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**Continuous-Estimator Representation for Monte Carlo Criticality Diagnostics**


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## INTRODUCTION

Within the last decade, diagnostics for Monte Carlo criticality calculations such as the Shannon entropy have been implemented into production-level software packages [1]. Typical implementations of the diagnostic involve an overlaid uniform, Cartesian mesh. The software uses this mesh as a means to tally fission source locations for computing the Shannon entropy.

While this mesh representation works very well for the Shannon entropy, extending it to other types of diagnostics, such as those for measuring whether or not the fission source has been sufficiently sampled, has complications. The issue, for this purpose, is that the mesh is entirely independent of the location of fissile material, and it becomes ambiguous as to how many, if any, fission source neutrons should lie within a particular mesh region.

To illustrate, the overlay may place the mesh such that only a very small corner of fissionable material is included, and, correspondingly, the amount of sampling in this region should be very small or might not even occur within the time of the simulation. A different mesh spacing would lead to this situation not occurring. Sampling statistics done in both the cases with and without the "corner" would be very different, yet, from the point of view of whether or not the fission source is adequately sampled, should yield the same conclusions. It is therefore difficult to create a robust, automatic process to assess fission source sampling.

It should, in principle, be possible to establish a conformal mesh over the fissionable material; however, Monte Carlo software typically uses a combinatorial solid geometry representation that is excellent for robust ray tracing, but creates practical difficulties for meshing. Alternatively, recent work on continuous tallies, such as the kernel density estimator [2], provides an alternative approach. Estimators are placed randomly with some spacing with centers exclusively within fissionable material, and fission source point locations are used to score the estimators based on their proximity.

With the appropriate choice of estimator spacing and basis (with closed support) for scoring that cover all fissionable material, the Shannon entropy is essentially equivalent (within an additive offset) to that obtained from an adequately spaced mesh representation. The advantage of the continuous-estimator representation arises because the estimators cover all fissionable material, and, unlike with the mesh, it is unambiguous whether or not each estimator should be sampled.

## CONTINUOUS-ESTIMATOR REPRESENTATION

### Estimator Placement

The cloud of estimators need to be placed throughout the problem and spaced appropriately. The spacing should be defined in such a way that it is based upon some physical quantity. Ideally, the spacing would be based upon resolving important regions and details of the fission source; however, this requires knowing the answer a priori.

For a large class of criticality problems of interest, a choice that produces a reasonable estimator spacing is based on some representative average distance between where a neutron is produced in an iteration to where it creates another fission neutron, which will be called the fission distance $L$. Ideally, $L$ would be based on some robust statistic such as the median or maximum-likelihood estimator, but these pose practical difficulties in terms of algorithmic complexity and memory storage. Simple means or root-mean squares of distances are non-robust and tend to be overly influenced by the few histories that traveled relatively far. A compromise that is still simple to calculate and works well empirically bases $L$ on the square of the mean square-roots of distances,

$$L = \left[ \frac{1}{M} \sum_{i=1}^{M} ||\mathbf{r}_s - \mathbf{r}_f||^{1/2} \right]^2 , \tag{1}$$

where $L$ is the representative distance between fissions, $M$ is the total weight per iteration, $\mathbf{r}_s$ is the position of a source point, $\mathbf{r}_f$ is a corresponding fission termination point, and $||\cdot||$ is the distance (L2 norm) operator. This type of averaging reduces the effect of far traveling histories, and produces values that are more representative of actual fission distances.

For most problems and source guesses tested, $L$ appears to converge to within about ten percent of its stationary value within about five iterations. For that reason, the estimators are placed based upon the value of $L$ computed in the fifth iteration, although this can be changed by the user. Practically speaking, it is only necessary to get an approximate value for this quantity.

To place the estimators, a bounding box covering the domain of fissionable material is required. For now this is either defined by the user or based on the range of fission source neutrons in the first few iterations, which is not an entirely satisfactory solution – further development will need to be performed to answer this question. The bounding box is subdivided into uniform regions with a spacing of approximately $2L$. This mesh serves as a "scaffolding" to provide a data structure to increase the efficiency of placing the estimators and searching for which estimators are scored by each fission source point, and is not a necessary feature of the algorithm. The "scaffolding" elements are defined as the set $S$ containing an enumerated list of its elements with index $s$. The set $E$ starts as empty and will contain the placed estimators. The algorithm for placement of the estimators is as follows:

```
while S not empty do
  S ← random permutation of S, S′ ← empty
  for all elements s in S do
    k ← 1, K ← T, flag ← false
    while k ≤ K do
      randomly sample r = x, y, z in s
      if r not in fissionable material then
        k ← k + 1, cycle
      end if
      if flag is false then
        flag ← true, K ← 2K
      end if
      if distance between r and any estimator in E < L then
        k ← k + 1, cycle
      end if
      add r to E, add s to S′, break
    end while
  end for
  S ← S′
end while
```

