Title: Continuous-Estimator Representation for Monte Carlo Criticality
Diagnostics

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Continuous-Estimator Representation for Monte Carlo Criticality Diagnostics

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Abstract

An alternate means of computing diagnostics for Monte Carlo criticality calculations is proposed. Overlapping spherical regions or estimators are placed covering the fissile material with a minimum center-to-center separation of the "fission distance", which is defined herein, and a radius that is some multiple thereof. Fission neutron production is recorded based upon a weighted average of proximities to centers for all the spherical estimators. These scores are used to compute the Shannon entropy, and shown to reproduce the value, to within an additive constant, determined from a well-placed mesh by a user. The spherical estimators are also used to assess statistical coverage.

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Outline

- Towards Automating Diagnostics
- Spherical Estimators
- Shannon Entropy Results
- Coverage and Sampling Results

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Diagnostics in Criticality Calculations

- Modern analysis often requires detailed spatial- and energy-resolved results.
- Source convergence necessary to get the correct answers.
- Is the local fission source sufficiently sampled for a well-behaved solution?

- Many diagnostics available, e.g., Shannon Entropy.
- Some automation for users, but improvements desirable.

Shannon Entropy Requirements

- Shannon entropy provides a measure of how "spread out" a distribution is.

$$H = -\sum_{j=1}^{J} p_j \log(p_j)$$

- User of program must define J spatial regions.
- Uniform grid in MCNP with specified or estimated extent.
- Automated spacing based on total population of particles – no physics.
- Generally robust, but possible to get bad meshes, especially for problems with separated discrete regions.

Sampling Diagnostics

- Good local tally results depends on sufficiently sampling nearby fission source.

- For high dominance ratio problems, are all higher modes activated by stochastic noise either sufficiently suppressed or sampled?

- No automatic diagnostic currently in MCNP.

- Shannon entropy mesh may not be suitable because of "small corners" or other non-conformality.

Spherical Estimator

- Approach: Instead of a regular mesh, overlay a collection of spheres for tallying fission source points.

- Properties:
  1. Center of spheres guaranteed to be in fissionable material.
  2. All regions with fissionable material covered by a sphere.
  3. Have a physics-based radius and minimum separation distances.
  4. May overlap, and then fission source points contribute based on proximity to center.

Fission Distance

- Define the *fission distance* as some average straight-line distance between source and fission site.

- Empirically determined that square of the average of square-root of distances appears to work well.

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

Placement Algorithm

1. Bounding box is defined to cover the problem, and a temporary regular "scaffolding" mesh with approximate edge length $2L$.

2. In a random order for each scaffolding mesh, randomly sample points until one lies in fissionable material or some maximum samples exceeded.

3. If/when a point is found:
   - Check to see if it is within distance L of another (previously placed) estimator center.
   - If it is not, create a new spherical estimator centered at that point.
   - Store this element as a candidate for more elements and continue to the next element.

4. Go back to 2 if new estimators were added, else end.

Scoring the Estimators

- If fission source point i in only one estimator, score 1 to that estimator.

- Otherwise score a fraction to each estimator j, w_{ji}, based upon proximity to center using a 3-D tent function.

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

$$w_{ji} = \frac{\tau_{ji}}{\displaystyle\sum_{j;\tau_{ji}>0} \tau_{ji}}$$

Calculating Shannon Entropy

- Entropy computed similarly, except that fission source points may have more than one "state".

$$H = -\sum_{j=1}^{J} p_j \log(p_j)$$

$$p_j = \frac{1}{M} \sum_{i=1}^{M} w_{ji}$$

Test Problems

1. <u>Godiva:</u> Bare HEU sphere.
2. <u>3-D Full Core PWR:</u> Hoogenboom-Martin benchmark.
3. <u>k-eff of the World:</u> $9 \times 9 \times 9$ array of Pu-239 spheres.
4. <u>OECD Fuel Storage Pool:</u> Source convergence benchmark (very hard).

- Each calculation uses 20,000 neutrons per cycle.

Estimator Stats

Table: Estimator Placement Information.

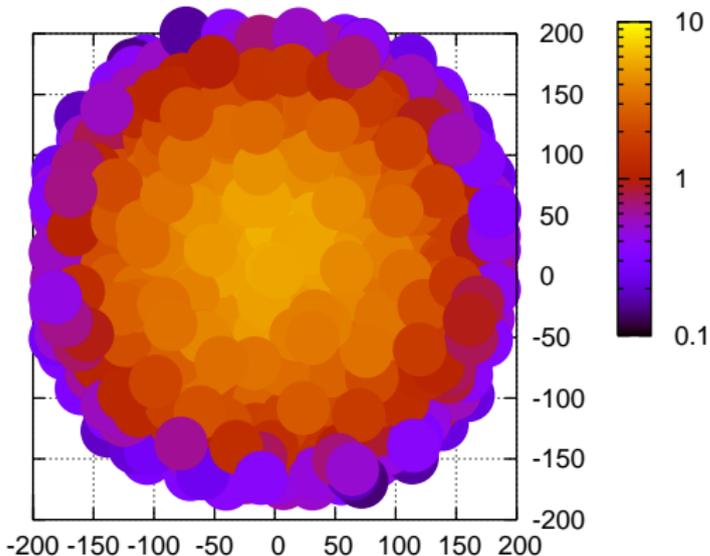|	L (cm)	Number
Godiva	3.10	88
PWR	13.66	10,762
k-Eff World	12.10	729
Fuel Pool	8.81	8,153

