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Title: AN ASSESSMENT OF MCNP WEIGHT WINDOWS

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AN ASSESSMENT OF MCNP WEIGHT WINDOWS

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ABSTRACT

The weight window variance reduction method in the general-purpose Monte Carlo N-Particle radiation transport code MCNP™ has recently been rewritten. In particular, it is now possible to generate weight window importance functions on a superimposed mesh, eliminating the need to subdivide geometries for variance reduction purposes. Our assessment addresses the following questions:

(1) Does the new MCNP4C treatment utilize weight windows as well as the former MCNP4B treatment?
(2) Does the new MCNP4C weight window generator generate importance functions as well as MCNP4B?
(3) How do superimposed mesh weight windows compare to cell-based weight windows?
(4) What are the shortcomings of the new MCNP4C weight window generator?

Our assessment was carried out with five neutron and photon shielding problems chosen for their demanding variance reduction requirements. The problems were an oil well logging problem, the Oak Ridge fusion shielding benchmark problem, a photon skyshine problem, an air-over-ground problem, and a sample problem for variance reduction.

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Our conclusions are:

(1) MCNP4C utilizes cell-based weight windows comparably to MCNP4B.
(2) MCNP4C generates cell-based weight windows 15% - 67% better than MCNP4B.
(3) Mesh-based windows can outperform cell-based windows. Cell-based windows are superior only if the geometry is optimally subdivided for variance reduction.
(4) Subdividing geometries for importances is no longer needed.

1. INTRODUCTION

The weight window variance reduction method in the general-purpose Monte Carlo N-Particle radiation transport code MCNP[1] has recently been rewritten. In particular, it is now possible to generate weight window importance functions on a superimposed mesh, eliminating the need to subdivide geometries for variance reduction purposes. Our assessment addresses the following questions:

(1) Does the new MCNP4C treatment utilize weight windows as well as the former MCNP4B treatment?

(2) Does the new MCNP4C weight window generator generate importance functions as well as MCNP4B?

(3) How do superimposed mesh weight windows compare to cell-based weight windows?

(4) What are the shortcomings of the new MCNP4C weight window generator?

Our assessment was carried out with five neutron and photon shielding problems chosen for their demanding variance reduction requirements.

First, we will review MCNP, the weight window variance reduction method, and the weight window generator. Then we will present the five shielding problems, and our results. Finally, we will answer the above questions and make recommendations.

2. MCNP AND WEIGHT WINDOWS

MCNP is a general purpose, three-dimensional, time-dependent, continuous-energy Monte Carlo N-Particle code that is used to calculate coupled neutron-photon-electron transport. Neutrons are modeled from 0 - 20 MeV; photons and electrons are modeled from 1 keV to 100 GeV. MCNP is widely used internationally for shielding, criticality safety, nuclear safeguards, detector design and analysis, nuclear well logging, health physics, medical physics, aerospace, and more. MCNP and its predecessors have existed at Los Alamos since 1963. Every few years a new version is released with sufficient quality that it can stand for a few years without modification. MCNP4C[2] was released early in 2000 along with a comprehensive user manual.[1] The rewriting of the weight windows, the weight window generator, and the addition of the superimposed mesh capability for weight windows was a major new enhancement for MCNP4C.

3. VARIANCE REDUCTION, GEOMETRIC IMPORTANCES, AND WEIGHT WINDOWS

The problem with the Monte Carlo method is that a large number of statistical trials is required to model how radiation interacts with matter. This is because particles do a random walk, and do not usually go to the parts of the problem where we want to tally them. Consequently there is a large statistical error, or variance, for a given number of particle histories. Variance reduction techniques reduce the statistical error by sampling more particles in regions of interest than in regions of phase space where they do not contribute as much to the desired tally, thus reducing the variance for a given amount of computational time.

Importance sampling, or geometric splitting and roulette, is a relatively straightforward variance reduction technique. A problem geometry is subdivided into regions and assigned importances which increase in the direction of interest, and decrease towards unimportant regions. Particles passing into a region of higher importance are split into more samples, but the weight of each sample is reduced so that total weight, or the total number of particles represented, is conserved. Particles passing into a region of lower importance play Russian roulette. They are killed, or no longer modeled, with a given probability, but the weight of those surviving the roulette is increased to again conserve total weight.

