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VACATION MATRIX METHOD FOR CORRECT SOURCE DISTRIBUTION IN MONTE CARLO CRITICALITY CALCULATIONS

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ABSTRACT

Monte Carlo criticality calculations typically use the power iteration method in which the fissions in one generation become source sites for the subsequent generation. The eigenvalue, k_{eff}, converges much faster than does the eigenfunction. The eigenfunction is physically the neutron source distribution that is, in turn, related to the flux, energy deposition, and other important quantities. Even though the eigenvalue, k_{eff}, may be converged to high precision, such as 0.01%, the source distribution, or eigenfunction, may be off by orders of magnitude in loosely coupled systems.

A new method has been developed to estimate the source distribution in Monte Carlo criticality calculations correctly. Results for symmetric, asymmetric, homogeneous, and inhomogeneous problems indicate that 1000 times fewer histories are needed to converge the source distribution.

The fundamental problem of the fission matrix method is that the fission matrix, A, cannot generally be estimated within the Monte Carlo calculation because of statistical noise that produces false asymmetry. The proposed method nearly eliminates the problem of statistical noise in A by separating A into a vacation matrix V, where the elements are related to the number of fissions in one cell from particles exiting other cells, and a diagonal matrix where elements account for the geometric and fluctuating statistical asymmetry of the system. By assuming that the eigenfunction of the more stable vacation matrix preserves the shape of the eigenfunction of the fission matrix, part of the asymmetry is strategically removed from the system, and then reintroduced when it causes less noise.

1 INTRODUCTION

The power iteration method is generally used to solve the source distribution problem in Monte Carlo criticality problems [1]. If the effective fission matrix is perfect

(effective indicates the fission matrix that is inherent to the problem, rather than an actual calculated fission matrix), this method works by definition because the source in each fissionable geometric region (or cell) from one generation is effectively multiplied by the spatial proportionalities which comprise the fission matrix to generate the source in each cell for the next generation. However, for iterative solutions, the effective fission matrix is only approximate due to statistical error, and therefore the eigenfunction may never converge to the actual solution. Until a perfect effective fission matrix is constructed (which strictly speaking *never* happens in the Monte Carlo method), the eigenfunction solution is suspect. The failure of convergence of the eigenfunction is most pronounced in weakly coupled nuclear systems [2].

During the presettle period, in which fission source sites are spatially redistributed to more accurately reflect the actual eigenfunction, the fission source distribution is wrong, and therefore the effective fission matrix is populated with anomalous values. For instance, during the presettle cycles, if in a given problem the source distribution in each cell is wrongly central (this is often the case for problems where the initial source distribution is guessed), the effective fission matrix will be overly diagonal. The actual contribution from the off-diagonal would then be somewhat discounted and the resultant redistribution of the source sites would have a disproportionate dependence on the diagonal terms of the effective fission matrix.

The proposed method works by solving the fission matrix, A, the elements of which are related to the number of neutrons in each geometric region from each other's geometric region. The Vacation Matrix Method is introduced to produce a more accurate solution by considering proportionalities that are more reliable than those in the fission matrix. Namely, the number of sources produced in a given cell from those sources which began in and *left* another cell is considered, rather than the number of sources produced in a given cell from all sources which *began* in another cell. The probability of a source being created in one cell from a source which began in and vacated another is assumed to be a more reliable proportionality because it is less dependent on the source site redistribution process of the presettle cycles, especially for a diagonally dominant system, and because it disregards the probability that a source leaves the cell from which it originated. The vacation matrix approach is a significant improvement over our previous renormalization symmetrization approximation for A [3].

Others have approximated the eigenfunction using deterministic calculations of the flux [4,5,6,7,8], fixed source Monte Carlo estimations of A [5,9], and hybrid methods have emerged.

Figure 1 shows the results of a short run (130 cycles at 1000 histories/cycle) with standard Monte Carlo on a symmetric hexagonal lattice of fissionable cells. It is easy to see that, although the eigenvalue has quick convergence, the flux distribution is wrongly asymmetric. Preliminary results of the Vacation Matrix Method show that this problem can be fixed.

