International Conference on Mathematics, Computational Methods & Reactor Physics (M&C 2009)
Saratoga Springs, New York, May 3-7, 2009, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2009)

IMPROVED CRITICALITY CONVERGENCE VIA A MODIFIED MONTE CARLO POWER ITERATION METHOD

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ABSTRACT

Nuclear criticality calculations with Monte Carlo codes are normally done using a power iteration method to obtain the dominant eigenfunction and eigenvalue. In the last few years it has been shown that the power iteration method can be modified to obtain the first two eigenfunctions. This modified power iteration method directly subtracts out the second eigenfunction and thus only powers out the third and higher eigenfunctions. The result is a convergence rate to the dominant eigenfunction being $|k_3|/k_1$ instead of $|k_2|/k_1$. One difficulty is that the second eigenfunction contains particles of both positive and negative weights that must sum somehow to maintain the second eigenfunction. Summing negative and positive weights can be done using point detector mechanics, but this sometimes can be quite slow. We show that an approximate cancellation scheme is sufficient to accelerate the convergence to the dominant eigenfunction. A second difficulty is that for some problems the Monte Carlo implementation of the modified power method has some stability problems. We also show that a simple method deals with this in an effective, but ad hoc manner.

Key Words: Monte Carlo, second eigenfunction, criticality, power method

1. INTRODUCTION

The power iteration method is used extensively in many fields to obtain the dominant eigenfunction and eigenvalue. Recently, the power method has been extended to get the two (or more) eigenfunctions with the largest absolute eigenvalues. Though the focus of our work has been on Monte Carlo calculations[1–4], it is worth noting that deterministic eigenvalue calculations (e.g. discrete ordinates) sometimes use power iteration methods as well. Having noted the general applicability of the power method, the paper now focuses exclusively on the Monte Carlo nuclear criticality problem.

Monte Carlo transport codes typically estimate the fundamental mode of a nuclear system via a power iteration method. If the eigenvalues of the system are denoted k_1, k_2, $k_3 \cdots$, with $k_1 > |k_2| \geq |k_3| \geq \cdots$, and corresponding eigenfunctions ψ_m, it is well known that the ψ_m mode disappears after n iterations as $(|k_m|/k_1)^n$. When the dominance ratio $|k_2|/k_1$ is near unity, the convergence to ψ_1 can be very slow, even if the convergence to k_1 is fast. The convergence to ψ_1 sometimes can be dramatically improved by estimating ψ_1 *and* ψ_2. To see this, note that if ψ_2 can be estimated directly, then any ψ_2 component in the estimate of ψ_1 can be subtracted out instead of powered out; this leads to an improved convergence rate $(|k_3|/k_1)^n$ [2, 5].

A Monte Carlo implementation of the modified power iteration method in a nuclear criticality calculation requires the neutrons representing ψ_2 to have both negative and positive weights because ψ_2 cannot be of one sign. Thus, ψ_2 is a sum of negatively and positively weighted neutrons. Particles with positive and

negative weights must occasionally cancel each other. An exact cancellation procedure that sums negative and positive weights using point detector methods [1, 6] is available, but it is sometimes too slow in practice. Instead of summing by using point detector methods, we show that a new simple binning procedure can provide a summing procedure that leads to an approximate ψ_2 which then can be used to accelerate the convergence to a statistically exact ψ_1; that is, no approximate cancellation procedure is applied to the weights associated with the ψ_1 estimate, so the ψ_1 estimate only has the usual statistical variations.

The paper also discusses some apparent stability problems with the new method that has been effectively solved with an ad hoc modification. The source of the stability problems is unknown, though the paper gives some speculations as to possible reasons.

2. REVIEW OF THE STANDARD POWER ITERATION METHOD

The power iteration method is used to get the largest eigenvalue and eigenfunction of a linear operator by repeated application of that operator on an arbitrary function [7, Section 9.6]. Let A be the operator and k_i and $\psi_i(P)$ be the eigenvalues and eigenfunctions of that operator; that is,

$$A\psi_i(P) = k_i\psi_i(P) \tag{1}$$

For convenience, let the eigenvalues be ordered according to their magnitudes $k_1 \geq |k_2| \geq |k_3|...$ and choose the normalizations of the eigenfunctions so that

