

# SOURCE CONVERGENCE IN CRITICALITY SAFETY ANALYSES

## Phase II : Guidance for Analysts

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*Key Words:* convergence, criticality, Monte Carlo

### 1 INTRODUCTION

In this report, progress in fission source convergence in the programme of the OECD/NEA Expert Group on Source Convergence in Criticality Analysis is reviewed. Efforts by the participants in the Phase II programme have concentrated on three strategies: source iteration acceleration, statistical tests, and computational strategies. The efficacies of the most relevant of the acceleration algorithms and several statistical methods that were explored in this phase are described. This includes ease of use for analysts and simplicity of implementation in Monte Carlo codes for code developers. Computational strategies to prevent or identify source convergence problems are also briefly discussed.

Fission source convergence in Monte Carlo criticality calculations has been an issue since the early implementations of the method[1]. In 1971, Whitesides identified a specific case exhibiting source distribution problems -- a 9x9x9 array of decoupled spheres[2]. In the mid-1990s, An informal US Department of Energy Seminar on Misapplication of Monte Carlo Codes to Criticality Calculations highlighted the need greater care in criticality safety analyses. Since the 1990s, work intensified after unconverged sources influenced results for an international benchmark comparison [3]. This work has been carried out by members of the NEA Working Party on Nuclear Criticality Safety's Expert Group on Source Convergence in Criticality Analysis and by others.

The first Phase of the Expert's group was completed with the publication of its report in 2006[4]. The work program consisted of the specification of four test problems that exhibited slow convergence, under-sampling, or seemingly intractable noise. It also included the analysis of these systems using various criticality codes and methods, and the compilation of results. These four and some other systems have since been used to explore the efficacy of various methods in addressing slow or false convergence, noise, bias, and uncertainty bias. The test problems are briefly described in Figures 1 – 4, and full detail is specified in Reference 4.

To standardize comparisons between codes and methods in Phase I, the Monte Carlo computational parameters were specified. This made the computations unusually (and unrealistically) challenging so the effects of the methods would be more apparent. For example, test problem 4 was an undersampling problem with a dominance ratio of only 0.91 -- a 5x5x1

widely spaced array of identical 8.71 cm radius HEU spheres, with the central one replaced with a (critical) 10 cm radius sphere. Only 125 histories per cycle were used. Stratified sampling and superhistory powering both improved the chances of source convergence in this problem, but, of course, the simplest approach is to use many more histories per generation than were specified for the test problem. One can easily estimate how many by using each fissile component's volume fraction and its material's neutron multiplication properties.

Phase II was to be the collection and description of methods and techniques that can be useful in avoiding the pitfalls of incomplete source convergence, particularly in Monte Carlo criticality calculations. Furthermore, guidance on their applications to criticality calculations was to be provided for analysts in the field.

Fortunately, between 2006 and today, much good work has been done in this area to supplement earlier efforts on the subject. Most or all of these developments were carried out independently by Expert Group participants. Whether this was in response to the underlying needs of the community or because of the Expert Group's program, the improvements in source convergence tools and techniques are striking, and should contribute to more robust analyses.

We summarize here the aggregate work in source convergence emphasizing benefits and limitations of methods and techniques. It is hoped that code developers will implement the best of the algorithms, as well as develop better ones; and that analysts will make use of them.

## 2 CONVERGENCE TESTS

When applied to Monte Carlo calculations, stochastic fluctuations sometimes obscure the convergence trend signals that are normally much more apparent in deterministic calculations. It should be noted that the underlying slow convergence problem is not due to the Monte Carlo algorithm; deterministic calculations are also subject to false convergence of source distributions in high dominance ratio problems. A sample set of eigenvalue estimates from two Monte Carlo cases of the checkerboard fuel storage array demonstrate the noise problem in Figure 5.

Normally,  $k_{eff}$  converges at a much earlier iteration than does the source distribution[5], so a converged eigenvalue may mask an unconverged source. To observe source convergence, however, requires some detailed arrangements for display and analysis of source statistics, including autocorrelation, trends, etc. When source convergence is established, the convergence of  $k_{eff}$  is guaranteed. If the source has not been proven to be converged, then the analyst must show that  $k_{eff}$  is. An effective fission distribution convergence test is therefore useful for determining eigenvalue convergence even if, strictly speaking, only a converged  $k_{eff}$  is needed. Naturally, the fission source must be converged if reaction rates are desired, e.g., in depletion calculations.

