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Title: Difficulties Computing k in Non-Uniform, Multi-Region Systems with Loose, Asymmetric Coupling

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DIFFICULTIES COMPUTING k IN NON-UNIFORM, MULTI-REGION SYSTEMS WITH LOOSE, ASYMMETRIC COUPLING

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ABSTRACT

Using the Monte Carlo method for k-eigenvalue calculations has several well-documented issues that can lead to incorrect answers should users not exercise caution. One such issue that has garnered little attention is the problem of undersampling or statistical coverage, which is often confused with bias in k. Three problems are developed that specifically demonstrate this issue, often resulting in an incorrect calculation of k; all of these have features of containing multiple discrete fissile regions with loose, asymmetric coupling that is unfavorable toward the most reactive region in the problem. Given these problems, the impacts of failure to provide adequate statistical coverage is discussed and advice to practitioners is provided.

Key Words: Monte Carlo, eigenvalue, criticality, pitfalls

1. INTRODUCTION

There is often a temptation among practitioners, especially those new to the field, to treat simulation software as a "black box" that somehow produces correct answers to any problem. MCNP5 [1] is a Monte Carlo radiation transport package that is used widely in the criticality safety program to compute k-eigenvalue and related quantities, and can be used well or poorly. The reality is that eigenvalue calculations have several associated subtleties that can serve as pitfalls for uninformed practitioners. Several papers, presentations at conferences, and workshops from the MCNP team [2–13] have been devoted to relaying these issues – namely: convergence [14], bias [15, 16], and correlation [17] – to the community.

In this discussion, it is assumed (often tacitly, to the disadvantage of newcomers) that all regions of the problem are always adequately sampled. For typical nuclear reactor calculations, this is almost always the case and is of only academic concern for those in the reactor physics community. The criticality safety practitioner, however, may encounter and analyze systems with multiple discrete regions of fissile material where this may not be true. When analyzing these types of systems, a non-observant user of MCNP5, or any other Monte Carlo package, can get misleading or drastically wrong results even when diagnostics indicate everything is fine.

Three pathological problems are developed that illustrate the issues associated with poor sampling or coverage, and how traditional diagnostics such as the Shannon entropy, can fail to detect problems. Some observations are that asymmetric coupling leads to problematic behavior, and choosing a good starting source guess to seed the calculation is the most important step a practitioner can take to defeat these problems. The three problems may also be useful in the development of new diagnostics [18] to act as a "safety net" to warn practitioners.

2. PATHOLOGICAL PROBLEMS

There are three pathological problems developed that illustrate where a practitioner may encounter difficulties because of statistical coverage. These also show some weaknesses to current diagnostics and where the conventional wisdom may fail to hold. The three problems are: the "Revised k-Effective of the World Problem", the "Two-Room Vault Problem", and the "Near-Infinite Plutonium Plane Problem". The specifications of each problem and their specific features that make them pathological are discussed.

2.1. Revised k-Effective of the World

The original "k-Effective of the World" problem was devised by Elliot Whitesides in 1971 [19] to illustrate issues in Monte Carlo eigenvalue calculations at the time. The problem is a 9 x 9 x 9 array of plutonium-239 spheres suspended in vacuum. The entire array is surrounded by a thick water reflector, and this configuration is subcritical. The central sphere is replaced by a sphere that is exactly critical, by itself, in vacuum. The combined configuration is supercritical for physical reasons. Can a Monte Carlo calculation accurately compute k?

This problem is easy to solve today if a sufficient number of particles per batch are used and an adequate number of cycles skipped. In 1971, computers were too small and slow to run more than a few hundred particles per batch, not enough for even one neutron per sphere. Also, convergence diagnostics, such as the Shannon entropy, were not available, so it was very difficult to know exactly how many cycles to skip – it turns out that 100-150 is adequate to converge the fission source. The net result being that the predicted k was (and still is with the same parameters, of course) subcritical, even though that is not physically possible.

While coverage is an issue using 1971 batch sizes, it also suffers from the issue of biasing k because of stochastic fluctuations in renormalizing the fission source. The issue of bias is fairly well understood theoretically (it decreases as $1/M$, where M is the batch size, assuming M is large enough), but the issue of coverage is less so. A question to pose is as follows: Is it possible to construct a problem where the concern is coverage alone?