$$\int \psi_i^2(P)dP = 1 \tag{2}$$

(Note that this paper follows the notation of reference [7] so that the first eigenfunction is the fundamental eigenfunction.) An arbitrary function can be expressed as a linear combination of the eigenfunctions; that is,

$$\psi(P) = \sum_i a_i\psi_i(P) \tag{3}$$

In general, the a_i are not explicitly known, but the standard power iteration method does not need to know them to produce the fundamental eigenfunction. From Eqs. 1 and 3 one gets

$$A^n\psi(P) = \sum_i k_i^n a_i\psi_i(P) \tag{4}$$

The essence of the power method is that for large n and $k_1 > |k_2|$

$$A^n\psi(P) = \sum_i k_i^n a_i\psi_i(P) = k_1^n \sum_i \left(\frac{k_i}{k_1}\right)^n a_i\psi_i(P) \approx a_1 k_1^n \psi_1(P) \tag{5}$$

then

$$\lim_{n\to\infty} \frac{1}{k_1^n} A^n\psi(P) = \psi_1(P) \qquad and \qquad \lim_{n\to\infty} \frac{A^n\psi(P)}{A^{n-1}\psi(P)} = \lim_{n\to\infty} \frac{A^n\psi_1(P)}{A^{n-1}\psi_1(P)} = k_1 \tag{6}$$

Thus, only the first eigenfunction remains after many iterations and the ratio of successive iterates is equal to k_1 at all points P where $\psi_1(P) \neq 0$. The fact that Eq. 6 is true at *all* points is a key observation for the modified power method below.

3. REVIEW OF THE MODIFIED POWER ITERATION METHOD

The modified method starts with two arbitrary functions, ψ' and ψ'', expressed as linear combinations of the eigenfunctions,

$$\psi'(P) = \sum_i a_i \psi_i(P) \tag{7}$$

$$\psi''(P) = \sum_i b_i \psi_i(P) \tag{8}$$

and a parameter x. We subsequently will adjust x to obtain both the first and the second eigenfunction from the power method. Now let us take a linear combination of $\psi'(P)$ and $\psi''(P)$ using x.

$$\psi(P) = \psi'(P) + x\psi''(P) = \sum_i a_i \psi_i(P) + x \sum_i b_i \psi_i(P) = \sum_i (a_i + x b_i)\psi_i(P) \tag{9}$$

In general, the a_i and b_i in Eq. 9 are unknown in the same manner as the a_i in Eq. 3 are unknown. Applying A^n to $\psi'(P)$ and $\psi''(P)$ would eventually project out the $\psi_1(P)$ component in each sum. From Eqs. 7-9 we can make the standard power iteration approximation to get the approximate result for large n

$$A^n\psi(P) = \sum_i k_i^n (a_i + x b_i)\psi_i(P) \approx k_1^n (a_1 + x b_1)\psi_1(P) \tag{10}$$

Thus nothing is gained by using Eq. 10 because only the ψ_1 component remains. Now instead of the approximation in Eq. 10, we use the slightly better approximation for large n

$$A^n\psi(P) = \sum_i k_i^n (a_i + x b_i)\psi_i(P) \approx k_1^n (a_1 + x b_1)\psi_1(P) + k_2^n (a_2 + x b_2)\psi_2(P) \tag{11}$$

Now we adjust x to prevent the *sum* on the right hand side from collapsing to ψ_1 upon further application of A. In particular, if x is such that $(a_1 + x b_1) = 0$ with which Eq. 11 becomes

$$A^n\psi(P) = \sum_i k_i^n (a_i + x b_i)\psi_i(P) \approx k_2^n (a_2 + (-a_1/b_1) b_2)\psi_2(P) \tag{12}$$

There is also a value of x such that $(a_2 + x b_2) = 0$ with which Eq. 11 becomes

$$A^n\psi(P) = \sum_i k_i^n (a_i + x b_i)\psi_i(P) \approx k_1^n (a_1 + (-a_2/b_2) b_1)\psi_1(P) \tag{13}$$

The problem now is how to find these two values of x. To do this we use the key fact from Eq. 1 that if $\psi_i(P)$ is an eigenfunction then for any point P such that $\psi_i(P) \neq 0$ the corresponding eigenvalue must satisfy

$$k_i = \frac{A\psi_i(P)}{\psi_i(P)} = \frac{A^n\psi_i(P)}{A^{n-1}\psi_i(P)} \tag{14}$$

