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Title: USE OF DETERMINISTIC METHODS TO GENERATE
FISSION SOURCE POINTS FOR MCNP

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Use of Deterministic Methods to Generate Source Points for MCNP (U)

LA-UR-04-XXXX

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Abstract

To improve the convergence of the fission source distribution in criticality calculations a technique has been developed to use deterministic methods to generate initial fission source points for the Monte Carlo transport code MCNP. This technique employs the multigroup discrete-ordinates code PARTISN to calculate the initial fission source points for MCNP. THE MCNP weight window generator mesh is used to map the three-dimensional MCNP geometry to a geometry suitable for PARTISN. After the fission source distribution has been calculated with PARTISN, this distribution is used to create a set of initial fission source points for MCNP.

This method is evaluated using two test problems. Test problems are problems proposed by the OECD Nuclear Energy Agency Expert Group on Source Convergence in Criticality Safety Analysis. The two problems include a problem with two loosely coupled uranyl nitrate slabs separated with water and a problem of a 5x5 array of uranium metal spheres. The results obtained by using deterministic methods to produce the initial fission source distribution are compared with results obtained by using a user selected fission source distribution.

Introduction

For Monte Carlo criticality calculations come loosely coupled criticality problems can be slow to converge to the static source distribution. This slow convergence and the statistical nature of the Monte Carlo solution can produce unreliable fission source distributions which may lead to a non-conservative estimate of k_{eff} .

Often estimates of k_{eff} converge before the source distribution converges. While the k_{eff} produced by an unconverged source may match the k_{eff} produced from an converged source, the user is not guaranteed of this result. A converged fission source distribution must be used to produce a reliable k_{eff} . In order to increase the reliability of the fission source distribution, a method of generating an initial fission source distribution using deterministic methods has been developed. This method uses PARTISN⁽¹⁾ to calculate the initial fission distribution for MCNP⁽²⁾. This method is evaluated against user input source points for two test cases. The test cases are derived from the OECD/NEA Source Convergence Benchmark Program⁽³⁾.

Method

In order to convert a MCNP input deck to a PARTISN input deck the MCNP geometry is converted to voxel geometry using the MCNP weight window generator mesh⁽⁴⁾. Currently the material assigned to each voxel is the the material at the center point of the voxel. Future versions of this capability will provide volume fractions of each material in the voxel. An example of a MCNP 3-D geometry converted to voxel geometry for input into PARTISN is given in Figure 1.

MCNP materials, which are specified with ZAIDs (isotopes), must be matched to materials contained in the user specified multigroup cross-section library. To do this the user aliases the ZAIDs to the multigroup materials. For example the material water (m1) can be converted using the `dm1` card:

```
m1      1001 2      ! MCNP material for water
        8016 1
dm1     1001 h-1    ! Conversion to materials in SAILOR library
        8016 o-16
```

Currently, only the ASCII XSLIBB multigroup cross-section library format is supported. However, since MCNP outputs an ASCII text file as the input file for PARTISN the user can use any multigroup cross-section library and edit the PARTISN input deck as needed.