A few additional comments: While random sampling cannot guarantee it, and still may miss some elements, the probability of missing regions of space is quite low should $T$ be high enough. Generally speaking, a choice for $T$ that guarantees high probability is found empirically to be 100 plus 100 times the ratio of the volume of the scaffolding mesh element to $L^3$. When fissionable material is found, the value of $K$ is doubled, and this improves the number of estimators found in regions where fissionable material is known, while not wasting too much time sampling regions with no material. Once the cloud of estimators is established, it is fixed for the duration of the simulation, except when a region is found during the transport simulation such that no estimator is within a distance $hL$ (see next section for explanation of $h$); a new estimator is then placed at that point.

### Tallying the Estimators

A tally of fission source distribution neutron production is made each cycle following the creation. If each estimator is given an index $j$, and each fission source point is given an index $i$, then $w_{ji}$ is the score (or weight) imparted to estimator $j$ from fission source neutron $i$. These scores are related to the distance between estimator $j$ and source point $i$ defined by some basis function.

Almost unlimited possibilities exist for basis functions for the estimators. Since information about sampling is desirable, choosing the basis function to have closed support is a useful property. Closed support means that once the distance (a radius of influence) exceeds a certain value (call it $hL$), the score to $w_{ij}$ is zero, meaning that source neutrons contribute nothing to faraway estimators. A radius of influence that appears to work empirically is $h = 2$. Other values of $h$ are possible, so long as they are greater than one. There is a trade off such that $h = 1$ will lead to every small gap between the estimator spheres having a new estimator (the rejection distance is $L$), and, for $h$ very large, having all estimators score may not lead to meaningful sampling estimates.

The basis function selected decreases linearly with distance until zero is reached, or a 3-D tent function:

$$\tau_{ji} = 1 - ||\mathbf{r}_i - \mathbf{r}_j|| \, /2L \qquad (2)$$

If the distance is less than $2L$, the weight $w_{ij}$ is calculated by cycling through all fission source neutrons $i$, finding all estimators $j$ with a positive $\tau_{ji}$ by

$$w_{ji} = \frac{\tau_{ji}}{\sum\limits_{j;\tau_{ji}>0} \tau_{ji}}, \qquad (3)$$

otherwise it is zero. The total score in each estimator $w_j$ is found by taking the sum over $i$ of all $w_{ji}$.

### Computing Diagnostics

Once the estimator scores are known, various diagnostics may be computed. The Shannon entropy of fission source can be calculated using the estimator scores as opposed to the mesh. Define $p_j$ as the $w_j$ divided by $M$ (the sum of all $p_j$ should sum to unity) and take

$$H = -\sum_j p_j \log_2 \left(p_j\right), \qquad (4)$$

where $H$ is the Shannon entropy of the fission source. This statistic computed with the continuous estimators matches, within an additive offset, the mesh computed value if the mesh is well spaced.

In addition to the Shannon entropy, an assessment of sampling may be made by computing means and standard deviations of the estimator scores during the active cycles. Some crude, but easily automatable, global checks can be performed such as searching for any estimators with no scores, or determining if large regions of the fission source have a relative standard deviation in excess of ten percent. The point cloud with means and relative standard deviations can also be written to a text file and plotted using freely available graphics software such as *gnuplot* to visualize any regions that may be suspicious.

## TEST PROBLEM RESULTS

The method is implemented in a research version of MCNP [3]. Four problems are used to test the estimator-based approach: the Godiva sphere [4], the Hoogenboom-Martin performance benchmark – a 3-D full core pressurized water reactor (PWR) – [5], the "$k$-Effective of the World Problem" [6, 7], and the fuel pool source convergence test problem [8]. For each calculation a batch size of 20,000 neutrons per cycle is used.

Results of the fission distance $L$, the number of estimators $J$, and the ratio of the volume covered by the estimators $V_r$ is given. The Shannon entropy computed with both mesh- and estimator-based approaches is shown to have matching trends. Finally, sampling statistics of the estimators with zero scores and those relative uncertainty of greater than ten percent are given for each of the problems.