From Eqs. 1 and 9

$$A^n\psi(P) = \sum_i k_i^n (a_i + x b_i)\psi_i(P) \tag{15}$$

Defining $\nu(x)$ and using Eq. 14, we find that

$$\nu(x) \doteq \lim_{n\to\infty} \frac{A^n\psi(P)}{A^{n-1}\psi(P)} = \lim_{n\to\infty} \frac{(a_1 + x b_1)k_1^n\psi_1(P) + (a_2 + x b_2)k_2^n\psi_2(P)}{(a_1 + x b_1)k_1^{n-1}\psi_1(P) + (a_2 + x b_2)k_2^{n-1}\psi_2(P)} \tag{16}$$

As $n \rightarrow \infty$ the eigenfunction estimate at any point P is a mixture of just ψ_1 and ψ_2. If $a_1 + xb_1 = 0$, then $\nu = k_2$ and if $a_2 + xb_2 = 0$ then $\nu = k_1$. Because Eq. 15 is true at all points P_i

$$\frac{(a_1+xb_1)k_1^n\psi_1(P_1)+(a_2+xb_2)k_2^n\psi_2(P_1)}{(a_1+xb_1)k_1^{n-1}\psi_1(P_1)+(a_2+xb_2)k_2^{n-1}\psi_2(P_1)} =$$

$$\frac{(a_1+xb_1)k_1^n\psi_1(P_2)+(a_2+xb_2)k_2^n\psi_2(P_2)}{(a_1+xb_1)k_1^{n-1}\psi_1(P_2)+(a_2+xb_2)k_2^{n-1}\psi_2(P_2)} \tag{17}$$

Cross-multiplication produces a quadratic equation in x whose two solutions generate k_1, ψ_1 and k_2, ψ_2. This is the conceptual idea. Point estimates of the eigenfunction are inefficient, so the actual algorithm estimates $\nu_i(x)$ in two regions R_1 and R_2 and then solves for the two x's satisfying $\nu_1(x) = \nu_2(x)$ [1–3]; that is,

$$\nu_1(x) = \frac{\int_{R_1}\Big[(a_1+xb_1)k_1^n\psi_1(P_1)+(a_2+xb_2)k_2^n\psi_2(P_1)\Big]dP_1}{\int_{R_1}\Big[(a_1+xb_1)k_1^{n-1}\psi_1(P_1)+(a_2+xb_2)k_2^{n-1}\psi_2(P_1)\Big]dP_1} =$$

$$\frac{\int_{R_2}\Big[(a_1+xb_1)k_1^n\psi_1(P_2)+(a_2+xb_2)k_2^n\psi_2(P_2)\Big]dP_2}{\int_{R_2}\Big[(a_1+xb_1)k_1^{n-1}\psi_1(P_2)+(a_2+xb_2)k_2^{n-1}\psi_2(P_2)\Big]dP_2} = \nu_2(x) \tag{18}$$

Rearranging yields

$$\nu_1(x) = \frac{(a_1+xb_1)k_1^n\int_{R_1}\psi_1(P_1)dP_1+(a_2+xb_2)k_2^n\int_{R_1}\psi_2(P_1)dP_1}{(a_1+xb_1)k_1^{n-1}\int_{R_1}\psi_1(P_1)dP_1+(a_2+xb_2)k_2^{n-1}\int_{R_1}\psi_2(P_1)dP_1} =$$

$$\frac{(a_1+xb_1)k_1^n\int_{R_2}\psi_1(P_2)dP_2+(a_2+xb_2)k_2^n\int_{R_2}\psi_2(P_2)dP_2}{(a_1+xb_1)k_1^{n-1}\int_{R_2}\psi_1(P_2)dP_2+(a_2+xb_2)k_2^{n-1}\int_{R_2}\psi_2(P_2)dP_2} = \nu_2(x) \tag{19}$$

Again we note that if $a_1 + xb_1 = 0$, then $\nu_1(x) = \nu_2(x) = k_2$ and if $a_2 + xb_2 = 0$ then $\nu_1(x) = \nu_2(x) = k_1$. The associated eigenfunctions are projected out per Eqs. 12-13. This is the general idea of the modified power method explained as $n \rightarrow \infty$. The details for finite n can be found in references [2–4].

