in the convergence properties for the 0.3 density Godiva sphere were had by simply changing from an initial Watt spectrum to a uniform in lethargy spectrum, and setting α_{initial} to a negative value. This is very much similar to the recommendation to start particles in all regions in space with fissile material.

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