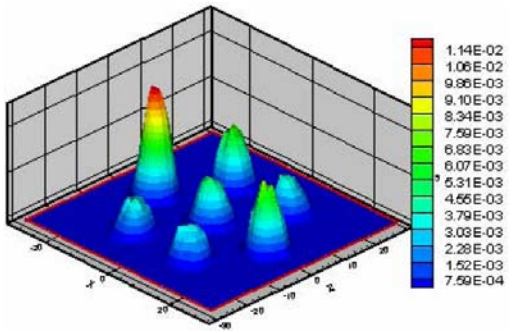

Figure 1. Standard Monte Carlo results

1.1 Probabilities approximated throughout the calculation

Note: *source* and *source particle* are used interchangeably in the following definitions.

Vacative probability: the probability that a source particle beginning in cell i will leave cell i

$$\alpha_i = \frac{l_i}{n_i} = \frac{\#\text{ sources which began in and left cell i}}{\#\text{ sources which began in cell i}}$$

Vacative source probability: probability that a source produced in cell j is from a source particle that left cell i

$$A_{ij} = \frac{L_{ij}}{N_{ij}} = \frac{\#\text{ sources produced in cell j from those which began in and left cell i}}{\#\text{ sources produced in cell j from those which began in cell i}}$$

Fission matrix probability: probability of producing a source in cell j from a source beginning in cell i

$$P_{ij} = \frac{N_{ij}}{n_i} = \frac{\#\text{ sources produced in cell j from those which began in cell i}}{\#\text{ sources which began in cell i}}$$

Vacation matrix probability: probability of producing a source in cell j from a source particle that began in and left cell i

$$V_{ij} = \frac{L_{ij}}{l_i} = \frac{\#\text{ sources produced in cell j from those which began in and left cell i}}{\#\text{ sources which began in and left cell i}}$$

1.2 The Fission Matrix Method

The fission matrix consists of elements $P_{ij} = N_{ij}/n_i$ where N_{ij} = # sources in cell j from those starting in cell i and n_i = # sources starting in cell i, generation k. The total number of sources expected in a given cell x in generation k+1 is given by

$$\left(n_x\right)_{k+1} = \sum_{i=1}^{R} \left(N_{ix}\right)_{k+1} = \sum_{i=1}^{R} \left[\frac{\left(N_{ix}\right)_{k+1}}{\left(n_i\right)_k}\right] \cdot \left(n_i\right)_k = \sum_{i=1}^{R} P_{ix} \cdot n_i \tag{1}$$

for a system of R fissionable cells, and where it is henceforth understood that $n_i = (n_i)_k$ unless explicitly stated otherwise (also for l_i and α_i in the future). Given the fission matrix $\mathbf{P} = \{P_{ij}\}$, and the target vector $\mathbf{T} = \{n_i\}$, the equivalent vectorial representation is

$$\mathbf{T}_{k+1} = \mathbf{P}_{k+1} \cdot \mathbf{T}_k \tag{2}$$

Note that in general the eigenvalue problem $\mathbf{PT} = \lambda\mathbf{T}$ implies the iterative dominant eigenvector solution $\mathbf{T}_n = \mathbf{P}^n\mathbf{T}_0$, corresponding to the dominant eigenvalue (assuming $\lambda_1 > \lambda_2 \geq ... \geq \lambda_m$ where λ_1 is dominant).

Given an initial source distribution, $\mathbf{T}_0$, the best current approximation of the fission matrix is used to iteratively solve for the corresponding flux target vector $\mathbf{T}_n$ $\{n \rightarrow \infty\} \rightarrow \mathbf{T}$. However, criticality calculations using the Monte Carlo method do not favor this method because of the presettle cycles in which the fission source is spatially redistributed to more accurately reflect the actual source distribution and because of aforementioned statistical fluctuations in the fission matrix probabilities [10]. During the presettle cycles, the fission matrix approximation may be insufficient for an accurate estimation of the flux.

In summary, fixed source estimations of the fission matrix are inefficient because of the computational expense, but the iterative estimation of the fission matrix is unreliable due to the statistical uncertainty and sensitivity of the fission matrix. Therefore, a different, more stable approximation of the solution matrix is required for the effective utilization of the more efficient iterative scheme.