In practice, n is finite, but the procedure is similar. On the $(n-1)^{st}$ iteration Eqs. 7- 8 yield

$$\hat{\psi}' = \sum_i k_i^{(n-1)} a_i \psi_i(P) \tag{20}$$

$$\hat{\psi}'' = \sum_i k_i^{(n-1)} b_i \psi_i(P) \tag{21}$$

Then

$$A^n\psi(P) = A\hat{\psi}' + xA\hat{\psi}'' \tag{22}$$

Then setting the eigenvalues in the two regions equal results in

$$\nu_1(x) = \frac{\int_{R_1}(A\hat{\psi}' + xA\hat{\psi}'')dP}{\int_{R_1}(\hat{\psi}' + x\hat{\psi}'')dP} = \frac{\int_{R_2}(A\hat{\psi}' + xA\hat{\psi}'')dP}{\int_{R_2}(\hat{\psi}' + x\hat{\psi}'')dP} = \nu_2(x) \tag{23}$$

which is a quadratic equation in x.

Using the above ideas, we have shown that two simple refinements of the standard power method [3] can explicitly separate the component multiplied by x into the first eigenfunction estimate and the other

component into the second eigenfunction estimate. The essence of these refinements is as follows: If C_i are normalizing constants and x_2 is the root that gives k_2, then the $(n+1)^{th}$ guess at ψ_2 is

$$\psi_2(P) \approx \psi_2^{(n+1)} = C_2[A^n\psi]_{x=x_2} \tag{24}$$

Similarly, if x_1 is the root that gives k_1, then the $(n+1)^{th}$ guess at ψ_1 is

$$\psi_1(P) \approx \psi_1^{(n+1)} = C_1[A^n\psi]_{x=x_1} \tag{25}$$

These two estimates suggest using

$$\psi^{(n+1)}(P) = \psi_1^{(n+1)} + x\psi_2^{(n+1)} \tag{26}$$

as the next iteration guess. Next, we set

$$\hat{\psi}' = \psi_1^{(n+1)} \tag{27}$$

$$\hat{\psi}'' = \psi_2^{(n+1)} \tag{28}$$

and insert them into Eq. 23 and solve for the two x roots.

One root for x attempts to subtract out any remaining ψ_1 in the estimate of ψ_2 and the other attempts to subtract out any remaining ψ_2 in the estimate of ψ_1. Subtracting ψ_2 from the estimate of ψ_1 means that ψ_2 is *not* powered out, but ψ_3 needs to be powered out, so convergence goes as $(|k_3|/k_1)^n$.

4. MONTE CARLO IMPLEMENTATION

A Monte Carlo implementation of the modified power method uses most of the technology of a Monte Carlo implementation of the standard power method with only minor extra requirements. In the standard method, each neutron tracked carries a single weight associated with the first eigenfunction estimate. In the modified power method, each neutron tracked carries two statistical weights, one weight is positive and associated with the first eigenfunction estimate and the other is of mixed sign and associated with the second eigenfunction estimate. In a critically problem the second mode must have regions of opposite signs. The transport process within a fission generation is unchanged. Two points on which the new approach require procedure changes are population control and the weight cancellation for the second mode. We executed population control at the end of each iterative step on both weights simultaneously through the use of the combing technique described in [5]. A number of options exists for weight cancellation.

5. COMMENTS ON WEIGHT CANCELLATION

The second eigenfunction cannot have the same sign everywhere. Particles representing the $\pm$ parts of the eigenfunction thus have $\pm$ weights. Where there is an overlap of $-$ and $+$ weights, these weights must sum so that there is a proper cancellation of $-$ weights entering a $+$ eigenfunction region and vice-versa. In a continuous Monte Carlo transport problem two particles will not be at *exactly* the same phase-space point to produce cancellation unless special procedures are used. While there is an exact method [1, 6] to effect this cancellation, it requires computationally expensive point detector mechanics. We have found we can avoid the point detector mechanics by summing the weights of nearby particles in the same region. This

approximation means that the second eigenfunction estimation is no longer exact, but we show that it is close enough to accelerate the convergence to the fundamental.

To effect the weight cancellation for ψ_2, we divided the phase-space into small regions, and for each cycle we calculated the average ψ_2 weight in each region and assigned it to each neutron in the region in place of its actual weight. The neutron phase space position was unchanged. Yamamoto [8] uses a similar cancellation approach in which the average fission weight in a region is estimated and the fission sites for the next generation are then sampled uniformly within the region. Our method retains more shape information about the fission density, but for small enough regions results obtained with Yamamoto's method should be similar to ours. We have not compared the methods, as ongoing research (to be published later) is pointing to another cancellation method that is superior to both methods. We will report this method elsewhere.