Statistical tests commonly available to Monte Carlo users include plots of individual cycle  $k_{eff}$  or cumulative  $k_{eff}$  vs. cycle (with estimated errors), second half – first half  $k_{eff}$  (drift-in-mean) comparisons, and autocorrelation coefficient edits. Using the first test problem from Phase I, the checkerboard fuel storage system, several additional statistical tests were also evaluated. Designed for fixed source Monte Carlo problems, these are premised on the independence of estimates in different cycles, which is not the case in Monte Carlo criticality calculations,

especially high-dominance ratio ones. (They are still quite useful for fixed source calculations of unlikely events, however.) The Shapiro-Wilk normality test[6] was unable to detect the slow trend in cycle-by-cycle  $k_{eff}$  estimates common in slowly converging calculations[7]. Similarly, the R-test [8], and the "1/N" test[8] all proved insensitive to slowly evolving  $k_{eff}$  or reaction rate estimates[7].

Additional work has been done in automated (eigenvalue) transient suppression using Brownian Bridge methods [9]. This is accomplished by computing all of the autocorrelation coefficients of  $k_{eff}$  once the Monte Carlo calculation is complete, and determining the optimal number of skip cycles retrospectively. This method is used in MORET4[10] to retrospectively select the number of skip cycles. It can work even when noise obscures an underlying trend in  $k_{eff}$ . It is easy to use, but it does not evaluate the evolving source distribution.

Autocorrelation in fission source distributions, more pronounced than for eigenvalues, provides information for additional statistical tests. Such tests require that spatial subdomains unique to each system be analyzed. Identifying and specifying these subdomains might add modestly to code input and introduce some unreliability. Except in one of the test problems, these methods were a small part of the Expert Group's Phase I work.

To date, the most promising statistical tests aimed at checking source convergence in high-dominance-ratio Monte Carlo calculations are entropy-based informatics methods[11] that analyze the source distribution rather than  $k_{eff}$ . In the relative entropy method, the source distribution entropy is computed at the end of each cycle using a spatial mesh specifically established for source entropy tallies. If a uniform initial source is used, a reasonable initial mesh can be established automatically after the first cycle's fission site bank is filled. Even if an unrealistic initial source is used, the mesh can be modified by the during subsequent cycles to provide the right granularity. The method is simple: it does not require modification of the random walk or source site selection procedure.

It is the trend in entropy that signals source convergence, not the value of the entropy. At the extremes, a point source has an entropy of  $\ln_2(N_s)$ , where  $N_s$  is the number of source entropy bins. A uniform source has an entropy of zero, with other cases lying in between. At the end of a calculation, the statistical distance of each cycle's entropy from the average second-half entropy is compared, and convergence is determined to occur when this distance is within statistics of zero.

The entropy methods are quite easy to use -- there is only one output parameter to monitor. Because the entropy tally mesh can be determined automatically, there is no need for additional input or foreknowledge of the distribution or even of the problem geometry. It assesses the source distribution, so the eigenvalue convergence can be guaranteed. This is currently implemented in MCNP5 and MORET5[12].

### 3 ACCELERATION METHODS

One obvious strategy for problems with slow source convergence is the acceleration of the outer (power) iterations. Unfortunately, most of the methods that work for deterministic transport calculations are difficult to implement successfully and reliably in Monte Carlo codes because of

noise. Nevertheless, several noteworthy methods have been developed and implemented in Monte Carlo codes.

One of the earliest of these, the superhistory powering method [13], was originally aimed at reducing the bias of the  $k_{eff}$  estimators and the fission source distribution that stems from frequent fission source renormalization, but it also improves the convergence reliability of Monte Carlo criticality calculations [14]. In this method, a set of starters from the previous batch is tracked, along with their fission neutron progeny through generation N (typically 10). Only the last generation produces the fission sites for the next batch, so source renormalizations are less frequent.