2 THE VACATION MATRIX METHOD

The Vacation Matrix Method solves both problems introduced by the fission matrix by separating the fission matrix into two matrices containing separable probabilities. The vacation matrix is composed of elements $V_{ij} = L_{ij}/l_i$ where L_{ij} = # sources in cell j from those that began in and left cell i, and l_i = # sources that began in and left cell i. The equivalent fission matrix solution for a given cell x is

$$\left(n_x\right)_{k+1} = \sum_{i=1}^{R}\left(N_{ix}\right)_{k+1} = \sum_{i=1}^{R}\left[\frac{\left(N_{ix}\right)_{k+1}}{\left(L_{ix}\right)_{k+1}}\right]\cdot\left[\frac{\left(L_{ix}\right)_{k+1}}{\left(l_i\right)_k}\right]\cdot\left[\frac{\left(l_i\right)_k}{\left(n_i\right)_k}\right]\cdot\left(n_i\right)_k = \sum_{i=1}^{R}\left(A_{ix}\right)^{-1}V_{ix}\cdot\alpha_i n_i \quad (3)$$

This solution is identical to the fission matrix solution [Eq.(1)], and is given by

$$\mathbf{T}_{k+1} = (\mathbf{V} - \mathbf{V}_d + \mathbf{A}\cdot\mathbf{V}_d)_{k+1}\cdot\boldsymbol{\alpha}_k\cdot\mathbf{T}_k = \mathbf{P}_{k+1}\cdot\mathbf{T}_k \quad (4)$$

where $\mathbf{A} = \{A_{ii}^{-1}$ - diagonal n × n matrix$\}$, $\mathbf{V} = \{V_{ij}\}$, $\boldsymbol{\alpha} = \{\alpha_i$ - diagonal n × n matrix$\}$, and $\mathbf{V}_d = \{$n × n diagonal of $\mathbf{V}\}$. The fission matrix has been separated as

$$\mathbf{P} = (\mathbf{V} - \mathbf{V}_d + \mathbf{A}\cdot\mathbf{V}_d)\cdot\boldsymbol{\alpha} \quad (5)$$

The above target vector (eigenfunction solution) approximation [Eq.(4)] suggests that, instead of approximating $\mathbf{T}$ directly, the more reliable vacation matrix may be used to directly approximate $\boldsymbol{\alpha}\cdot\mathbf{T}$, using only the modified vacation matrix:

$$\mathbf{V}_m = \mathbf{V} - \mathbf{V}_d + \mathbf{A}\cdot\mathbf{V}_d \quad (6)$$

The primary assumption of the Vacation Matrix Method is that the modified eigenfunction of the vacation matrix is a good approximation to the eigenfunction of the system:

$$(\boldsymbol{\alpha}\mathbf{T})_{k+1} = \mathbf{V}_m \cdot (\boldsymbol{\alpha}\mathbf{T})_k \tag{7}$$

$$\mathbf{T} \approx \boldsymbol{\alpha}^{-1} \cdot (\boldsymbol{\alpha}\mathbf{T})_n = \boldsymbol{\alpha}^{-1} \cdot (\mathbf{V}_m)^n \cdot \mathbf{T}_0 \tag{8}$$

This assumption removes the error introduced by the faulty source distribution of the presettle cycles, and the noise introduced by the fluctuating vacative probability (probability that source will leave source cell) contained in the fission matrix.

To enhance the speed of convergence (reduce n), the following identity from linear algebra is used:

$$\text{if } \mathbf{A}\mathbf{x} = \lambda\mathbf{x}, \text{ then } (\mathbf{A} + c\mathbf{I})\mathbf{x} = (\lambda + c)\mathbf{x} \tag{9}$$

In other words, the eigenfunction **x** is unchanged by the addition of some arbitrary constant c to the diagonal of the matrix **A**. For the current problem, $\mathbf{A}=\mathbf{V}_m$, $c=-\min(\mathbf{A}\cdot\mathbf{V}_d)$, and $\mathbf{x}=\mathbf{T}$. The more refined Wielandt's Method used for an accelerated solution to (4) has recently been borrowed from the deterministic approach and implemented in the Monte Carlo method [11].