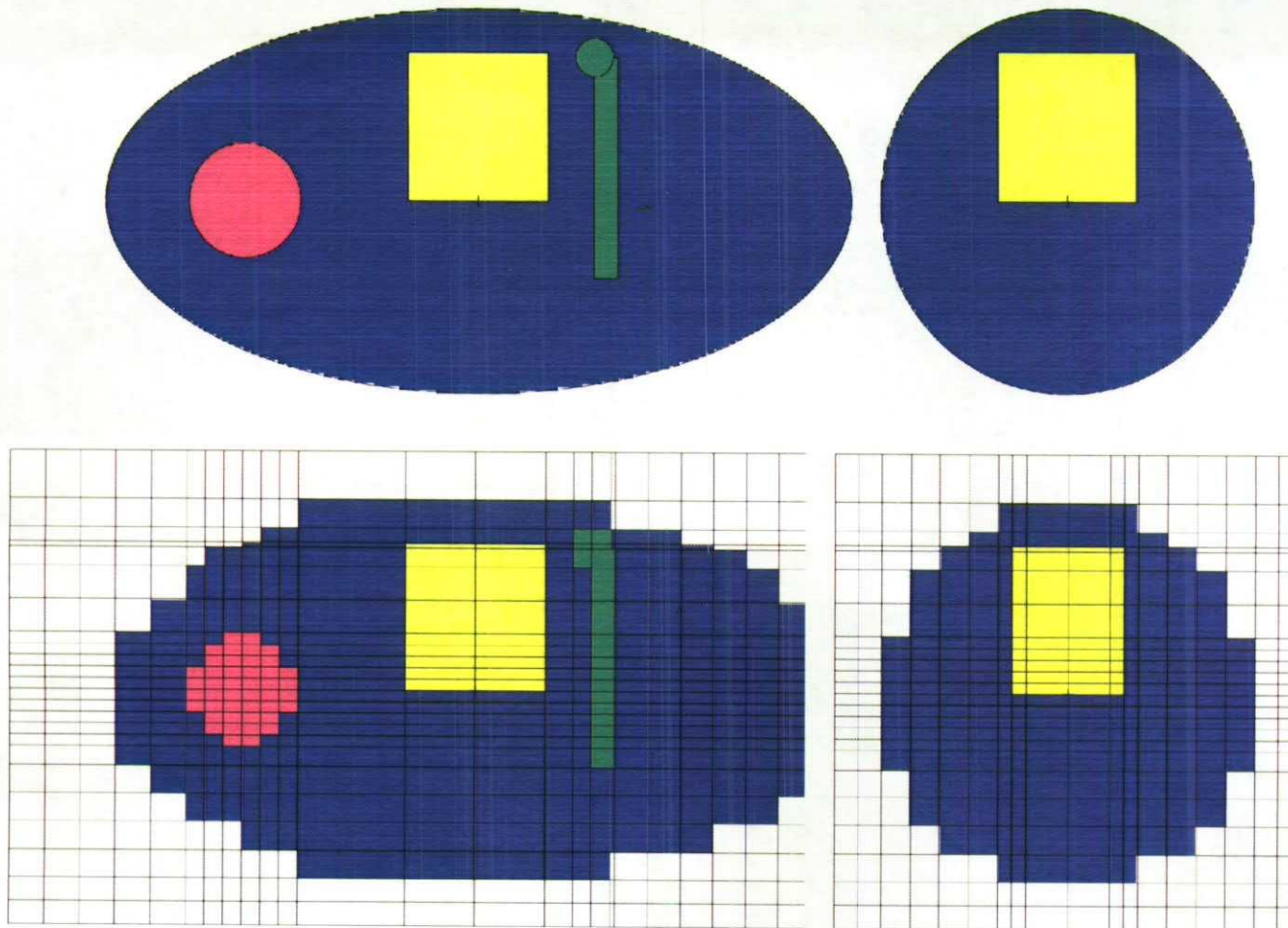


Figure 1: MCNP 3-D geometry converted to voxel geometry for input into PARTISN.

Method

After executing PARTISN, the calculated fission densities on the ASCII text file 'edtogx' were converted into a cumulative distribution function, which was sampled to select a voxel cell into which a source point could be placed. Once the voxel cell was selected, then the x, y, and z coordinates were sampled uniformly within the cell, and the point was written to the MCNP fission source point file 'srctp'. The energy of each particle in the initial source is sampled from a Watt fission spectrum hardwired into MCNP. This source energy probability is given in Equation 1.

$$p(E) = C \exp\left(\frac{-E}{0.964 \text{ MeV}}\right) \sinh\left((2.29 \text{ MeV}^{-1}) * E\right)^{1/2} \quad (1)$$

Method

In order to test for convergence of the fission source the stationary diagnostic proposed and implemented in MCNP5 by Ueki and Brown⁽⁵⁾ were used. This diagnostic provides a measure of the entropy of the fission source distribution. The convergence of the entropy of the fission source is compared to the convergence of the single cycle keff.