The larger number of generations between tallies reduces the autocorrelation between batches is reduced because each flux or reaction rate tally aggregates scores from N generations of neutrons spreading though the system. As a result, uncertainty estimates are more realistic (i.e., larger). Depending on the problem these can be much larger. The method is effective and easy to use, requiring only one input parameter (N). (Autocorrelations in reaction rate tallies can also be reduced in the same way by batching tallies to include N generations without using the superhistory method.) Either method reduces the uncertainty underprediction bias, which depends only on autocorrelation. Superhistory powering has been implemented in MONK and MORET4.

Yamamoto, Nakamura, and Miyoshi applied a fission matrix method to address the problem of anomalous fission distributions arising from autocorrelation in a high dominance ratio two-component multiplying system[15]. This system consisted of two nearly identical fissile solution slabs separated by a thick slab of water, very similar to the Phase I test problem 3, for which the most difficult case had a dominance ratio of 0.9974. Consequently, the  $k_{eff}$  error resulting from non-convergence of the fission source would normally be quite modest, i.e., less than 0.0026, but the aim of the method is a stable, accurate estimate of the fission distribution among the slabs. The procedure is to estimate the fission matrix elements in two steps: (1) collect a set of fission sites during a criticality calculation, and run fixed source calculations from the fission sites to estimate the fission matrix elements, and (2) use the fission matrix to adjust fission neutron weights as if applying a "restoring force" to reduce the source distribution fluctuations. This method is effective and can be used to estimate dominance ratios, but is not helpful for large 3D reactor problems.

A very promising method is Wielandt's[16], in which a portion of the fission (determined by the parameter  $k_e$ ) source is subtracted from both sides of the transport equation, effectively increasing the interactions between decoupled fissionable zones. This reduces the eigenvalue of the first harmonic. The lower dominance ratio of the modified equation results in faster convergence, remarkably so when the control parameter  $k_e$  is optimal. Furthermore, the faster convergence makes the usual convergence tests considerably more sensitive due to reduced autocorrelation. This is one of the methods that has been used to accelerate iterations in deterministic calculations[17].

Applied to Monte Carlo codes, the Wielandt method modifies the random walk in a way similar to the superhistory method, i.e., more than one generation of fission neutrons are followed during a single cycle. In this case, the algorithm randomly continues a fraction of the

histories within the current cycle according to the control parameter,  $k_e$ . Furthermore, a collision in any generation within a cycle can produce a fission neutron for the next cycle, not just the final generation of the cycle. As the initial source transient is worked off by iteration,  $k_e$  is gradually adjusted. It is optimal to pick late iteration values of  $k_e$  to be slightly above  $k_{eff}$  to lengthen the fission chains within a cycle. If  $k_e < k_{eff}$ , then the fission chains within a cycle will not terminate, and if  $k_e$  is too large, then the iterations are not accelerated. As with the superhistory method, the number of individual neutron histories is not decreased, so there is no savings in computational effort.

Yamamoto and Miyoshi first implemented Wielandt's method in a simple test code, and then in MCNP4C using a procedure of repeated MCNP fixed source calculations in which each calculation represents one iteration. For a system very similar to the Phase I test problem 2 (an infinite lattice of depleted fuel pins with axially-dependent burnup and a high dominance ratio), the calculation converged the fission distribution in 35 cycles vs. the hundreds required for conventional power iteration. They noted that, especially in the early cycles, the method amplified source distribution fluctuations from cycle to cycle.

More recently, Brown[18] implemented Wielandt's method in a test version of MCNP5. To mitigate the large fluctuations in flux estimates in the early cycles,  $k_e$  is initially set to  $k_{eff}+1$  and then gradually reduced to the user-input value during cycles 3-20. When applied to a 2D PWR reactor case, convergence was achieved in 5 cycles vs. 80 for the standard power iteration method. The results were similar for several other systems. Figure 6 shows the dramatically different source entropy histories for one of the checkerboard fuel storage calculations performed both without and with Wielandt acceleration. Like the superhistory method, Wielandt acceleration has been shown to reduce or eliminates autocorrelation of reaction rate and flux tallies[19], providing more realistic uncertainty estimates.