Assuming that the results of long runs in standard Monte Carlo are correct, preliminary results of the Vacation Matrix Method indicate that it is best to *wholly* subtract the diagonal of $\mathbf{V}_m$ for systems where all parts of the iterated target vector are non-zero. If at any point in the iteration any part of the target vector iterates out or becomes zero, the diagonal of $\mathbf{V}_m$ is added, which is $\mathbf{A}\mathbf{V}_d$, to achieve a solution closer to the results of standard Monte Carlo, which are steady-state solutions (time goes to infinity), not merely static solutions.

2.1 The Decoupled Matrix Method

All real problems have some coupling between all parts (cells) of the problem. There is no real black-body, and no real infinite distance. For most problems, the modified vacation matrix is therefore sufficient, no matter how weak the coupling. However, for artificially decoupled problems, the modified vacation matrix is a diagonal (there is no source in j from $i \neq j$ when decoupled) or zero. This artificial problem has a trivial solution, and must therefore be treated trivially, as a special case.

In a real problem, if $k_{eff} > 1.0$ in cell 1 and $k_{eff} < 1.0$ in cell 2, in a problem with two cells of unit importance, the decoupled solution would correctly be $\mathbf{T} = [1\ 0]^T$. However, if both cells are subcritical, the Monte Carlo solution gives all sources to whichever cell has the higher k_{eff}, and likewise for supercritical decoupled cells. A target vector $\mathbf{T} = [k_1\ k_2\ \ldots\ k_n]$ is therefore imposed, where k_i = eigenvalue of decoupled cell i, given the fact that the flux $\boldsymbol{\varphi}$ is proportional to k_{eff}. For extremely weakly coupled problems, this approximation is used until sufficient information is gathered for an accurate solution.

2.2 Flux Imposition

Imposition

The difference between the actual source distribution and the target flux calculated with the vacation matrix is proportional to the bias applied to the source distribution. Various damping factors ensure the absence of oscillations and other computational instabilities.

The bias B_i for sources in cell i is calculated with respect to the unit target vector T in i as

$$B_i \cdot \left[\left(n_i \right)_{k+1} \right] = T_i \cdot \sum_{j=1}^{k+1} \sum_{i=1}^{R} \left[\left(n_i \right)_j \right] - \sum_{j=1}^{k} \left(n_i \right)_j \tag{10}$$

or, B_i times the sources generated (generation k+1) in cell i is the number of sources that must be added to the accumulated (up to current generation k) source in cell i so that the biased source in i is in correct proportion to the entire source throughout all generations ($1 \rightarrow k+1$) and all cells ($1 \rightarrow R$).

Renormalization

After the bias is calculated, the biased source is renormalized to preserve the eigenvalue of the system. If $F_i > 1.0$, let modified bias $F_i = F^+_i$, and if $F_i < 1.0$, let modified bias $F_i = F^-_i$. Thus, a statement of the conservation of sources is

$$\Sigma_+ (F^+_i - 1) \cdot (n_i)_{k+1} + \Sigma_- (F^-_i - 1) \cdot (n_i)_{k+1} = 0 \tag{11}$$

The biases are modified to satisfy this condition with stabilizing factors applied.

3 DESCRIPTIONS OF ILLUSTRATIVE TEST PROBLEMS

3.1 Hexagonal Lattice

Seven cylindrical configurations are placed in the hexagonal arrangement shown in Figure 2. Each configuration consists of material-less cylinder of height 8cm and radius 5cm placed atop a cylinder of height 12cm and radius 5cm that consists of pressurized-water-reactor (PWR) fuel (1.0889e-4 at-% ^{235}U, 1.0909e-3 at-% ^{238}U, 3.2929e-2 at-% ^{16}O, 5.7058e-2 at-% ^{1}H). Both cylinders are surrounded by a cylindrical iron shell of thickness 1cm. This lattice is placed in a cylinder of radius 30cm and height 22cm of nitrous oxide. The outside world has zero importance (neutrons not tracked). At the beginning of the run, each cylinder has an isotropic point source at its center.