Test #1: Two Uranyl Slabs

The first test problem consisted of three sandwiched slabs surrounded by a void. The outer two slabs were a uranyl solution, and the inner slab was water. Each slab was of thickness 20 cm with sides of 600 cm making them almost infinite. The first test problem is depicted in Figure 2.

This problem was run in PARTISN with the SAILOR 47-neutron-group cross-section library. The MCNP KCODE run was performed with 10,000 source points per cycle for 500 cycles. The results of the run using fission source points from PARTISN were compared to results obtained by starting on one source point in each slab. The results of the source entropy for the two methods are given in Figure 3. For the case where source points were generated with PARTISN the fission source distribution appears converged from the first cycle. However, the case using only 2 initial source points shows that the source distribution does not converge until after 400 cycles.

Figure 4 depicts the single cycle keff for the two methods of initial source point generation. The single cycle keff appears converged after only a few cycles for both methods. This problem illustrates the importance of utilizing the source entropy diagnostic

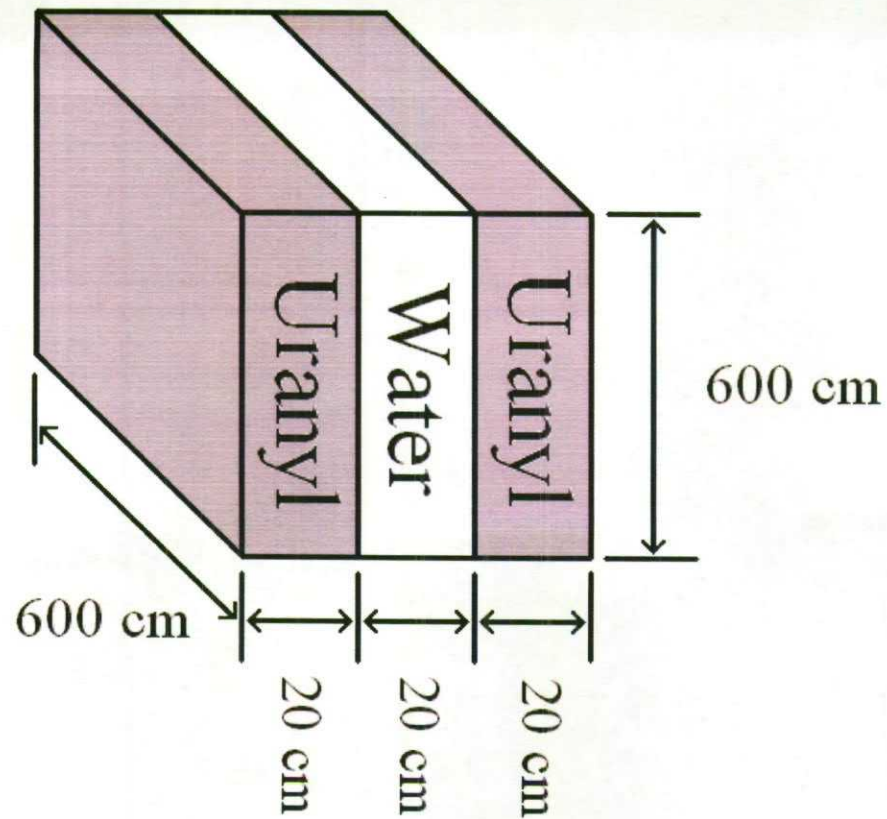


Figure 2: Test problem #1, 20-cm thick Uranyl slabs separated by 20-cm of water.