The answer is that a problem similar to the "k-Effective of the World" can be defined that specifically stresses statistical coverage. This is called the "Revised k-Effective of the World" problem [20], or simply the Revised Problem. The Revised Problem is still a 9 x 9 x 9 array of plutonium-239 spheres with radii of 3.75 cm and densities of 20 g/cc. The space between the spheres is flooded with water at 1.0 g/cc and the spheres have center-to-center distances of 20 cm. Like with the original problem, k in this configuration is subcritical (k is approximately 0.95). As before, the central sphere is replaced by a larger sphere (radius of 4.33 cm), but this time with a thick cadmium coating (0.5 cm thick, natural composition, and solid density) – the reason for this is discussed shortly. This sphere is critical when submerged in an infinite bath of water, so the combined system, as with the original problem, is supercritical. The initial source guess is also specified to sample points, at the center of each sphere, with equal probability, in accordance with the modern best practices. The number of cycles to skip is 500 and the total number of cycles run is 1,000.

The question is as follows: how large should the batch size be, given these constraints, so as to

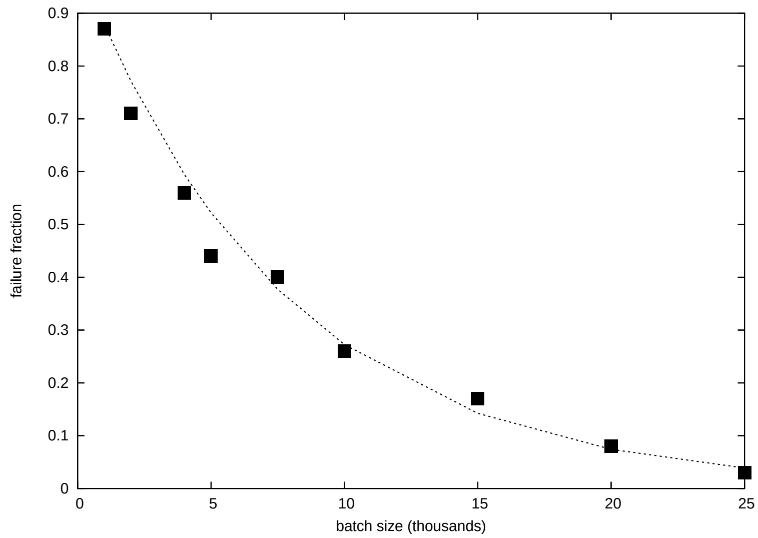


Figure 1: **Failure Rate of Computing k for the “Revised k-Effective of the World” Problem.**

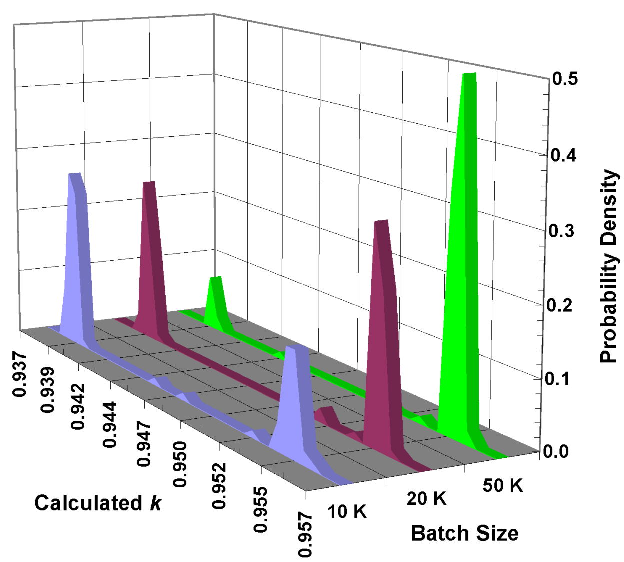


Figure 2: **Distribution of Predicted k for the “Revised k-Effective of the World” Problem.**

guarantee that the Monte Carlo calculation converges to the correct value of k? It turns out this number is quite high for this configuration, as seen in Fig. 1, where the probability of getting an incorrect k is plotted as a function of the batch size. This percentage is determined by running 100 independent random trials (MCNP5-1.60 used for all calculations) and observing the fraction that predict k to have a value far below 1.0. Notice that even for a batch size of 25k, there is still about a few percent chance of getting k incorrect. Many engineers would find this a rather large probability considering the consequences of under-predicting k by 0.05.