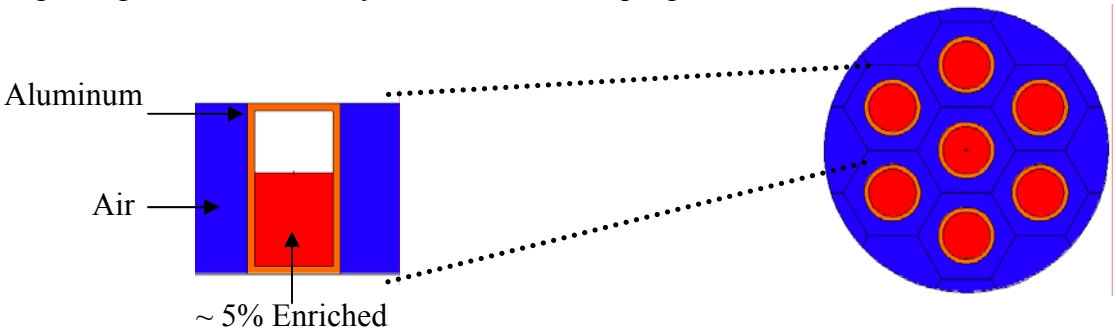

Figure 2. Hexagonal arrangement

3.2 Fuel Pin

In Figure 3, a 330-cm-long rod with radius 0.40cm of 3 at-% ^{235}U and 97 at-% ^{238}U surrounded by Zircaloy of thickness 0.06cm (typical PWR fuel pin dimensions and composition) is segmented axially into 11 equal parts, each part initially having an isotropic point source at its center, and placed in pool of water with reflecting rectangular parallelepiped surface with 2.926cm sides and 334cm height (2cm gap between reflector and rod at each end). All runs use an initial k_{eff} of 1.0. The fuel pin problem was chosen specifically as an extreme case, where computational difficulties were expected to arise because of the weak coupling.

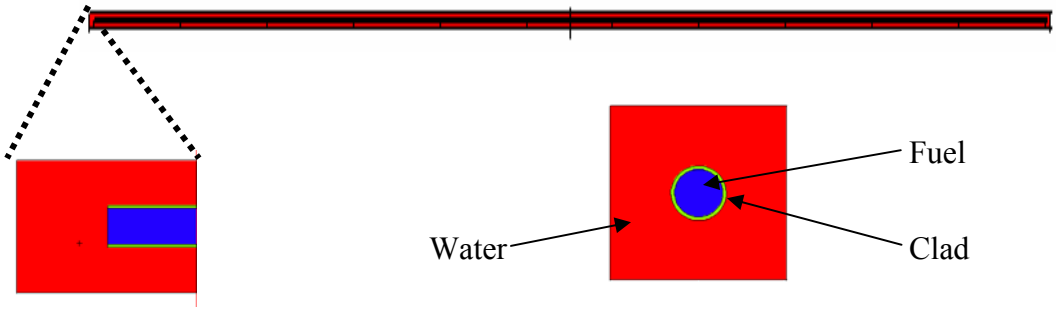

Figure 3. Fuel Pin arrangement

4 PRELIMINARY FINDINGS

Results for the symmetric hexagonal lattice are illustrated again in Figure 4, where the central peak corresponds to the central cylinder. The Converged run corresponds to a 130 million history calculation (130 cycles, 1 million histories per cycle, 30 inactive cycles). The Standard run corresponds to the results of standard Monte Carlo after 130 thousand histories (130 cycles, 1000 histories per cycle, 30 inactive cycles), and the Proposed run corresponds to the results achieved with the Vacation Matrix Method after 130 thousand histories.

Longer runs up to 4 billion particles with standard Monte Carlo indicate the peak of the Converged result should actually be closer to 0.213, which is actually nearer the Proposed peak than the Converged peak. This suggests that the proposed method converges well over 1000 times faster than conventional Monte Carlo.