Stratified fission source sampling[20] was evaluated for problems where undersampling important fissile components is a possibility. In this method, at least one fission site is selected in each fissile component during each generation. This is accomplished by forcing collisions in components in which neutrons travel uncollided and by forcing low-weight fission sites into the site bank for the next cycle, with appropriate weight reductions. The efficacy of the method is comparable to the superhistory method, but it obviously requires intrusive intervention in the random walk and source selection procedures. Furthermore, to prevent substantial slowdowns in computing speed due to tracking insignificant neutrons, it is necessary to set a cut-off weight below which sites are removed by roulette from the stratified sample. Overall, when applied optimally, the method increases the computational effort only marginally. The method is currently implemented in MORET4.

Of the methods explored, Wielandt's method and superhistory powering seem to be best suited to criticality calculations. They require little or no advanced knowledge of the system being analyzed, they use only one input parameter, and their iterations fit nicely into existing convergence tests, uncertainty estimates, etc. Unfortunately for code developers, however, they require modification of the random walks, complicating their application to criticality codes that already use other intrusive non-analog techniques for variance reduction of flux and reaction rate tallies. The MORET-5 code planned for release to the NEA Data Bank is to include Wielandt acceleration.

## 4 COMPUTATIONAL STRATEGIES

Even without the methods discussed above, use of engineering knowledge to identify important neutronic characteristics of the system being analyzed is one of the strongest protections against source convergence failure and erroneous uncertainty estimates. For example, some experienced Expert Group participants understood immediately that the most effective reflection in the fuel storage test problem would occur in the single location where the fuel bundle was stored at an interior corner of the concrete structure. A less experienced analyst could easily identify this effect with a few short Monte Carlo calculations, each representing a fuel bundle with concrete bordering on two sides, on one side, and on no sides. In many such complex systems, performing a few additional calculations can be very helpful in identifying challenging convergence characteristics and in establishing bounds for the full system eigenvalue.

One procedure useful for all high dominance ratio systems is to repeat the criticality calculation with a several radically different initial sources (uniform, in or near a high-worth component, far from the high-worth component), in which case statistically identical results indicate convergence[3]. This was tested thoroughly in the fuel storage problem and the high-burnup pin cell lattice. Of course, it can be used with any code, Monte Carlo or deterministic.

The simplest procedure of all, of course, is to apply more computational power of the right kind. More histories per generation will reduce uncertainties but not uncertainty biases, and will reduce  $k_{eff}$  and reaction rate/flux distribution biases. More skip cycles will generate source iteration progress.

The single most useful procedure to detect statistical problems (as opposed to slow convergence) arising from the Monte Carlo method is to perform a set of calculations identical except for the pseudorandom number sequence, and to estimate uncertainties directly from the ensemble of reaction rate, flux, or  $k_{eff}$  estimates. These estimates are truly independent, so the resulting uncertainty estimates will be accurate to within statistics. Assuming enough replicas are completed, any anomalies will emerge, as is shown in Figure 7.

## 5 CONCLUSIONS

Work on source convergence detection and acceleration has produced considerable progress during Phase 2 of the Expert Group. The statistical tests can generally be implemented without much difficulty. Acceleration methods involve some intervention in the random walk procedures, so it is more difficult to implement them, particularly in codes not aimed solely at criticality calculations.

Today, the strongest combination is either the Wielandt or superhistory method plus an entropy test. This combination will make source convergence both more reliable and more reliably detectable. Although convergence of  $k_{eff}$  can occur without fully converging the fission source, a converged fission source will guarantee convergence of  $k_{eff}$ . These methods are not substitutes for good judgement, but they are tools to provide more information useful for understanding the physics and mathematics of specific cases.

Finally, when effective detection or acceleration methods are used, complacency remains as a risk for which the best antidote is vigilance, physical intuition, analytical thoroughness, and the application of brute computational force.