Source Entropy vs. KCODE Cycle

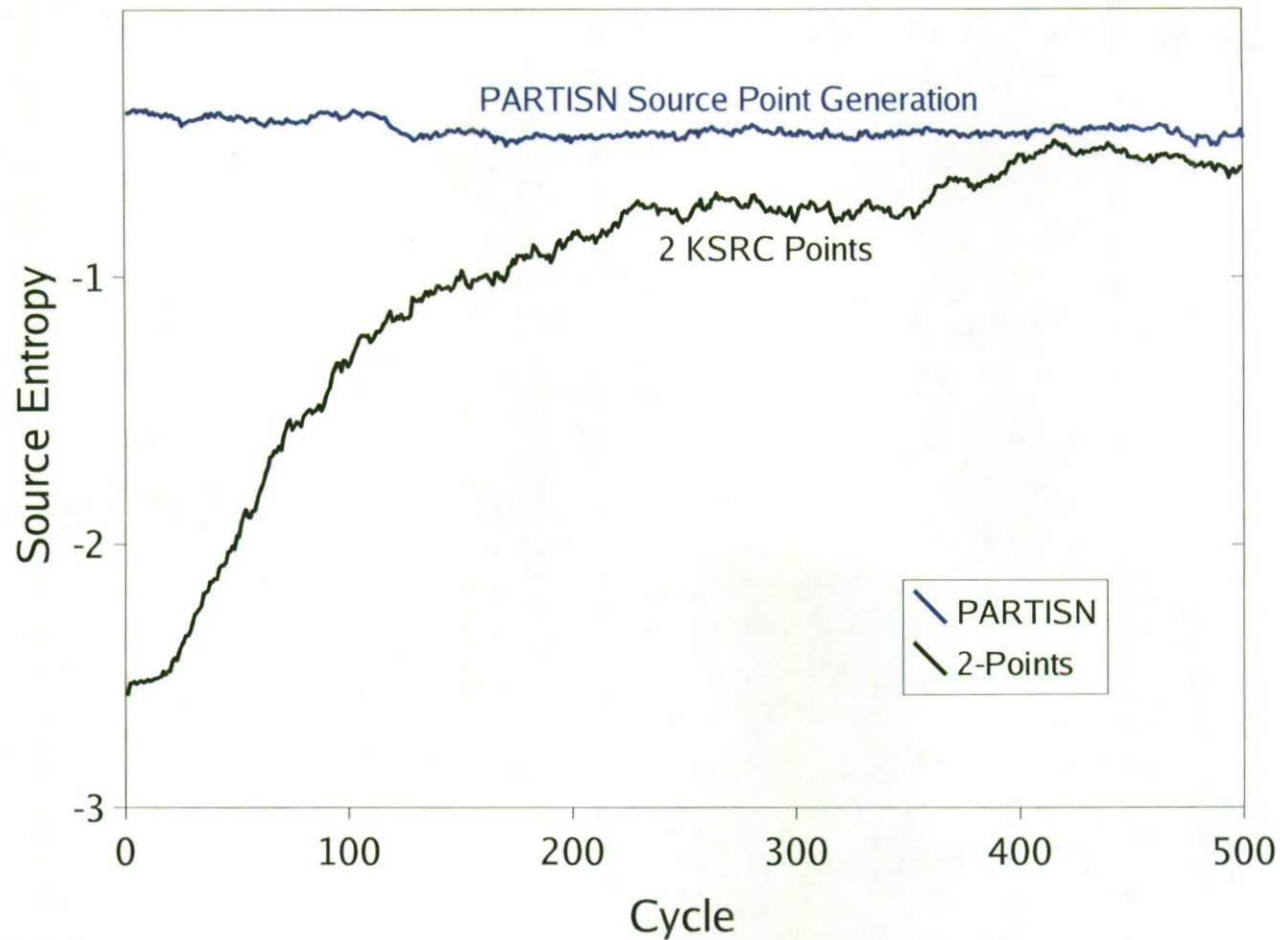


Figure 3: Source entropy versus KCODE cycle for the case using points generated from PARTISN and the case using one point in each of the slabs.