A plot of the distribution of k for a few batch sizes is displayed in Fig. 2. Note that the distribution is mostly bimodal with one peak representing the correct supercritical value of k and the other being around $k = 0.95$, or the system multiplication without the central sphere. Note that the mean value of the correct peak is consistent in all three cases (and others), and does not demonstrate the $1/M$ trend, indicating that bias is not an issue in this problem.

The reason for this irregularity is the characteristics of the coupling between the central sphere and the rest of the spheres. First, observe that the true value of k is dominated by the characteristics of the central sphere: the most reactive region. The system has components that are more or less reactive, and this creates an inherent difficulty because it is necessary (but not necessarily sufficient) to adequately sample the central sphere well to get k correct. Because of this, it is important to establish stable neutron chains in the central sphere.

Recall that there are 729 spheres, even a source guess of 10k will only start about 10-20 particles in each sphere. If the probability of establishing a stable fission chain in the central sphere is significantly less than 5-10%, then this batch size may be inadequate, and indeed it is as seen by the 25% failure rate. Because of a cadmium coating and the water reflector, neutrons that leave the system are most likely to thermalize and, should they backscatter at thermal energies into the sphere, will almost certainly be absorbed before causing fission. The only realistic pathway to establishing a fission chain is to have several successive generations of increasing populations of fast fissions within the sphere, which turns out to be a somewhat rare event.

Should a fission chain not be established from the initial source, it is also possible for neutrons from another sphere to initiate the chain reaction in the central sphere – indeed this does happen, as evidenced by the cases in between the two modes on the curves in Fig. 2. Because of the large number of mean-free paths between the spheres, it is unlikely a neutron will retain enough energy to be able to penetrate the cadmium coating. Rather, it is far easier for a neutron to leak out of the central sphere and initiate a stable fission chain in another sphere. In other words, the coupling between the spheres is not only loose (in that communication is infrequent), but also asymmetric because communication from the central sphere to other regions is favored over communication from other spheres with the central sphere. It turns out this asymmetry is the significant factor in determining whether or not a particular problem has coverage concerns.

Given this information, suppose the source specification is modified to incorporate only the central sphere. Will this yield more reliable results? The answer is yes, and remarkably so. Even with a batch size of 1k, the value of k is always predicted correctly for each of the 100 trials. This makes sense considering that for the previous guess, the number of chances of initiating a stable fission chain was a factor of 50-100 lower.

2.2. Two-Room Vault Problem

In the previous problem, the asymmetric coupling is caused predominantly by spectral properties. Geometry is also a possible cause of asymmetry as well should the more reactive region be much smaller in size than less reactive ones. The diagram in Fig. 3 shows the xy-plane cutaway at $z = 1.5$ m of the “Two-Room Vault Problem”. In the left room is the Jezebel sphere [21] 1.5 m above the concrete floor. The room on the right contains an array of stainless steel (approximated as pure iron-56) cans containing plutonium nitrate solution. The cans have an internal radius of

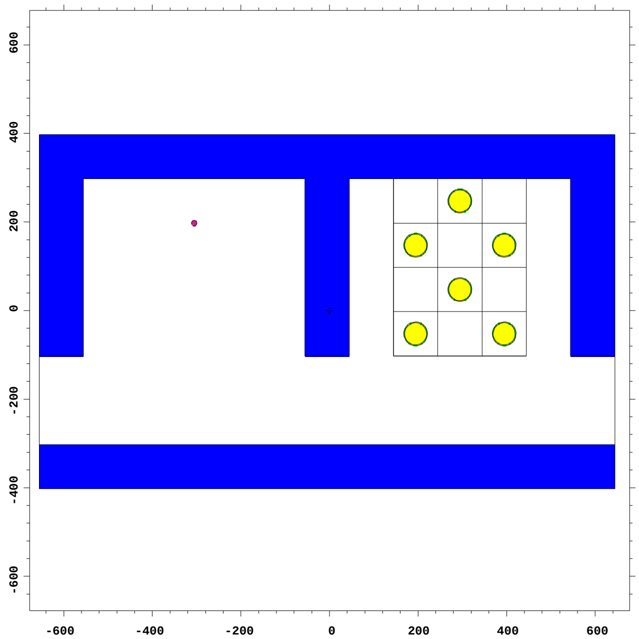


Figure 3: **MCNP Plotter Image of the Two-Room Vault Problem (Dimensions are in cm).**

25 cm, a thickness of 2 cm circumferentially, on top, and on bottom, and a height of 2 m. The solution height in the cans is 1.5 m. The plutonium nitrate solution composition is found in Table I, and uses a light-water $S(\alpha, \beta)$ law. The concrete material composition is from the PNNL Compendium of Material Composition Data [22].