## 6 ACKNOWLEDGEMENTS

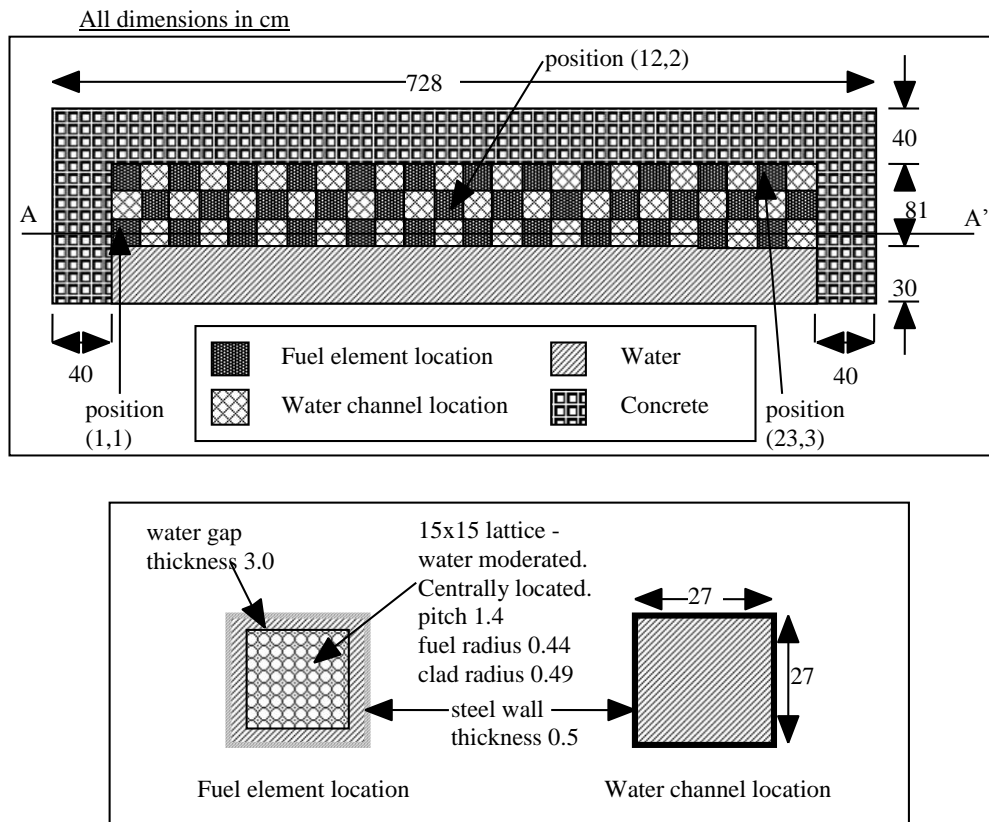
The author wishes to acknowledge the efforts of all of the participants in both Phases of the Expert Group's work. Results and their graphics reported here were contributed by Forrest B. Brown.

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**Figure 1. Test Problem 1: Checkerboard fuel storage array (2D features only)**

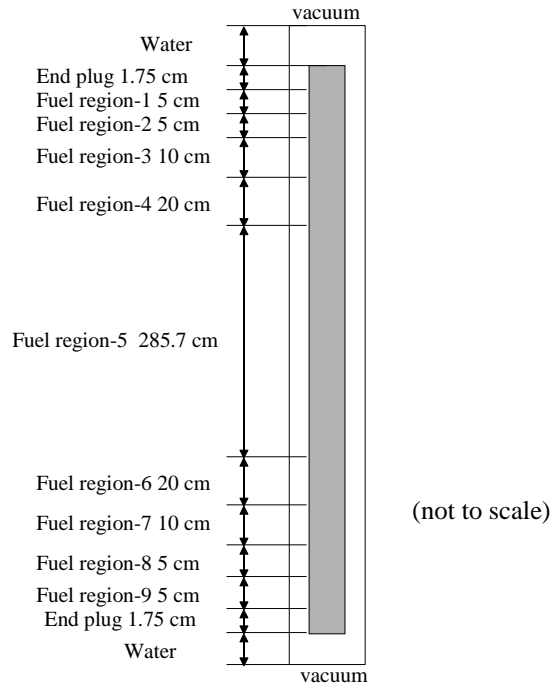


Figure 2. Test Problem 2: Infinite lattice of depleted fuel pins.