Cycle k (Collision) vs. KCODE Cycle

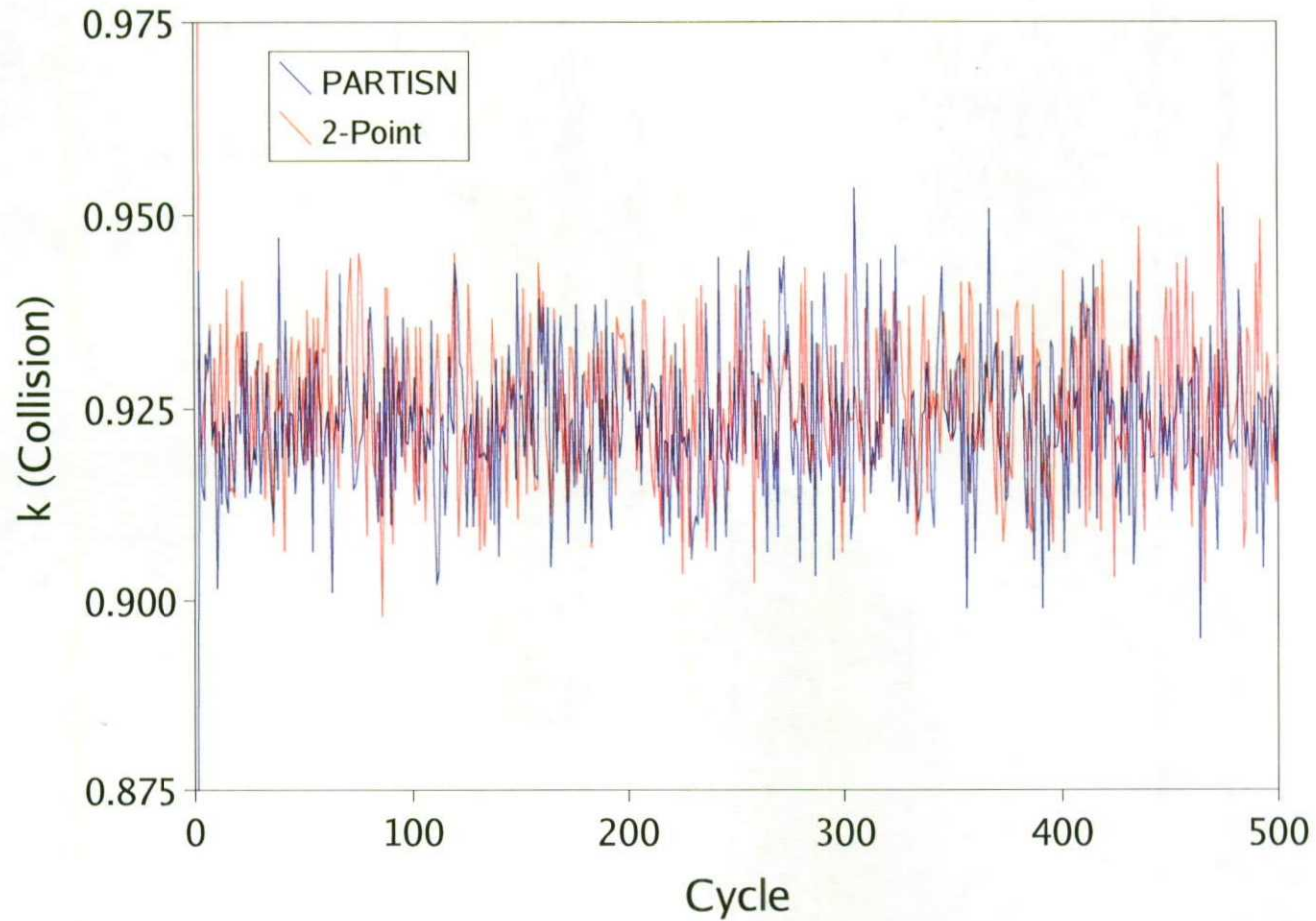
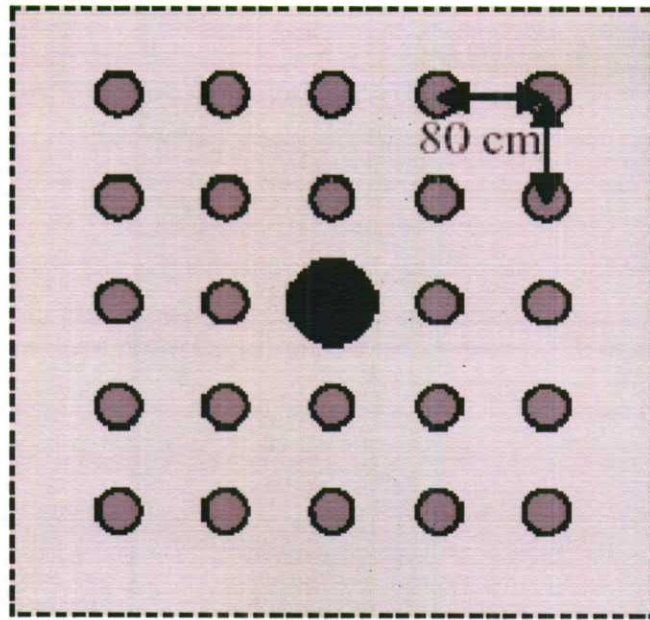