Estimators Illustrated

Figure: PWR Mid-Plane Slice of the Estimator Spheres.
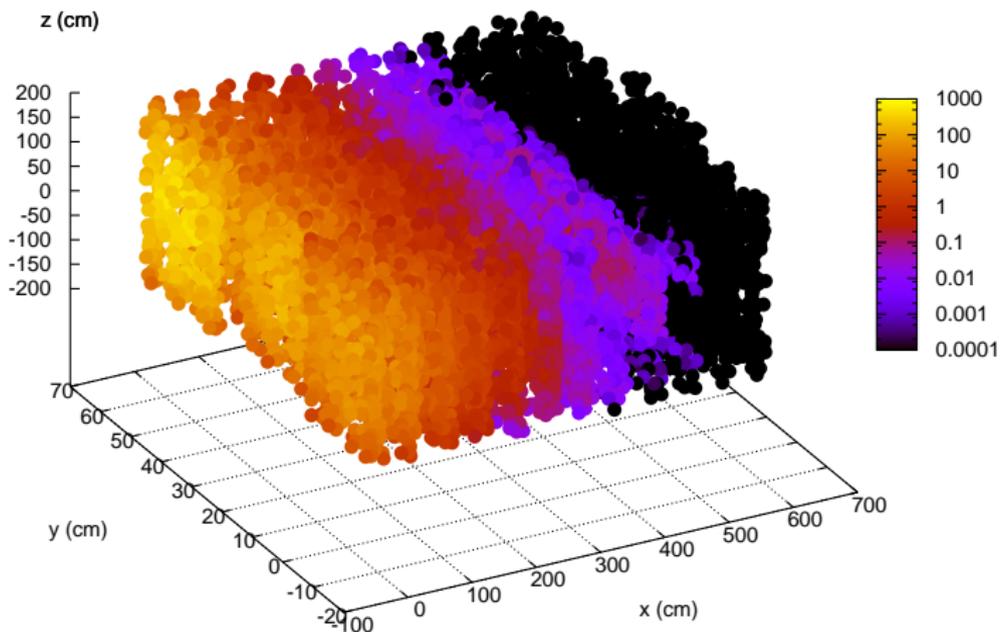
Estimators Illustrated

Figure: Fuel Pool Estimator Spheres.
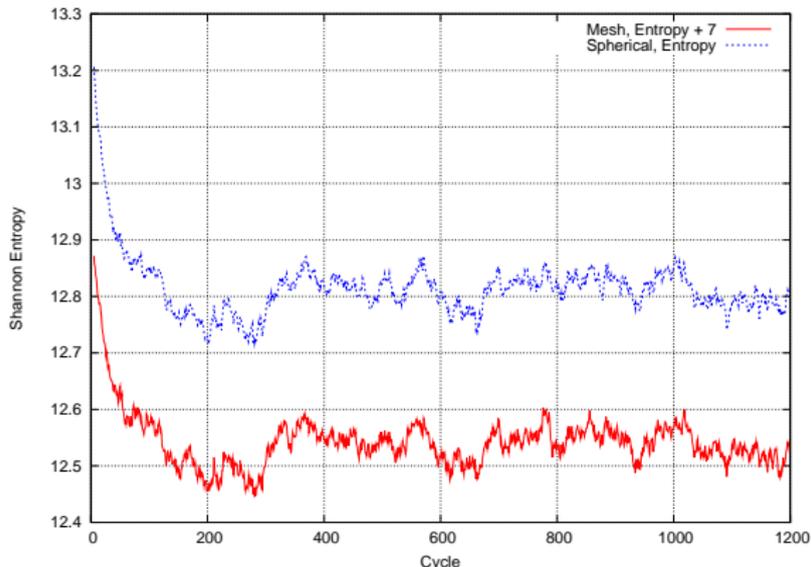
Shannon Entropy

Figure: Shannon Entropy User-Defined Mesh Versus Automated Spherical Estimators

Sampling Diagnostics

Table: Number of Histories Required to Satisfy Sampling Thresholds.

	>99.9% Sampled	>99% Error < 10%
Godiva	< 20k	960k
PWR	440k	8.8M
k-Eff World	< 20k	6.6M
Fuel Pool	>> 100M	>> 100M

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Conclusions

- Automated placement algorithm for spherical estimators developed.
- Distance is "physics based".
- Able to reproduce Shannon entropy to within additive constant.
- More research needed on sampling diagnostics, but provides a basis.

Questions?