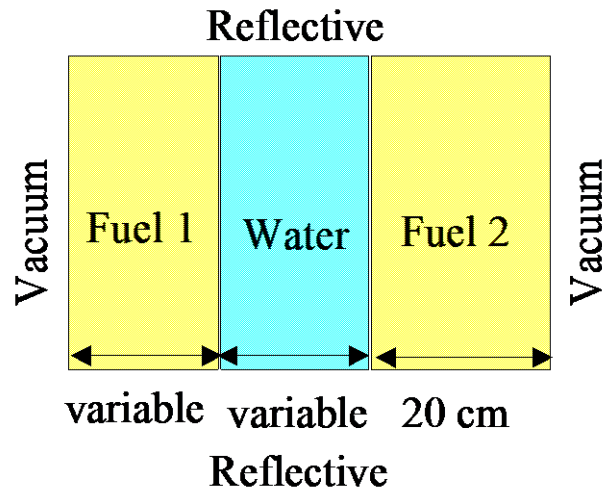
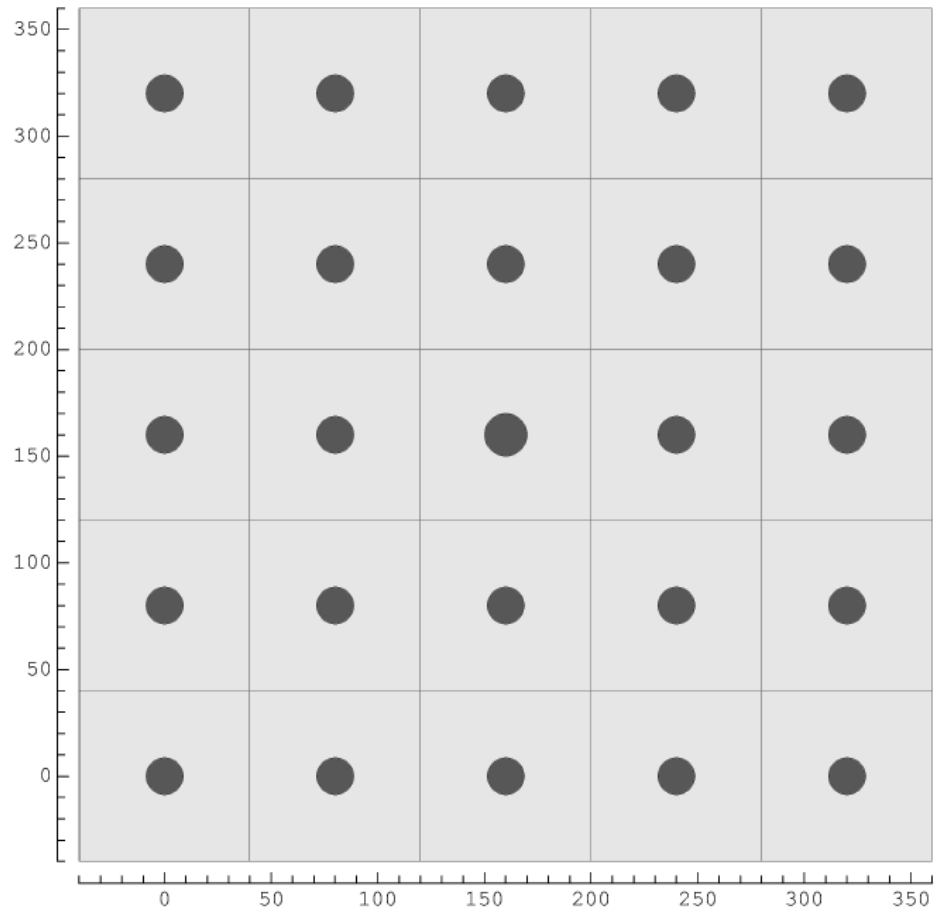
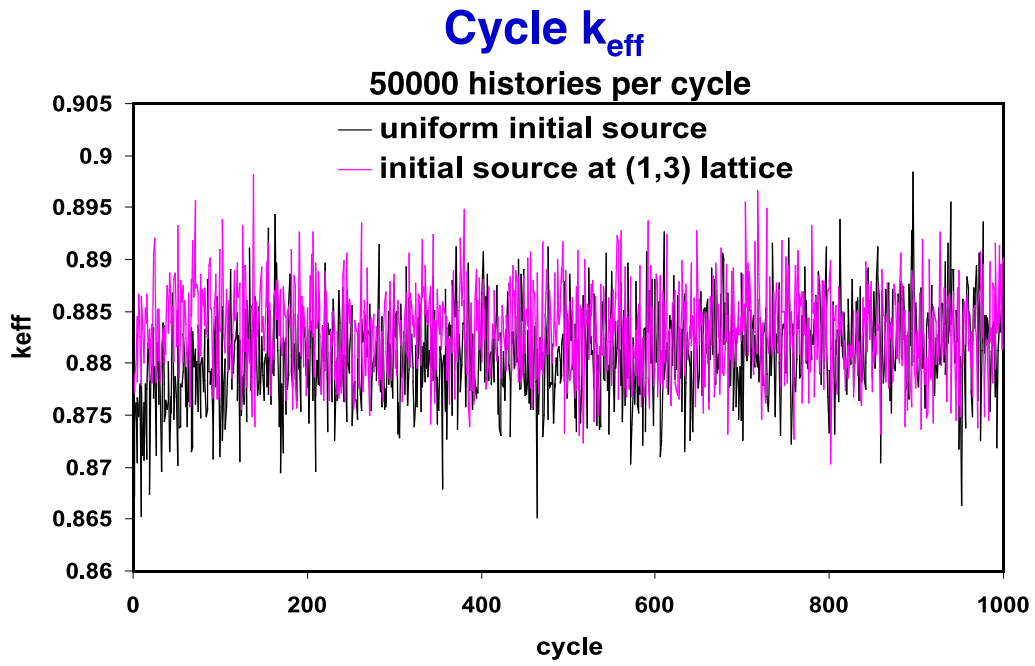