Figure 4: Single cycle keff versus KCODE cycle for the case using points generated from PARTISN and the case using one point in each of the slabs.

Test Problem #2: 5x5 array U spheres.

The second test problem consisted of a 5x5 array of subcritical uranium spheres with a central supercritical driving sphere. A diagram of the 5x5 array of spheres is given in Figure 5. Because of the large separation distance between the spheres, they have a limited amount of coupling, which makes convergence difficult especially if the initial source distribution is poorly defined. However, the coupling is very significant because the central sphere is driving the other spheres.

This problem was run in PARTISN with the SAILOR 47-neutron-group cross-section library. The MCNP KCODE run was performed with 10,000 source points per cycle for 1000 cycles. The results of the run using fission source points from PARTISN were compared to results obtained by starting on one source point in each sphere. The results of the source entropy for the two methods are given in Figure 6. For this problem the fission source distribution converges after the same number of cycles for both methods. The results of the single cycle keff for the two methods of initial source point generation are given in Figure 7. The keff converges at about 100 cycles for both methods. This is approximately the same number of cycles as required for the fission source distribution to converge. For this problem the method of generating the initial source distribution with PARTISN does not appear to have an advantage over simply picking individual source points. However, the method of generating the initial source distribution with PARTISN does perform as well and provides some confidence that a reasonable initial source distribution is used.






-  U_{metal} $R = 8.71 \text{ cm}$
-  U_{metal} $R = 10 \text{ cm}$
-  Air



Figure 5: Test problem #2, 5x5 array of subcritical spheres.

