

AN ALTERNATIVE METHOD OF BIASING THE COLLISION KERNEL IN MONTE CARLO CALCULATIONS

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SUMMARY

A simple alternative way of biasing the collision kernel for variance reduction is justified due to the great difficulties in implementing most techniques found in literature in the general Monte Carlo programs available. These difficulties are related to programming necessities and the extensive data amounts usually required for the general methods. The random walk of particles is heavily driven by the probability distribution of the azimuthal scattering angle in each collision, even though it has a very simple form. In this work, a variance reduction scheme is devised to sample azimuthal scattering angles as a means to guide the scattering particle towards a preferred direction. Therefore, the particles trajectories can be forced into a virtual pipeline drawn between the source and the point of interest. As an alternative method, it can be easily included in Monte Carlo programs and the results show a promising performance in the demonstration problem solved in this work.

INTRODUCTION

Problems that arise in the utilization of Monte Carlo methods often require variance reduction techniques which differ in complexity, applicability and efficiency. Techniques that are very efficient may require great efforts to be incorporated in the available codes and at the same time may be too specific to some kind of problem. Therefore, there is a need for simple techniques that are easy to improve in the existing codes and that can be made automatic in the code operation. In this context we devised a simple variance reduction technique, which is based on the opening of the particle trajectory towards the point-of-interest by acting only on the sampling of the azimuthal scattering angle. This is accomplished by importance sampling the scattering quadrant that leads the particle towards the point of interest. The results show a significant improvement in the figure of merit for the outer detectors in the sample problem presented. Also, it is important to note that the technique is easy to implement in existing codes.

The theoretical foundations are explained in the next section. Also, one application is presented to illustrate the performance of the technique.

ANALYSIS

The MORSE Monte Carlo radiation transport code[1] utilizes the Boltzmann integral transport equation for the emergent particle density. This equation in multigroup notation and time-independent may be written as

$$\chi_g(\vec{r}, \hat{\Omega}) = S_g(\vec{r}, \hat{\Omega}) + \Sigma_{g'} \int \int \chi_{g'}(\vec{r}', \hat{\Omega}') K^{g'-g}(\vec{r}', \hat{\Omega}' \rightarrow \vec{r}, \hat{\Omega}) d\vec{r}' d\hat{\Omega}' \quad (1)$$

The transition kernel K may be expressed by the product of two kernels, the transport and the collision kernels both multiplied by the non-absorption probability. The