6. CALCULATIONAL RESULTS

6.1 All Fuel Problem

Our modified power method was applied to two transport problems derived from the work of Ueki and collaborators [9]. The first problem was a 9 cm slab of fuel with isotropic scattering and fission with the following properties:

- $\Sigma_{total} = 1.0\ cm^{-1}$, $\Sigma_{scattering} = 0.8\ cm^{-1}$, $\Sigma_{capture} = 0.1\ cm^{-1}$. $\Sigma_{fission} = 0.1\ cm^{-1}$, $\nu = 3.0$

plus void boundary conditions. The slab was divided into 900 regions of 0.01-cm thickness. Fig. 1 shows the first two eigenfunctions derived from a long reference calculation with 15 million particles, 1000 total iterations and tallying over iterations 101-1000. This long calculation was then used as the "exact" result for the eigenfunctions.

$$rms = \sqrt{\frac{1}{900}\sum_{i=1}^{900}\Big(\psi_1(i) - \psi_e(i)\Big)^2} \tag{29}$$

where i is the bin number, $\psi(i)$ is eigenfunction estimate on the i^{th} iteration, and $\psi_e(i)$ is the reference result for the eigenfunction. The estimated eigenvalues from this reference calculation are $k_1 = 1.30534$ and $k_2 = 0.95488$. The eigenfunctions were fit with a tenth order polynomial to smooth out noise for what we used as our final "exact" eigenfunctions.

Figure 2 compares the convergence of the modified method with the standard method using 10 million particles per iteration. Note that the modified method converges substantially faster and that both methods' rms error is eventually limited to about 5×10^{-7} by the finite number of particles run. The results converge for much smaller numbers of particles in both methods; using 10 million particles simply permits the convergence display over a larger number of iterations until the convergence becomes limited by the finite number of particles. (The first eigenfunction initial distribution was $\psi_1(x) = 2$ for $x < 0$ and $\psi_1(x) = 4$ for $x > 0$. The second eigenfunction initial distribution was $\psi_2(x) = -2$ for $x < 0$ and $\psi_2(x) = 1$ for $x > 0$.)