### Estimator Placement Results

Table I gives a list of results for $L$, $J$, and $V_r$. The volume ratio is the volume of all the spheres with a radius $L$, that are guaranteed to be a distance of at least $L$ apart to the problem volume – for Godiva and "$k$-Effective of the World" the total volume of fissile material is used; for the 3-D PWR and fuel storage vault, the volume of the assemblies (including all fuel, clad, and coolant) are used because $L$ is much larger than the pin radius.

The value of $J$ for "$k$-Effective of the World", which is a $9 \times 9 \times 9$ array of interacting plutonium spheres, has exactly 729 elements, indicating that there is one for each sphere. All of the volume ratios are greater than one, as

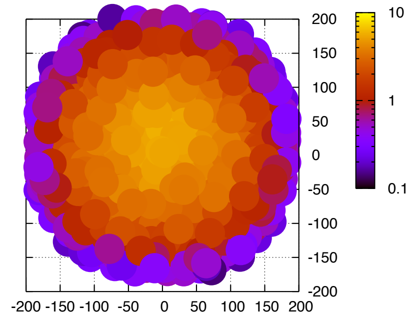

Fig. 1. PWR Mid-Plane Slice of the Estimator Spheres.

expected, since there are edge effects where the spheres formed by the estimators extend outside the fissionable material.

The volume ratio does not prove coverage of the spheres. To show coverage, a top-down view of the 3-D PWR is given in Fig. 1 where both the width of the slice in the axial direction and the radius of the spheres are set to be approximately to $2L$. There are no gaps from this top-down view, and other views of thin slices in this and other directions confirm this. While this still does not prove all fissionable material is covered, it does give a bit of evidence as such.

### Shannon Entropy Agreement

Table II shows the Pearson correlation coefficient $\rho$ comparing the mesh- and estimator-based computed Shannon entropies, along with the resolution of the entropy mesh used. All problems except Godiva have a correlation coefficient $> 0.95$, meaning strong agreement in the trends. Godiva shows a larger disagreement because the mesh-based Shannon entropy has significantly more noise than the estimator-based entropy, but after a least-squares fit additive offset has been applied, the means agree within $0.01\%$. As verification, the Shannon entropies of the "$k$-Effective of the World" agree exactly ($\rho$ = 1), since both mesh and the estimators have a one-to-one correspondence to each sphere.

Table I. Estimator Placement Information.

| Problem | $L$ (cm) | $J$ | $V_r$ |
|---|---|---|---|
| Godiva | 3.10 | 88 | 3.9 |
| PWR | 13.66 | 10762 | 2.8 |
| $k$-Eff World | 12.10 | 729 | 14.2 |
| Fuel Pool | 8.81 | 8153 | 2.5 |

Table II. Shannon Entropy Comparison.

| Problem | $H$ Mesh | $\rho$ |
|---|---|---|
| Godiva | $4 \times 4 \times 4$ | 0.702 |
| PWR | $4 \times 4 \times 4$ | 0.980 |
| $k$-Eff World | $9 \times 9 \times 9$ | 1.000 |
| Fuel Pool | $24 \times 3 \times 6$ | 0.999 |

### Sampling Statistics

Table III gives the approximate number of histories required to sample at least 99.9% of the mesh elements ($Z < 0.001$) and also to ensure that at least 99% of the elements have less than ten percent relative uncertainty ($N_{0.10} < 0.01$).

For Godiva, slightly less than 1 million neutrons are necessary to sample its fission source to within ten percent relative uncertainty. For the 3-D full core (PWR) model, over 8 million histories are required to resolve the at least 99% of the fission source to a standard deviation of ten percent. Additionally, the fuel storage vault requires much more than 100 million histories to sample all the regions. After this many, about one-third of the problem remains unsampled and about 45% of the elements have relative uncertainties of greater than ten percent. It may be that for this problem a source size of 20,000 is too small for a meaningful Monte Carlo sampling.

Table III. Number of Histories Required to Satisfy Sampling Thresholds.

| Problem | $Z < 0.001$ | $N_{0.10} < 0.01$ |
|---|---|---|
| Godiva | < 20k | 960k |
| PWR | 440k | 8.8M |
| $k$-Eff World | < 20k | 6.6M |
| Fuel Pool | >> 100M | >> 100M |

## CONCLUSIONS

A method of placing continuous estimators for computing convergence and sampling statistics for Monte Carlo criticality calculations has been developed. The method has been tested for four different criticality problems and the random sampling scheme based on a fission distance $L$ is shown to offer a representative spacing and cover the fissionable material of the problem. The continuous estimators are able to reproduce the trends of the Shannon entropy computed with a well-spaced mesh. Additionally, sampling statistics of the fission source on the continuous estimators are readily performed because all estimators lie in fissionable material, and therefore unambiguously must be sampled.

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