Table I: **Plutonium Nitrate Composition**

ZAID	Atomic Density (atoms/b/cm)
1001	6.0070e-2
8016	3.6540e-2
7014	2.3611e-3
94239	2.7682e-5

The initial source guess is specified as a point at 50 cm above the floor in the topmost can. An experienced practitioner will undoubtedly realize that this is an abysmal source guess for the problem, but it is chosen to illustrate what can go wrong when Monte Carlo simulation software is used incorrectly. The problem uses 500 inactive cycles and 1000 total.

The room with the steel cans has a k of approximately 0.95, and Jezebel is approximately critical. The multiplication of this system is therefore supercritical. Considering the terrible source guess

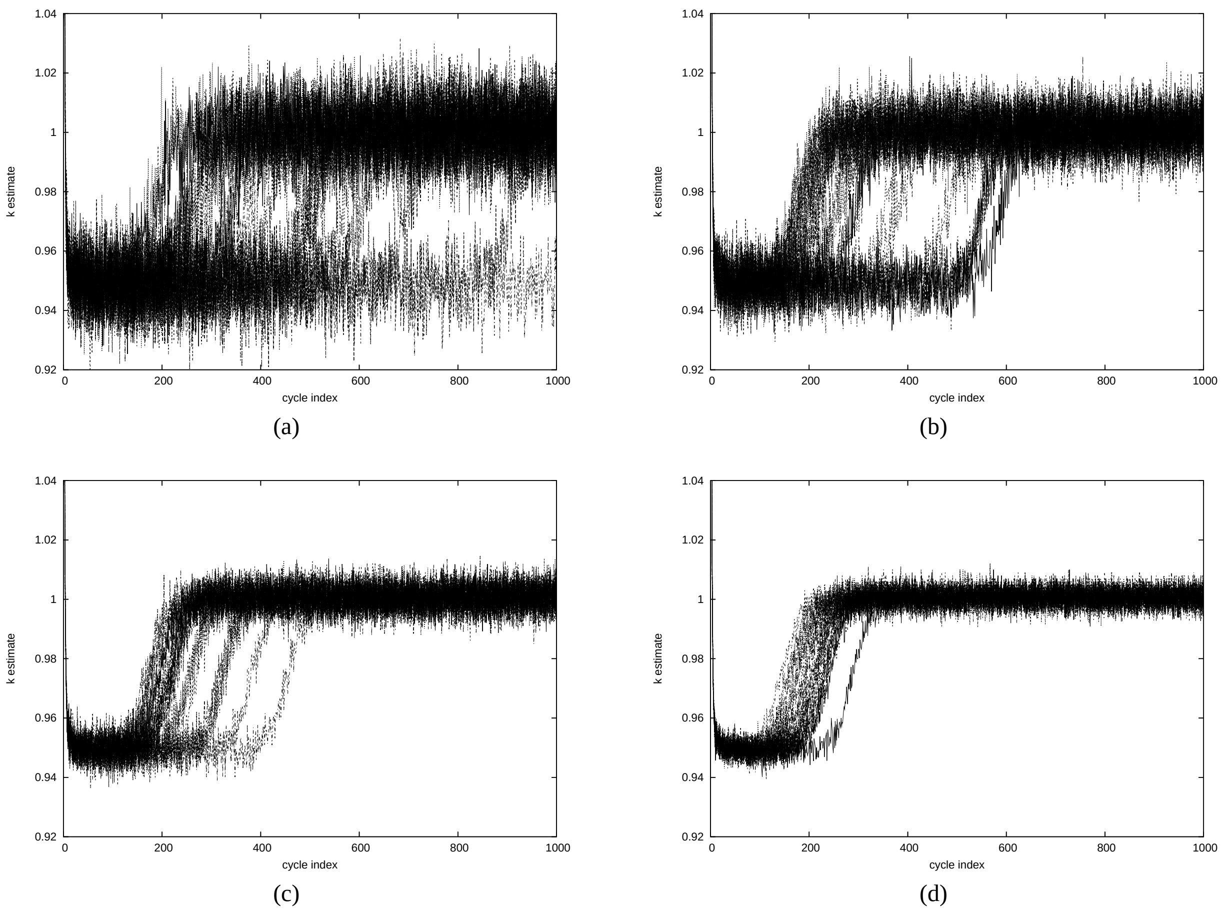


Figure 4: **Predicted k Estimate as Each Cycle for 25 Independent Runs for the Cases with Batch Sizes of (a) 10k, (b) 20k, (c) 50k, and (d) 100k.**

and the large amount of separation, it is quite likely that the predicted value of k will be 0.95. To reach the sphere, a neutron must travel from the cans either through 1 m concrete or scatter through the hallway and then, by chance, hit the target that has a very small cross-sectional area. Because of the relative cross-sectional areas, it is easier for neutrons to leak from Jezebel and find the cans than the other way around – the coupling is asymmetric.

25 independent runs are made with batch sizes of 10k, 20k, 50k, and 100k, and k as a function of cycle is plotted in Fig. 4. The results of these cases show a high degree of randomness in the number of cycles it takes the source distribution to converge, and this randomness is less significant as the batch size becomes large. The conventional wisdom is that larger batches do not lead to faster convergence, yet these results seem to indicate otherwise. More accurately, the statement of batch size versus cycles to convergence should be that larger batches