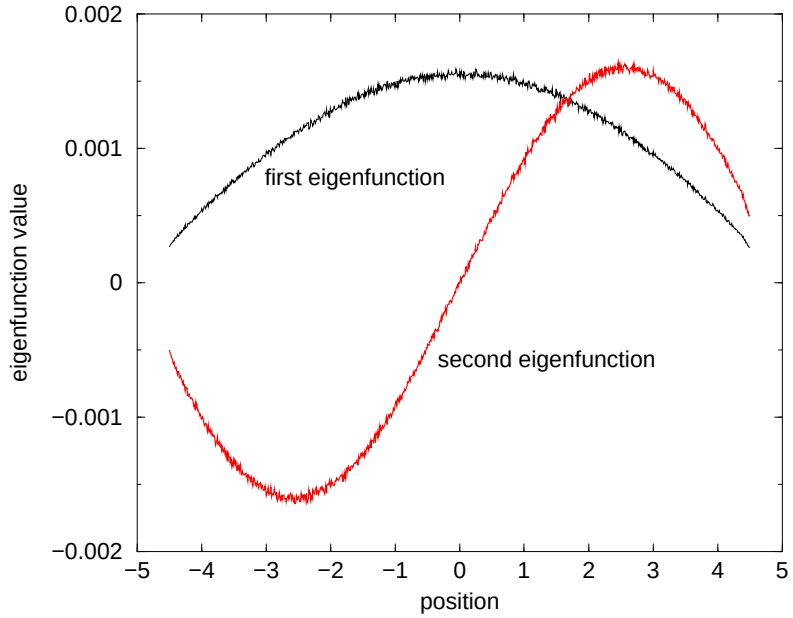

Figure 1. Full Fuel Eigenfunctions

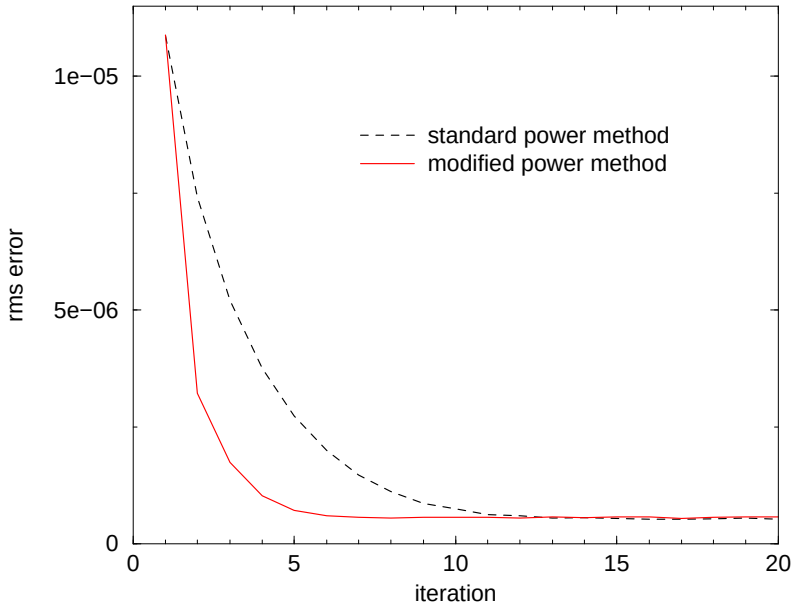

Figure 2. Full Fuel Problem with 10 Million Particles

Note this problem is pretty easy, even by the standard power method, because the first two eigenvalues are well separated. In the next section we turn attention to a much more difficult problem, in which the first two eigenvalues are very close, that others have characterized and studied.

6.2 Ueki's Asymmetric Split Fuel Problem

We also applied our modified power method to problem 1 in Ueki et al [9]. The problem is a 5 region slab of thickness 9.01-cm, with void boundary conditions on both sides, and one-group isotropic cross sections. The problem is *almost* symmetric with boundaries (shown in Fig. 3) given by vertical planes at -4.5, -3.5, -2.5, 2.5, 3.5, 4.51; the asymmetry is the -4.5 on the left boundary vs the 4.51 on the right boundary.

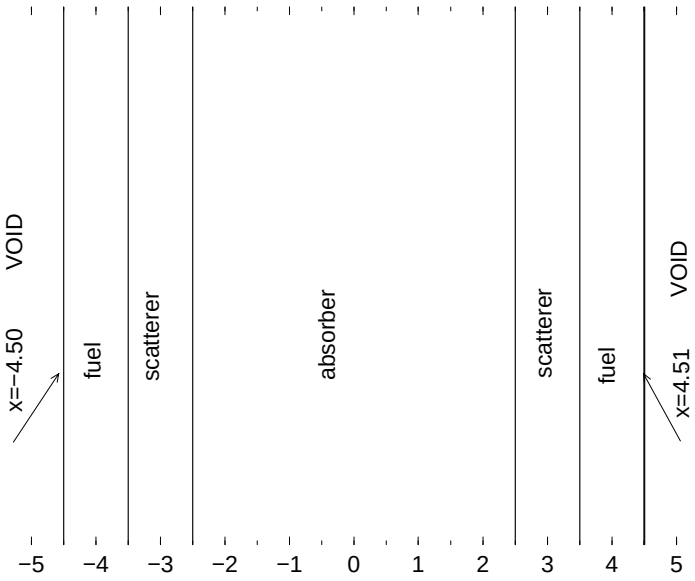

Figure 3. Split Fuel Problem Geometry

1. material 1 (scatterer): $\Sigma_{total} = 1.0\ cm^{-1}$, $\Sigma_{scattering} = 0.8\ cm^{-1}$, $\Sigma_{capture} = 0.2\ cm^{-1}$
2. material 2 (fuel): $\Sigma_{total} = 1.0\ cm^{-1}$, $\Sigma_{scattering} = 0.8\ cm^{-1}$, $\Sigma_{capture} = 0.1\ cm^{-1}$. $\Sigma_{fission} = 0.1\ cm^{-1}$, $\nu = 3.0$
3. material 3 (absorber): $\Sigma_{total} = 1.0\ cm^{-1}$, $\Sigma_{scattering} = 0.1\ cm^{-1}$, $\Sigma_{capture} = 0.9\ cm^{-1}$