Although importance sampling is very effective at producing more statistical samples (low weight particles) in regions of interest, the weights of the particles can still fluctuate widely thus contributing to statistical fluctuations. The weights are affected by other variance reductions techniques, including implicit capture which reduces particle weight at each collision.

The weight window method[3] was developed to both increase sampling in important regions of a problem and to control particle weights. Upper and lower weight bounds are assigned to each region of phase space. Particles with weights above the bounds are split so that there are more particles and their weights are within the window bounds. Particles with weights below the bounds are rouletted so that those that survive have weights increased into the window bounds. The weight bounds decrease in the direction of importance and increase away from important regions, just the opposite of importances, so that many lower weight particles are sampled in the regions of importance.

4. THE WEIGHT WINDOW GENERATOR

Setting the weight window bounds is difficult and non-intuitive. Therefore, MCNP has provided a weight window generator[3] for many years. The weight window generator statistically estimates the importance of each phase space region as the ratio of the weight of particles passing through a cell that eventually tally to the total weight of particles passing through. These estimated importances are then inverted and normalized so that they can become weight windows to be used in the next iteration of the problem.

The MCNP4B weight windows and weight window generator were still limited in spatial representation to geometric cells input by the user. Liu and Gardner[4] have demonstrated the usefulness of generating and applying weight windows on a superimposed grid, eliminating the need for code users to subdivide geometries sufficiently for spatial importances. They have also generated weight windows with a diffusion solver.[5]

The original MCNP weight window generator used up through version MCNP4B had a number of approximations to simplify the chore of the required bookkeeping. MCNP4C has eliminated those approximations, made a number of minor corrections both in the way weight windows are used and generated, and added a new method and capability to generate weight windows in a mesh that is not part of the physical geometry but rather is superimposed over it.[6] Presently there are no plans to add a diffusion or other deterministic solver to generate the weight windows in the mesh.

5. TEST PROBLEMS

Five shielding / deep penetration problems were chosen to assess the new MCNP weight window capabilities. These problems were chosen because they required importances to vary over several or many orders of magnitude and optimal importance functions had already been determined and published. We wanted to see if MCNP4C could generate importance functions as well as the experts.

Each of these problems was modeled in the "expert configuration," requiring many cells to subdivide the geometry for geometric importance sampling, and in the "simple configuration"—the fewest number of cells required to model the geometry with no subdivision for variance reduction. The numbers at the end of each problem description are the numbers of geometric cells required by the expert/simple configuration.

The five problems are:

(1) Oil: The oil well logging problem from the MCNP test set is a nuclear well logging tool which is off center in a borehole in a rock formation. The tool geometry is oversimplified to be non-proprietary. Neutrons are emitted from one end of the tool into the rock and scattered neutrons are detected at the other end of the tool. (231/8)

(2) Fusion: The Oak Ridge fusion benchmark[7] is a 14-MeV beam source penetrating a 55-cm iron/stainless steel shield with a detector off-center behind the shield. (179/53)

(3) Skyshine: The photon skyshine problem[8] consisting of a cesium-137 point source collimated into a 150-degree cone pointed skyward. The source sits on a plane of dirt and photons are tallied a meter above the dirt 700 meters away. (19/5)

(4) Air/Ground: The air-over-ground problem[8] is an infinite flat field of dirt emitting radioactive fallout with a detector a meter above the ground in the center of the field. (122/4)

(5) Class: The sample problem for variance reduction[9] is a fictitious problem that has been developed to challenge all the MCNP variance reduction features working together. It is referred to as the class problem because it is taught in the MCNP classes. It requires a 2 - 14 MeV neutron source to penetrate 180 cm of concrete, then pass through a 1820 cm void duct, then scatter off a 10 cm plate of light material to a detector 200 cm off to the side. (23/7)

6. METHODOLOGY

Performance of the weight windows was characterized by the Figure-of-Merit (FOM) automatically printed by MCNP. The FOM is

$$1/T\varepsilon^2$$

where T is the computer time for running particle histories and ε is the relative statistical error. The FOM is approximately constant because for N particle histories in the Monte Carlo simulation, ε decreases as $1/\sqrt{N}$ and time is proportional to N. The higher the FOM, the higher the efficiency of the problem.