do not change the **average** number of cycles it takes to converge. Time to convergence is a random variable because it arises from the random walks of very many particles. For tightly coupled systems, or for loosely-coupled ones with a decent initial guess, the variation in this time is typically very small (a few cycles at most) so the convergence may as well be considered deterministic.

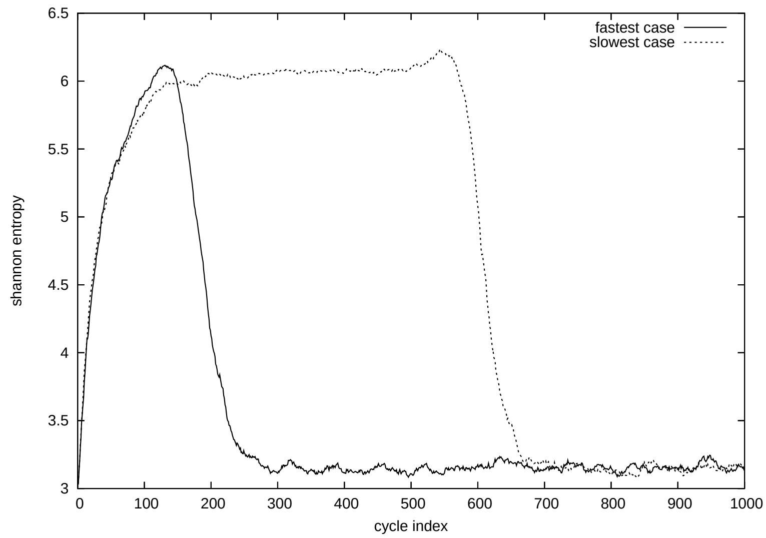


Figure 5: **Shannon Entropy for the Fastest and Slowest Cases to Converge (Batch Size of 20k).**

Figure 5 shows the Shannon entropy of the fission source as a function of cycle for the fastest and slowest to converge cases of the 20k batch size set. Visual inspection of the slow case shows that the fundamental mode of only the plutonium can array is achieved in about 150 cycles. At that point, the simulation will continue providing incorrect results until a chance event initiates a chain reaction in Jezebel and the source distribution shifts, as seen by the rapid decrease in the fission source Shannon entropy as the source becomes centralized within a much smaller region (a smaller Shannon entropy indicates a distribution is more centered).

Even for small batch sizes, this wildly random convergence behavior vanishes if the initial guess is chosen as being a point in the center of Jezebel. This illustrates the importance of taking a “good” initial source guess and what defines “good”; namely, an appropriate initial source guess focuses on the most reactive region in the problem, which, in this case, is the Jezebel sphere. An experienced practitioner would run each discrete region separately, determine the value of k for each, and pick and initial guess accordingly. Upon completing the calculation, the practitioner would perform a “sanity check” and ensure that the calculated k of the entire system is greater than that of any individual component.