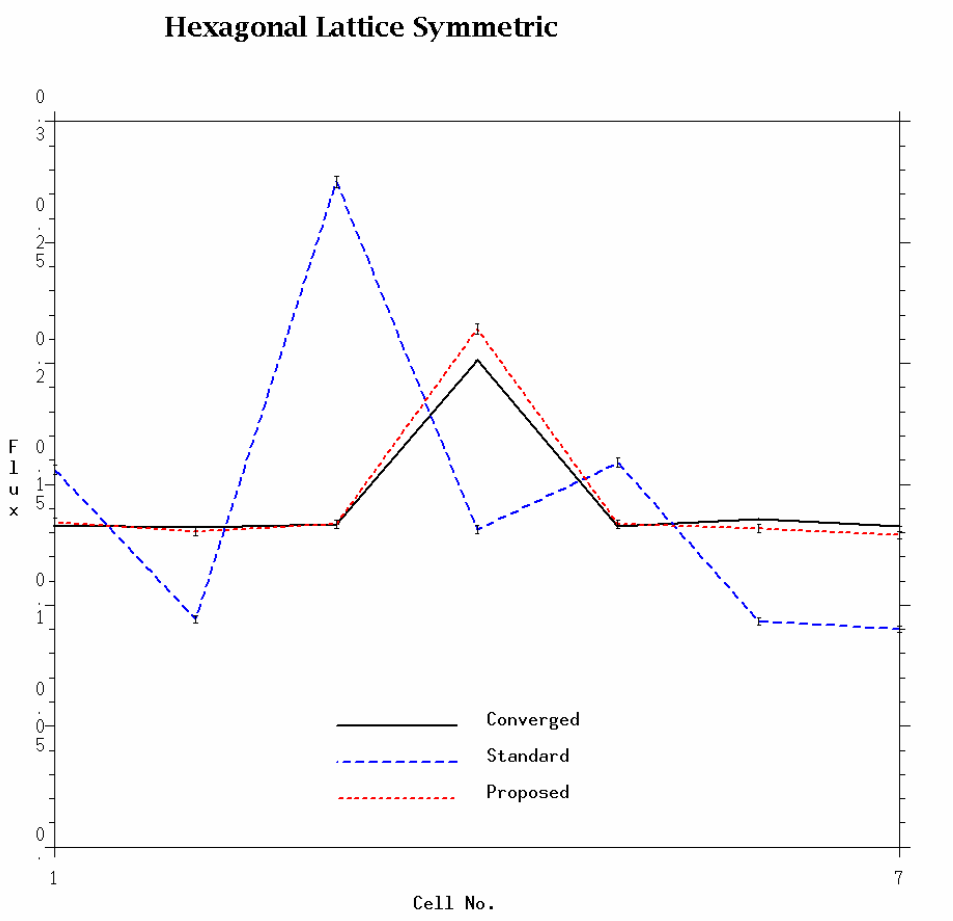

Figure 4. Quick convergence for the symmetric hexagonal lattice

Results for the asymmetric hexagonal lattice are shown in Figure 5. The Vacation Matrix Method again converges much more quickly than standard Monte Carlo.