Ueki reports [9] the first six eigenvalues were computed by means of a deterministic Green's function method to be 0.427425, 0.424221, 0.130633, 0.129265, 0.071924, and 0.071173 [10] with dominance ratio of 0.993. Accordingly, $k_3/k_1 = 0.306$. We divided the slab into 901 regions of 0.01-cm thickness. Fig. 4 shows the first two eigenfunctions derived from a long reference calculation with 15 million particles, 1000 total iterations and tallying over iterations 101-1000. Tenth order polynomial fits were then used to fit the eigenfunctions on the left and right sides. This fitted long calculation was then used as an "exact" result for the eigenfunctions. The first two estimated eigenvalues were 0.427406 and 0.424220, which agree well with the deterministic values.

As before, we define the rms error as:

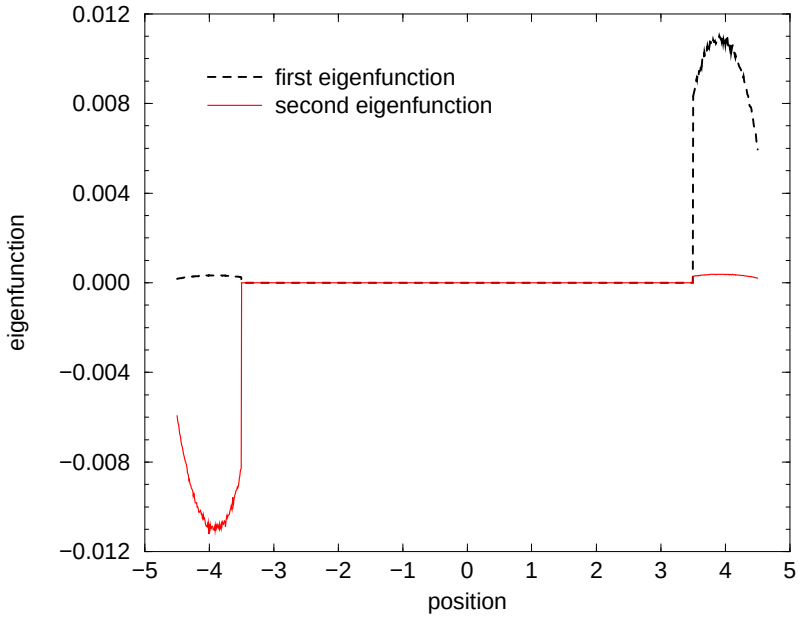

Figure 4. Split Fuel Eigenfunctions

$$rms = \sqrt{\frac{1}{901}\sum_{i=1}^{901}\Big(\psi_1(i) - \psi_e(i)\Big)^2} \tag{30}$$

Figure 5 illustrates the accelerated convergence benefits of the modified power iteration method. The initial first eigenfunction source distribution was uniform (1.0) over the entire range $-4.5 \leq x \leq 4.51$ and the initial second eigenfunction source distribution -2.0 for $x < 0$ and 1.0 for $x \geq 0$. Note the dramatic effect of the standard convergence of k_2/k_1 versus the modified convergence of k_3/k_1

Though the results displayed in Fig. 5 look good, stability problems emerge for reasons that are currently not understood when using smaller numbers of particles. Fig. 6 shows the rms error for starting 1 million particles per iteration. Fig. 6 also shows that the rms error can get quite low (4×10^{-6} at iteration 5), but then have huge lurches upward. This problem can be solved in an ad hoc manner by limiting the rapidity of the correction of the ψ_1 estimate by the ψ_2 estimate. That is, instead of using Eq. 25, use

$$\psi_1(P) \approx \psi_1^{(n+1)} = C_1[A^n\psi]_{x=x_{limit}} \tag{31}$$

where

$$x_{limit} = sign(x_1)min(|x_1|, \delta) \tag{32}$$

Fig. 6 also shows the results with the eigenfunction mixing limited by $\delta = 0.05$.

