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Title: Monte Carlo Variance Reduction Using Nested DXTRAN Spheres

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MONTE CARLO VARIANCE REDUCTION USING NESTED DXTRAN SPHERES

RADIATION PROTECTION

KEYWORDS: *Monte Carlo, variance reduction, angle biasing*

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Dxtran is a deterministic transport method typically used for increasing the sampling in a spherical region that would otherwise not be adequately sampled because the probability of scattering toward the region is often very small. Essentially, the dxtran method splits the particle into two pieces at each source or collision point: a piece that arrives (without further collisions) at the dxtran sphere and a piece that does not. One difficulty with the dxtran method is that it can introduce a large weight fluctuation between particles colliding just before the sphere and particles colliding after crossing the sphere. New work shows that it is possible to mitigate this difficulty by extending the dxtran sphere concept to a set of nested dxtran spheres. Each dxtran sphere then shields its interior from particles whose weights are too large so that weights are more commensurate with their locations. Shielding against the large weights not only increases the efficiency of the calculation but the reliability as well. The effectiveness of the technique in MCNP was demonstrated on a 1-km air transport problem and on a concrete duct problem.

I. CURRENT DXTRAN METHOD

The current dxtran (deterministic transport) method in MCNP is described fully in the MCNP manual[1]; here, only a brief overview is possible. The dxtran method uses a sphere (the "dxtran sphere") to partition the possible next events after a collision or source event into two categories:

1. the particle reaches the dxtran sphere before the next collision or escape, or
2. the particle does not reach the dxtran sphere before the next collision or escape.

The nondxtran particle is sampled and tallied (with its full weight) exactly as it would be sampled if no dxtran sphere were present, with one exception. If the nondxtran particle reaches the dxtran sphere on its next flight, it is killed. Nondxtran particles tend to have much higher weights than desirable inside the dxtran sphere, so killing the nondxtran particle tends to keep high-weight particles from entering the dxtran sphere. The weight of nondxtran particles that are killed on the dxtran sphere is balanced by creating appropriately weighted dxtran particles on the surface of the dxtran sphere.[1] Because dxtran typically reduces particle weight, the dxtran particles tend to have low weights. These low weights tend to be consistent with the weight window inside the dxtran sphere.

Dxtran works very well when the dxtran sphere is in a void. Statistical fluctuations arise when the dxtran sphere is in or near a scattering medium. These fluctuations are very similar to the statistical behavior of point detector estimates; this is not surprising because a point detector is the limit of a dxtran sphere with an infinitesimal radius. The dxtran method can introduce a large weight fluctuation between particles colliding just before the sphere (high weight) and particles colliding after crossing the sphere (low weight). The nested dxtran sphere concept was devised to control this large weight fluctuation.

II. NESTED DXTRAN METHOD

The nested dxtran method consists of an arbitrary collection of nonintersecting dxtran spheres. If sphere B is totally inside sphere A, then B is "nested" within A. Note that A and B need not be concentric. In addition, another sphere C might be nested within B, or both spheres B and C might be nested within A. For example,

$$x^2 + y^2 + z^2 - 10^2 = 0 \text{ (sphere A)} ,$$

$$x^2 + (y - 5)^2 + z^2 - 1^2 = 0 \text{ (sphere B)} ,$$

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or

$$(x-1)^2 + y^2 + z^2 - 2^2 = 0 \text{ (sphere C)} \ .$$

At every collision and source point, a dxtran particle is placed on *every* dxtran sphere that the collision is outside of, and correspondingly, the nondxtran particle is killed if it tries to enter any nested dxtran sphere from the outside (Fig. 1). Each dxtran sphere thus shields its interior from particles whose weights are too high so that weights are more commensurate with their locations. That is, in high importance regions inside the dxtran sphere, low weights that are inversely proportional to the importance are desired.