Source Entropy vs. KCODE Cycle

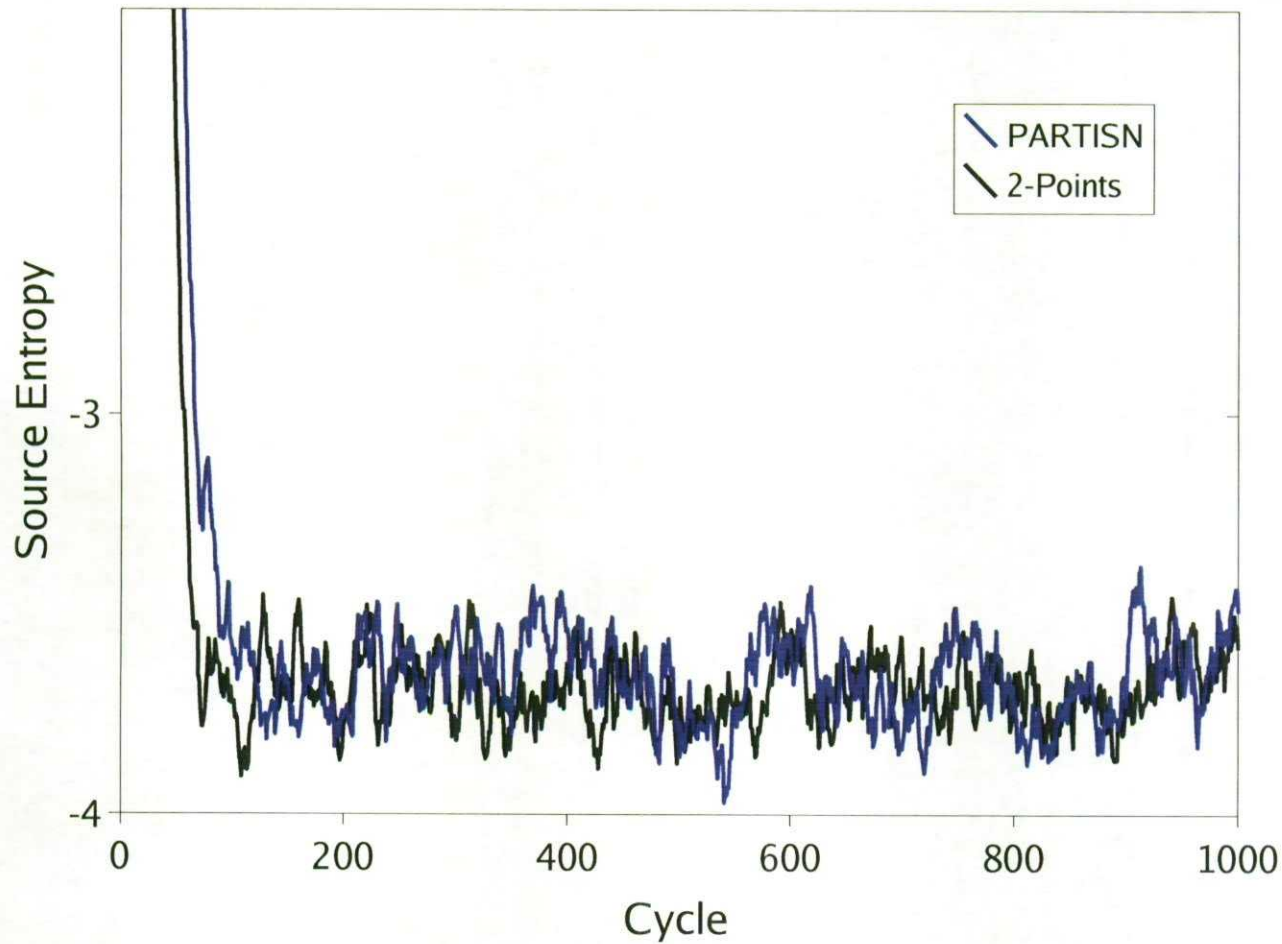


Figure 6: Problem #2 - Source entropy versus KCODE cycle for the case using points generated from PARTISN and the case using one point in each of the spheres.