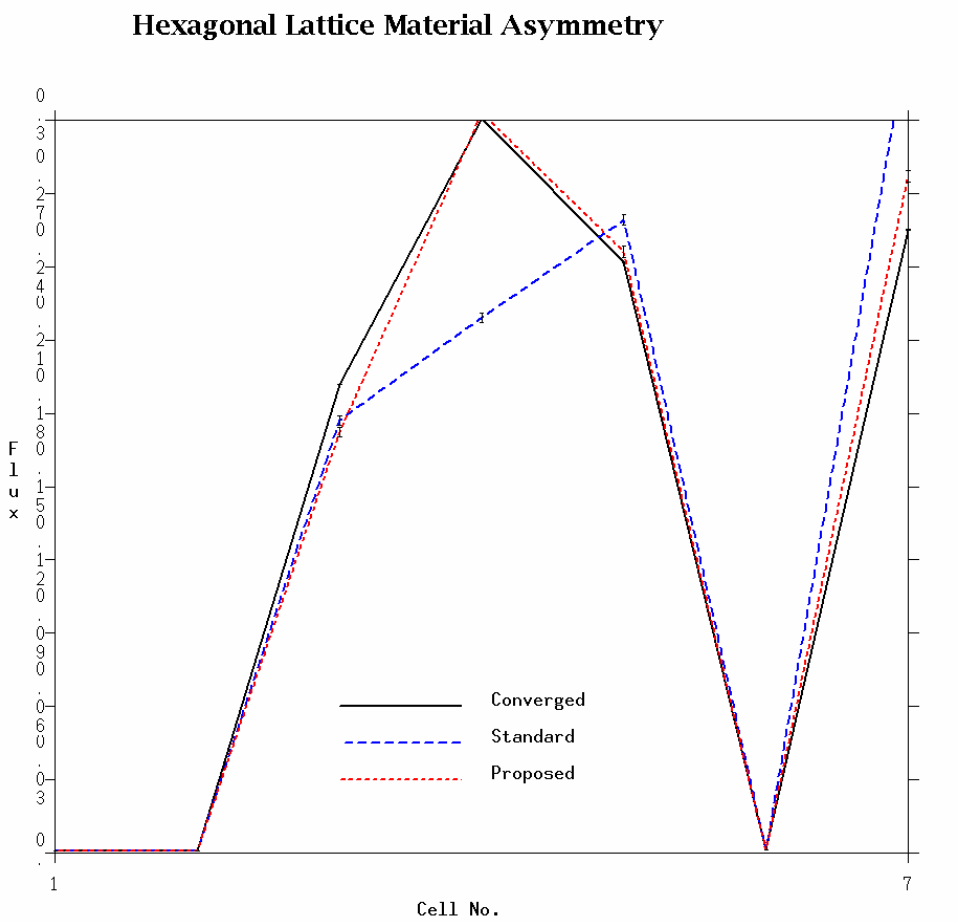

Figure 5. Quick convergence for the materially asymmetric hexagonal lattice

The symmetric fuel pin problem was chosen specifically to test extremely decoupled systems with a small number of histories per cycle. Shown in Figure 6 are the results of the current Vacation Matrix Method for the symmetric fuel pin. Runs up to 400 million histories have shown that the peak should be sharper, but should not be as sharp as indicated by the proposed method. Because the proposed method yields better results in all other tested problems, it is suspected that this faulty distribution is caused by computational anomalies. Figure 7 shows a similar anomaly for the geometrically asymmetric fuel pin case, where the sizes of the cells along the fuel rod are altered.

This suggests that the contribution of the diagonal be accounted for by the addition of a separate eigenfunction, which is directly proportional to the diagonal of the fission matrix, to the eigenfunction of the modified vacation matrix. It is expected that these two contributions of the diagonal and off-diagonal will be weighted with the relative values of the one-norms of the off-diagonal matrix and of the diagonal matrix. This would broaden the shape of the fluxes in Figures 6 and 7, causing the vacation matrix solution to approach the Converged solution.