III. TWO SAMPLE PROBLEM RESULTS

Problem 1 consisted of a track-length estimate of the flux inside a 7-cm sphere. The flux was produced by a 14-MeV isotropic neutron placed 1 km (100 000 cm) from the 7-cm sphere. Air at constant density was used everywhere in the problem. Weight windows alone (without nested dxtran spheres) in a 10-h calculation (21 685 582 source particles) produced the following mean, relative error, and figure of merit (FOM) [i.e., $(rel\ err)^{-2} \times time^{-1}$]: 1.6062×10^{-12} n/cm^2, 0.1574, and 0.067.

Ten nested dxtran spheres with radii of 7, 15, 30, 60, 125, 250, 500, 1000, 2000, and 4000 cm were used for the nested dxtran calculation by roughly quadrupling the solid angle from the source to the tally sphere. Weight windows and nested dxtran spheres in a 1-h calculation (154 816 particles) produced the following mean, relative error, and FOM: 1.7514×10^{-12} n/cm^2, 0.0189, and 46. This indicates a speedup factor of 686 over weight windows used alone.

Using the weight window and only the innermost dxtran sphere produced some erratic, but interesting, results. A 1-h calculation (781 007 particles) produced the following mean, relative error, and FOM: 1.7261×10^{-12} n/cm^2, 0.0096, and 181. The 1-h calculation passed MCNP's ten statistical checks. A 24-h calculation (18 301 168 particles) produced the following mean, relative error, and FOM: 1.7543×10^{-12} n/cm^2, 0.0020, and 171. Note that the 1-h calculation had a tail slope of 4.3, indicating that only the first three moments of the score distribution were finite. The central limit theorem is applicable if the first two moments are finite.[1,2] But, because the fourth moment is infinite, the variance of the variance (VOV) is infinite, and thus the sample variance may not be a good estimate of the true variance. Indeed, the 24-h calculation shows a nonmonotonic behavior in the estimated VOV and a slope of only 2.7, indicating a possibly infinite variance. Note that the estimate depends on a finite variance. Thus, while high, an FOM of 181 is statistically unreliable. Indeed, note that despite a small relative error estimate of 1% at 1 h, the FOM has a relatively large change after 24 h from 181 to 171. This is characteristic of the poor sampling in point detector estimates that often fools the unwary practitioner. Essentially, the tally behaves like a point detector tally because the radius (7 cm) is tiny compared to the mean free path (4300 cm) in the vicinity of the sphere. (There are many other indications of inadequate sampling in the output file as well.) A summary of these results can be found in Table I.

The concrete duct of problem 2 is another example where dxtran is often employed. Here the source is a 14-MeV point isotropic neutron source at the bottom of a straight 2.54-cm radius duct through 200 cm of concrete. The tally is the current exiting the far end of the duct. A 1-h calculation (7 995 273 particles) with weight windows alone produced the following mean, relative error, and FOM: 4.4154×10^{-5} n, 0.0522, and 6.1. A 1-h calculation (2 191 827 particles) with weight windows and 5 dxtran spheres at radii 2.54, 5, 10, 20, and 50 cm produced the following mean, relative error, and FOM: 4.3853×10^{-5} n, 0.0018, and 5344. Five separate calculations with single dxtran spheres of 2.54-, 5-, 10-, 20-, and 50-cm radii produced FOMs of 1561, 2864, 2329, 860, and 164, respectively. As with problem 1, the tail slope estimate is erratic for these single dxtran sphere

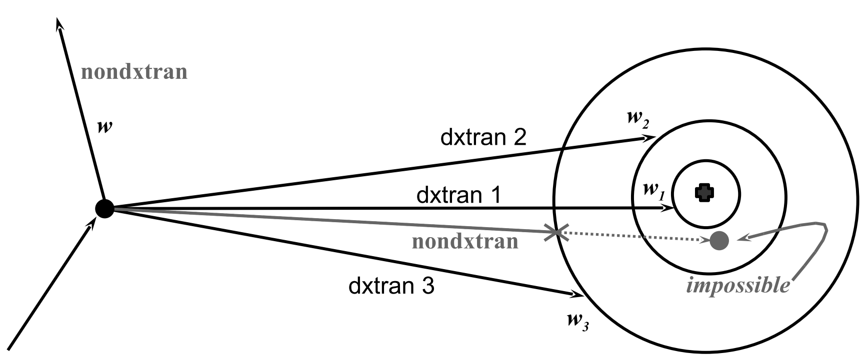

Fig. 1. Nested dxtran sphere scheme roughly configured by a solid angle and $w_1 < w_2 < w_3 \ll w$.