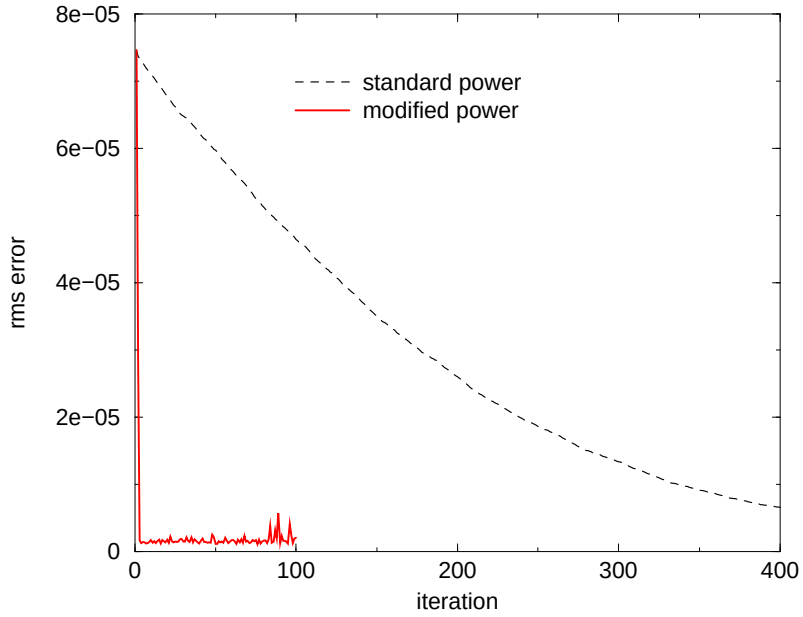

Figure 5. Standard vs Modified Convergence

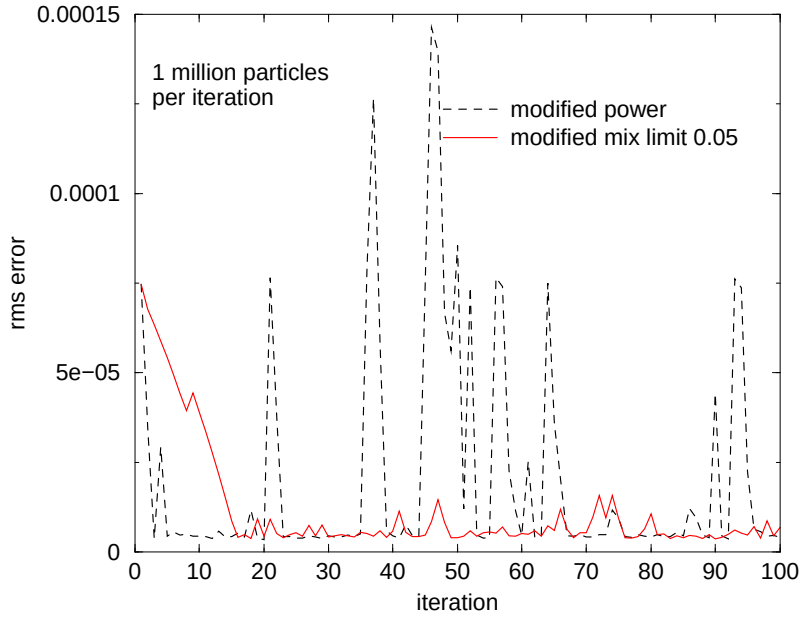

Figure 6. Split Fuel With/Without Mix Limit

The worst lurches upward seem to occur when the Monte Carlo procedure gets eigenvalue inverted estimates such that $\hat{k}_1 < \hat{k}_2$ associated with the eigenfunction estimates $\hat{\psi}_1$ and $\hat{\psi}_2$. When the eigenvalues are close, it is not hard for the statistical estimates to have an inverted order from the true order. The result is to intermix large amounts of the two eigenfunctions. After the mix, the estimated first eigenfunction has so much second eigenfunction component that the rms difference from the true eigenfunction is huge. The ad hoc mixing control is effective, as per Fig. 6, but the situation is unsatisfactory for two reasons. First, the mixing control slows down the accelerated convergence. Second, it is not clear apriori what δ should be

used.

7. CONCLUSIONS

We have shown that a simple region averaging of $\pm$ weights in the second eigenfunction estimate is sufficient to accelerate the convergence in the two test problems herein. This means that the time consuming point detector mechanics in [1] are not necessary for practical acceleration to the fundamental. A useful byproduct of the new method is that a good estimate of the second eigenfunction is obtained while accelerating convergence to the fundamental.

Although a simple ad hoc procedure solved the instability encountered in the split fuel problem, more work is needed to understand the instability and obviate the ad hoc procedure.

ACKNOWLEDGEMENTS

We gratefully acknowledge support of the U. S. Department of Energy through the LANL/LDRD program.

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