2.3. Near-Infinite Plutonium Plane

This problem is designed to illustrate geometric asymmetry, and is not representative of any practical problem; the specifications are as follows: Below $z = 0$ cm, the entire region is rock or silicon dioxide at a density of 2.5 g/cc. Along the z-axis is a cylinder of radius 50 cm and height 2.05 cm consisting of plutonium-239 at density 20.0 g/cc; this will be called Region I and has a computed $k = 1.004$ when all space $z > 0$ cm and outside cylinder is air 80% nitrogen-14, 20% oxygen-16) at a density of 0.0013 g/cc. Region II consists of all space $0 < z < 0.45$ cm that is not already defined by Region I, and consists of plutonium-239 at the same density; $k = 0.980$ for Region II when all space outside of Region II for $z > 0$ cm is air. The result of the composite

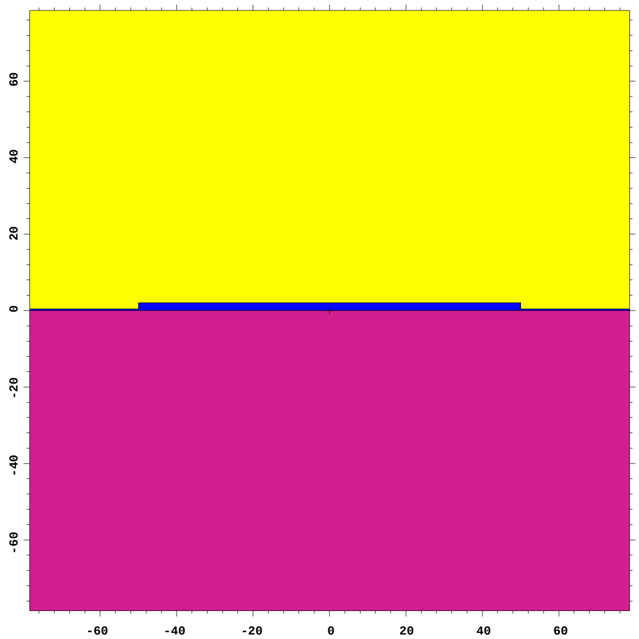


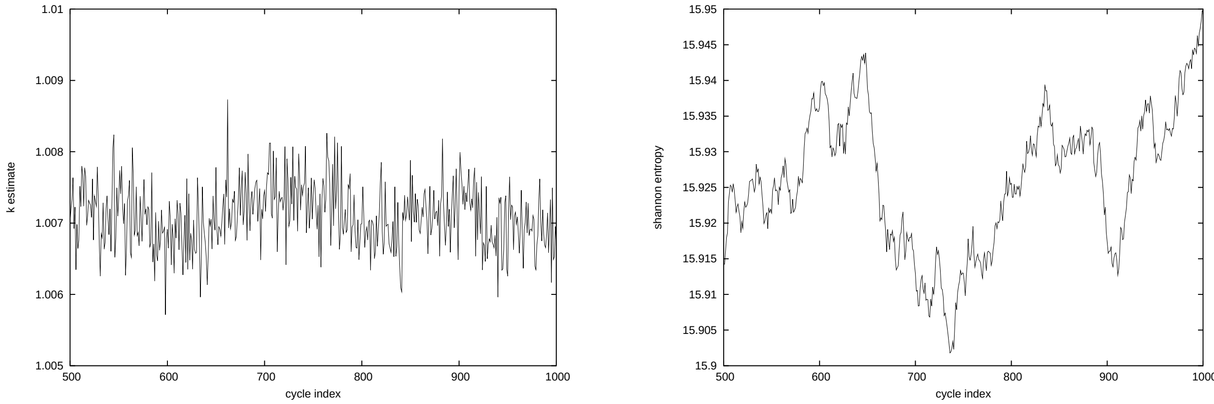
Figure 6: **MCNP Plotter Image of the Near-Infinite Plutonium Plane Problem (Dimensions are in cm).**

system of Region I and Region II (diagram in Fig. 6) is therefore supercritical. To circumvent MCNP's cell-based diagnostics for fission source sampling, Regions I and II are combined into one cell.

The source guess is defined as a cylindrical source, oriented about the z-axis, of radius 5 m with an extent from $0 \leq z \leq 0.45$ cm. The number of inactive cycles is 500, and the total number is 1,000.