TABLE I

Comparison of MCNP Nested Dxtran Sphere and Nonnested Results for Flux Transported 1 km in Air from Isotropic 14-MeV Neutrons

Dxtran Technique	Run Time (h)	Mean (n/cm^2)	Relative Error	VOV	FOM	Slope
None	10	1.6062×10^{-12}	0.1574	0.3845	0.067	2.0
1 dxtran (sphere 1)	1	1.7261×10^{-12}	0.0096	0.0012	181	4.3
1 dxtran (sphere 3)	1	1.7414×10^{-12}	0.0115	0.0006	126	10.0
1 dxtran (sphere 5)	1	1.7145×10^{-12}	0.0269	0.0020	23	5.3
1 dxtran (sphere 7)	1	1.7964×10^{-12}	0.0908	0.0226	2.0	0.0
1 dxtran (sphere 9)	1	1.9744×10^{-12}	0.2293	0.1280	0.032	0.0
1 dxtran (sphere 1)	24	1.7543×10^{-12}	0.0020	0.0002	171	2.7
10 nested dxtrans	1	1.7514×10^{-12}	0.0189	0.0017	46	10.0

TABLE II

Comparison of MCNP Nested Dxtran Sphere and Nonnested Results for Current in a Concrete Duct*

Dxtran Technique	Mean (n)	Relative Error	VOV	FOM	Slope
None	4.4154×10^{-5}	0.0522	0.0029	6.1	10.0
1 dxtran (sphere 1)	4.3742×10^{-5}	0.0033	0.0195	1561	4.1
1 dxtran (sphere 2)	4.3766×10^{-5}	0.0024	0.0096	2864	7.3
1 dxtran (sphere 3)	4.3873×10^{-5}	0.0027	0.0219	2329	3.2
1 dxtran (sphere 4)	4.3945×10^{-5}	0.0044	0.0109	860	3.7
1 dxtran (sphere 5)	4.3836×10^{-5}	0.0101	0.0052	164	2.4
5 nested dxtrans	4.3853×10^{-5}	0.0018	0.0001	5344	10.0

*All calculations took 1 h.

cases, indicating inadequate sampling. Thus, although the FOM gain is only a factor of 2 for this problem, the nested dxtran calculation has much better statistical properties and is therefore much more believable and reliable than the single dxtran sphere cases (Table II).

IV. CONCLUSION AND FUTURE WORK

The nested dxtran sphere method is a modest, though useful, extension to the basic dxtran method for two reasons. First, the method significantly improves the FOM. Second, the method tends to ameliorate the point detector–like statistical problems that often plague single dxtran sphere calculations in small solid-angle problems. Although this paper showed nice gains for the nested dxtran method, it may take some experience to decide on the number of dxtran spheres and their radii for various types of problems. Also, a forced collision technique in combination with an entering collision weight window (in addition to the free-flight window currently in MCNP) might provide additional improvements in conjunction with nested dxtran spheres.

For the future, noting that the nested dxtran method seems to ameliorate point detector–like statistical problems, it would be interesting to nest a set of dxtran spheres around a point detector. One can even imagine an infinite nest of dxtran spheres around the point detector in combination with a forced collision technique to ensure collisions at all levels of the nest and a stochastic termination technique for deciding how many levels of nesting to use at any collision. Such a technique might not only produce a finite variance (as do other point detector modifications) but a finite variance of the variance as well.

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