Figure 3. Test problem 3: Decoupled uranyl nitrate slabs



**Figure 4. Test Problem 4: Widely separated spheres, central sphere is critical.**



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Figure 5. Two eigenvalue estimate histories for the checkerboard fuel storage problem (*F B Brown*)

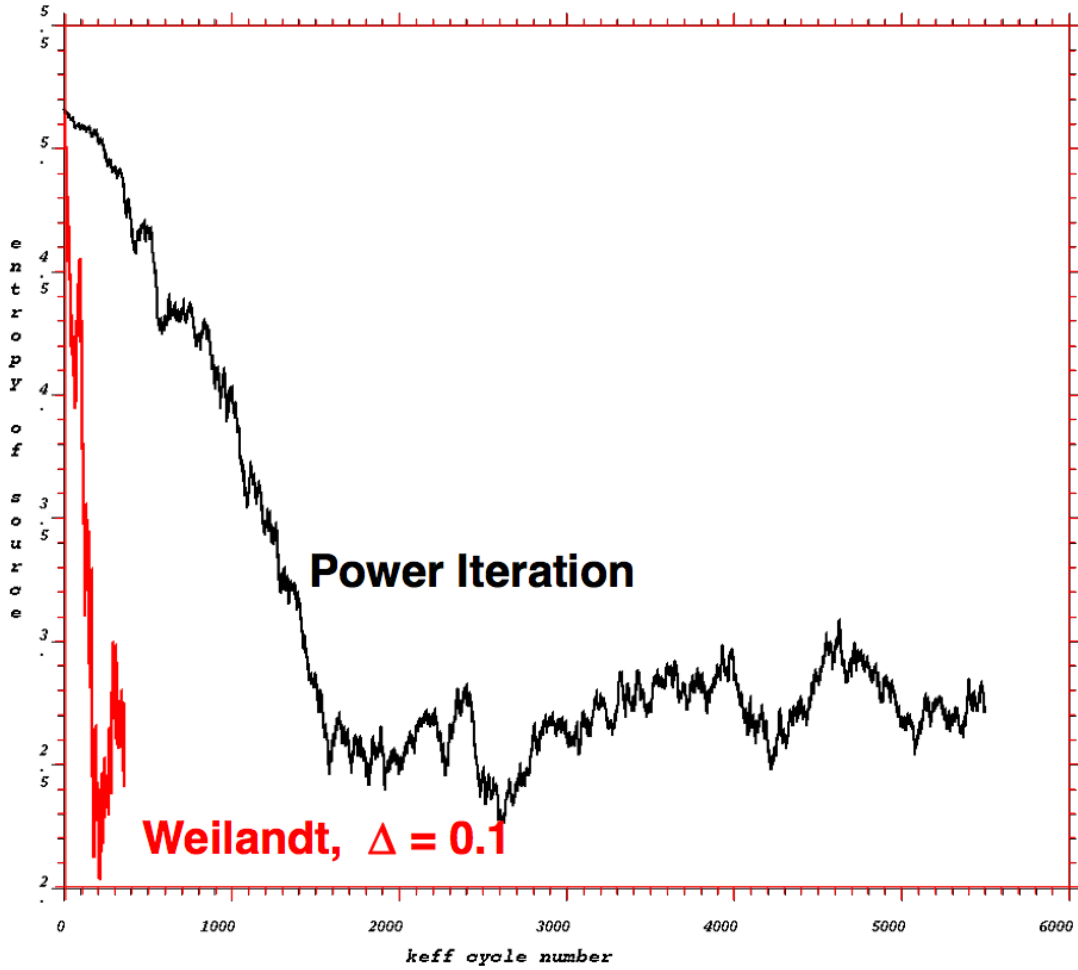
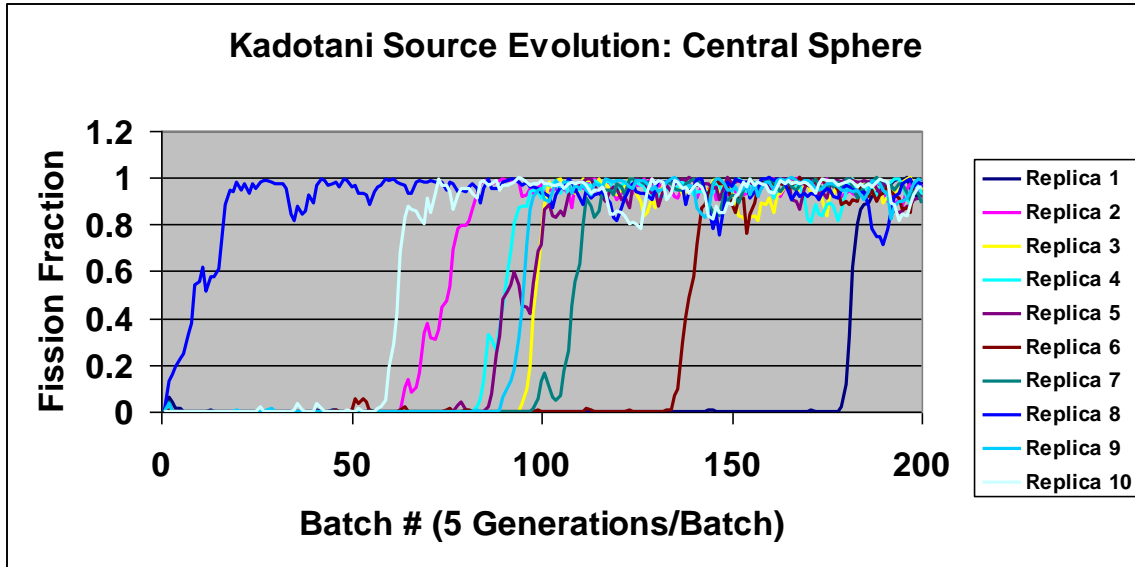


Figure 6. Source entropy shows the effectiveness of Wielandt acceleration in the checkerboard fuel storage problem. (F B Brown)



**Figure 7. Fission fractions in the central sphere of the 5x5x1 array for Monte Carlo replicas.**