There are two major features that make this specification problematic. The first is the source guess that does not focus on the central, most reactive region; the ratio of volumes for the source and Region I ($0 \leq z \leq 0.45$ cm portion) is 0.01, so about 1% of the neutrons will start in the most reactive region. The second is the high leakage from the active material allows neutrons to start fission chains, because of skyshine, very far away from where they originated.

These two effects work together to produce behavior that can lead to erroneous Monte Carlo results. One possible event is a failure to initiate, where all neutron chains travel to regions far away from Region I and never return because of the large extent of the problem. The purposeful joining of the two regions as a single cell defeats MCNP's cell-based sampling diagnostics; no problem will be indicated even if there obviously is one. Even if a neutron chain in Region I initiates, the ability to leak and start fission chains can lead to a later extinction, whose effect can be observed by a sudden decrease in cycle-predicted estimates of k, or simply long periods where too many neutrons are elsewhere, thereby leading to a low estimate of k far outside of the stated confidence intervals.



(a) (b)

Figure 7: **Cycle Estimates of (a) k and (b) Shannon Entropy for a Five Million Batch Size Run of the Near-Infinite Plutonium Plane Problem.**

The cycle estimates of k and the Shannon entropy versus cycle are given in Fig. 7 for a case with five million neutrons per cycle ($k = 1.0071$). The very small range of the Shannon entropy is because of the large number of elements in a mesh to cover a large enough region about the origin. Visual inspection of the Shannon entropy shows periods, typically 50-100 cycles long, where it takes on a certain range of values, followed by fairly sharp transitions taking 10-20 cycles, to other periods where it has another range.

Because of the inherent noise in the cycle estimates of k, visual inspection cannot yield obvious, definite conclusions about how to connect the Shannon entropy and k. Using the data, the Pearson correlation coefficient is computed. The coefficient has a value of approximately -0.4, and this indicates the cycle estimates for k and the Shannon entropy are anticorrelated. When the Shannon entropy is lower, the fission source distribution is more concentrated (likely in Region I), suggesting the estimates of k should be higher. The converse is also true; a more spread out fission source has a higher Shannon entropy and suggests a lower value of k. This anticorrelation coupled with the long periods in the Shannon entropy seem to indicate a "sloshing" of the fission source that impacts k. Further, results of calculating the ratio of the empirical (obtained from calculating the standard deviation of k from 25 independent MCNP trials of various smaller batch sizes) to quoted (averaging the 25 MCNP produced standard deviations the batch sizes) standard deviations of k show that the standard deviation is underestimated by a factor of four or greater; this is very large compared to typically observed values ranging from 1.0 to 1.5. Note that there appears to be no bias in k for these batch sizes; the average value of k for the 25 independent trials for various batch sizes all match around 1.007, which also agrees with the k found for the five million case.

This problem is particular interesting because this "sloshing" of the fission source has an observable impact on k. Such behavior is also observed in difficult problems such as the fuel storage vault from the OECD/NEA source convergence benchmark set [14], however, the impact on k itself is small. The conventional wisdom is higher-order modes in k that arise from statistical noise decay in proportion to the batch size M as $1/\sqrt{M}$ [17]. This does not appear to be occurring for the case with five million particle batch sizes, suggesting that, for this problem, five million is not sufficiently large (a coverage problem), or there is some assumption made that does not hold for this particular arrangement. In either case, there is likely to be some interesting analysis to perform on this problem.

3. LESSONS LEARNED & OUTLOOK

Three pathological problems are constructed that demonstrate the issue of statistical coverage, as distinct from the negative bias in k arising form small population sizes. All problems have some properties in common: they involve multiple regions that are loosely coupled, the regions vary in how reactive they are, and the coupling is asymmetric and unfavorable toward the most reactive region. This presents a lesson for practitioners using Monte Carlo software for analysis to be extra cautious when using these tools to analyze these problems – treating software as a black box can yield dangerously incorrect answers.

Another conclusion to draw is that the conventional wisdom and the current understanding of these problems is incomplete. This should be of no surprise to those experienced in the field, but is worth stating for the benefit of newer members who may have not yet been exposed to much of the theoretical work as applied to their practice. These three problems may be useful to help bridge the gap in understanding, and to aid the development of methods that might assist practitioners in determining if such problems are of concern.

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