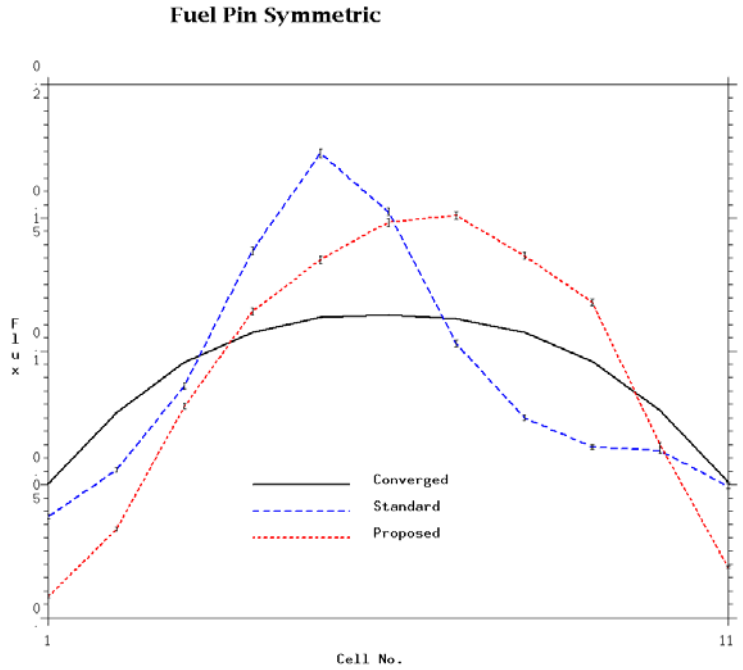

Figure 6. **Current Vacation Matrix Method for symmetric fuel pin case.**

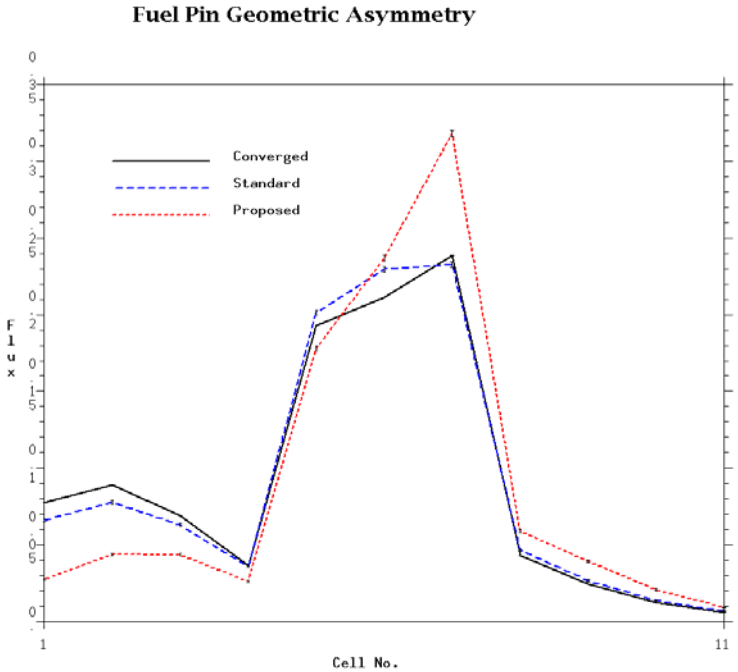

Figure 7. **Geometrically asymmetric fuel pin case.**

Figure 8 shows quick convergence for the materially asymmetric fuel pin case where the compositions of the geometrically symmetric cells are altered.

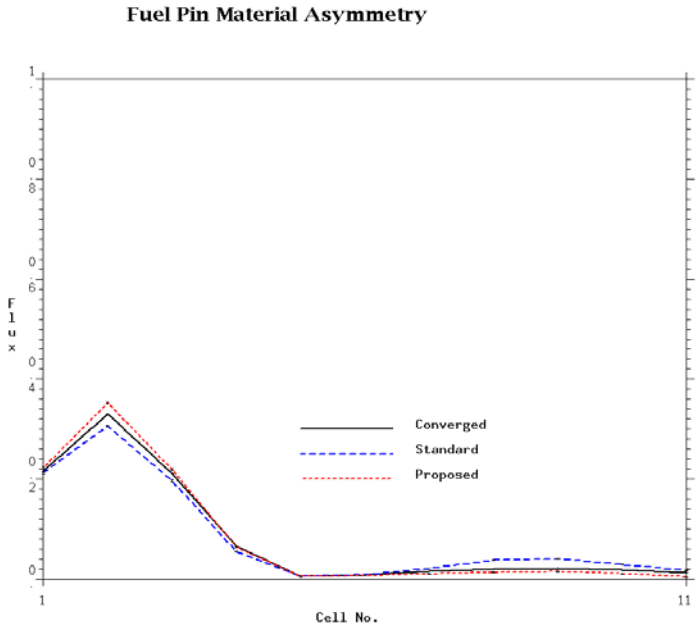

Figure 8. Quick convergence for the materially asymmetric fuel pin case

5 CONCLUSION

The standard power iteration method for solving criticality calculations with Monte Carlo can result in poor convergence of the eigenfunction (flux or source distribution) even when the eigenvalue, k_{eff}, is well converged. This poor convergence is most pronounced in loosely-coupled criticality problems.

The proposed Vacation Matrix Method converges the source distribution more efficiently, where is it found that the eigenfunction shape of the fission matrix is preserved in the more reliable vacation matrix. Furthermore, in many cases, the new method often yields *better* results than do long runs with standard Monte Carlo. In some problems 1000 times fewer source particles per power iteration cycle are needed to achieve a comparable source distribution. That is, the Vacation Matrix Method solves the source distribution problems 1000 times faster than do conventional methods in some loosely-coupled problems.

The Vacation Matrix Method still needs further development. In some problems the source distribution still does not converge well. Further generalization is required for the method to become part of a production Monte Carlo code. The method appears to have great promise.

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