Cycle k (Collision) vs. KCODE Cycle

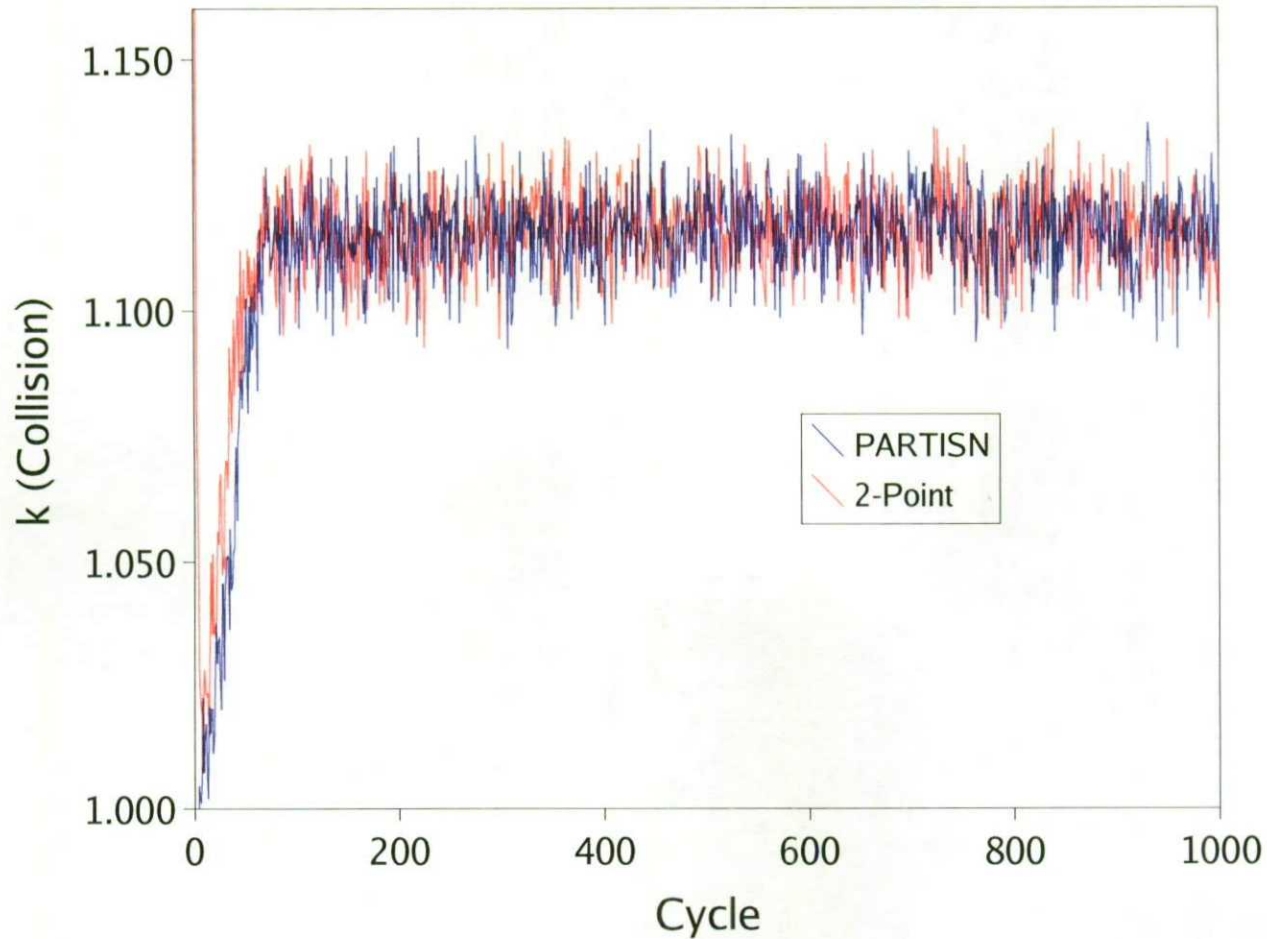


Figure 7: Problem #2 - Single cycle keff versus KCODE cycle for the case using points generated from PARTISN and the case using one point in each of the spheres.

Conclusions

For loosely coupled systems the method of producing an initial fission source distribution for MCNP using PARTISN can improve the rate at which the fission source distribution converges. However, this method does not always work better than other methods of choosing initial fission source points.

For the test problem of two 20-cm Uranyl slabs separated by 20-cm of water this method results in a converged fission source distribution in only a few KCODE cycles. The method of picking only one initial source point in each slab produced a single cycle keff that appeared to converge very quickly, however, a plot of the source entropy showed that the fission source distribution had not converged.

The second test problem of a 5x5 array of uranium spheres showed that the method of producing an initial fission source distribution for MCNP using PARTISN does not always result in a fission source distribution converging faster than just picking points in the spheres. The use of cell homogenization and other multigroup cross-section data libraries may improve the results obtained by the deterministic source point generation method.

References

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