Both MCNP4B and MCNP4C were compiled identically so that the only significant differences in running time were due to differences in the efficiency of the weight windows variance reduction technique. All runs were made on a single machine in the same environment.

7. RESULTS

7.1 INCOMPATIBILITY OF WINDOWS AND SOURCE BIASING

The air-over ground problem had an infinite source which was spatially biased to produce more particles near the center. It became apparent that there is no good way to match spatial source bias with spatial weight windows. All particles starting from the source started outside the mesh-based weight window bounds. Further, there were false convergence problems, even in the expert set-up reference problem, which had gone undetected because the reference air-over-ground problem was published before MCNP had the statistical checks to identify false convergence.[10] Consequently, most of the air-over-ground problem results are inconclusive and are omitted in the following results. Clearly a means is needed to match source bias with weight windows. Also a means of renormalizing weight windows is needed.

7.2 WEIGHT WINDOW UTILIZATION

For each of the five problems, cell-based weight windows were generated and then used with both MCNP4B and MCNP4C. For a given set of weight windows, MCNP4C is from 6%

slower to 12% faster than MCNP4B. That is, MCNP4B and MCNP4C utilize weight windows comparably.

7.3 WEIGHT WINDOW GENERATION

Both MCNP4B and MCNP4C run 15%-67% more efficiently when using weight windows generated by MCNP4C than when using weight windows generated in the same way on the same problem by MCNP4B. Thus MCNP4C generates weight windows significantly better than those generated by MCNP4B.

7.4 COST OF GENERATING WINDOWS

When the weight window generator is turned on, running time is increased. For the oil problem, the increase was 4% for cell based weight windows, 25% - 30% for rectangular xyz mesh-based weight windows, and 25% - 30% for cylindrical rzt mesh-based weight windows.

7.5 CELL-BASED vs MESH-BASED WINDOWS

The oil well logging benchmark problem had a geometry very carefully tuned by nuclear well logging experts to be sufficiently well subdivided for geometric importances. Consequently, the FOM with the best MCNP4C generated cell-based windows was 322. The best FOM with XYZ mesh windows was 192, and the best with RZT mesh windows was 161. The difference between the RZT and XYZ meshes is likely due to the increased difficulty and slower algorithm of the RZT geometry. Thus if a geometry is optimally subdivided for variance reduction, cell-based weight windows are better. They are also easier to understand and adjust, and they in effect provide a nice adjoint-solution like diagnostic for the problem.

However, users seldom have the resources or the advanced knowledge to set up a problem with an optimum variance reduction geometry. Mesh-based windows were superior to cell-based windows in the fusion problem by 3%, in the skyshine problem by a factor of four, and in the class problem by 25% after just one generation run. After 2-5 generation runs, the generated meshes were slightly better for the fusion and skyshine problems but a factor of two better than cell-based windows for the class problem. Thus mesh-based windows can provide a significantly better importance function than cell-based windows or importances if the problem geometry is less than optimally subdivided for geometric importances. Sometimes several iterations of the generator are required to get the best windows.

When no attempt is made to subdivide a geometry for variance reduction and the geometry is in its most simple, few-cell form, then mesh-based weight windows are the only viable alternative if the importance function has strong spatial dependence. In these cases the initial importance function for the weight window generator is necessarily cell-based and is very crude; it takes 3-5 iterations of the mesh based windows to get an efficient problem. But after several iterations the mesh-based windows will usually converge to a result comparable to generating the windows with an expert importance function. Further, generally the simple geometries run faster than the more complex ones subdivided for variance reduction.

8. CONCLUSIONS

MCNP4C utilizes cell-based weight windows comparably to MCNP4B.

MCNP4C generates cell-based weight windows 15% - 67% better than MCNP4B.

Mesh-based windows can outperform cell-based windows. Cell-based windows are superior only if the geometry is optimally subdivided for variance reduction.

Subdividing geometries for importances is no longer needed.

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