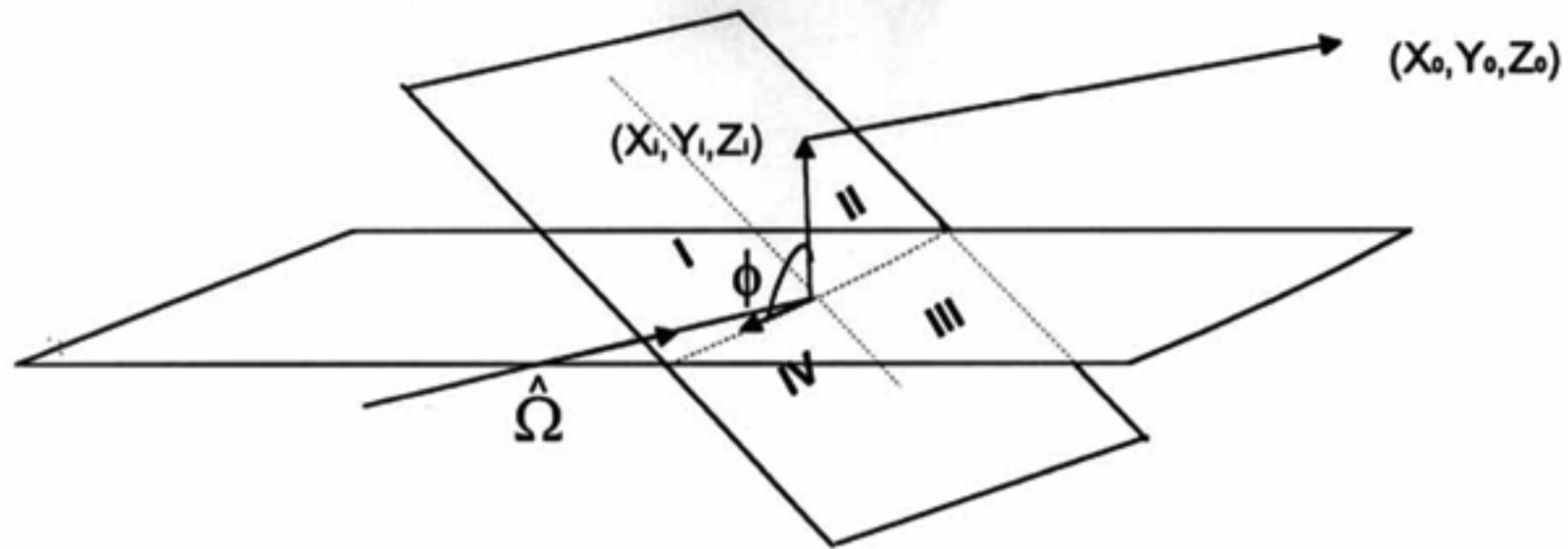


Figure 1: Geometrical Scheme of the Azimuthal Angular Biasing.

collision kernel is a joint probability distribution function for the random variables g and $\hat{\Omega}$. The g energy group of emergent particles is selected from a marginal p.d.f. and the $\hat{\Omega}$ directions are selected from the conditional p.d.f.

$$\frac{\Sigma_s^{g' \rightarrow g}(\vec{r}, \hat{\Omega}' \rightarrow \hat{\Omega})}{\Sigma_s(\vec{r})} = h(\phi)\omega(\mu). \quad (2)$$

Considering azimuthal symmetry, the differential scattering cross sections may be written as a function of the cosine of the polar angle and be expanded in a series of Legendre polynomials. This distribution is transformed in a discrete distribution by the utilization of a Gaussian quadrature scheme[1] which yields,

$$\frac{\Sigma_s^{g' \rightarrow g}(\vec{r}, \hat{\Omega}' \rightarrow \hat{\Omega})}{\Sigma_s(\vec{r})} = h(\phi)\omega^*(\mu). \quad (3)$$

Where the azimuthal angle distribution is given by

$$h(\phi) = \frac{1}{2\pi} \quad (4)$$

and the polar angle distribution[2] by

$$\omega^*(\mu) = \sum_{i=1}^N p_i \delta(\mu - \mu_i). \quad (5)$$

Where p_i is the probability associated to μ_i and N the number of possible polar scattering angles.

To select an outgoing direction at a collision site, a scattering polar angle is selected from the discrete distribution $\omega^*(\mu)$ of Eq. 5 and an azimuthal angle is selected from the uniform distribution $h(\phi)$ of Eq. 4. Because they are independent one or the other distribution can be selected first.

In the angular biasing of the collision kernel shown by Tang et al[2], N azimuthal angles are sampled first, forming a set of N possible outgoing directions and after that, one of these directions is selected

weighted by the point value function[3, 4] (or the adjoint angular flux). In this work, however, the polar angle distribution is not biased, but only $h(\phi)$, i.e., the azimuthal angle of scattering is chosen in the quadrant in which a straight line coming from the point of interest, trespass perpendicularly the plane defined by the incident particle direction cosines and the point of the collision coordinates (see Figure 1 and Eq. 6).

Consider a particle with direction cosines (u, v, w) colliding in (X_c, Y_c, Z_c) . The equation of a plane with direction vector (u, v, w) passing through (X_c, Y_c, Z_c) is

$$u(X - X_c) + v(Y - Y_c) + w(Z - Z_c) = 0. \quad (6)$$

The equation of a straight line perpendicular to this plane passing through the point of interest, (X_0, Y_0, Z_0) , which can be associated with the coordinates of a particular detector, is

$$\begin{aligned} X &= X_0 + ut \\ Y &= Y_0 + vt \\ Z &= Z_0 + wt. \end{aligned} \quad (7)$$

The point of intersection of this straight line with the plane defined by Eq. 6 above may be determined calculating t first,

$$\begin{aligned} u(X_0 + ut - X_c) + v(Y_0 + vt - Y_c) + \\ w(Z_0 + wt - Z_c) = 0, \end{aligned} \quad (8)$$

or

$$t = \frac{-[u(X_0 - X_c) + v(Y_0 - Y_c) + w(Z_0 - Z_c)]}{u^2 + v^2 + w^2}. \quad (9)$$

The intersection point, (X_i, Y_i, Z_i) , is obtained by substituting t in Eq. 7.

By defining the straight line

$$u(X - X_i) + v(Y - Y_i) + w(Z - Z_i) = 0, \quad (10)$$

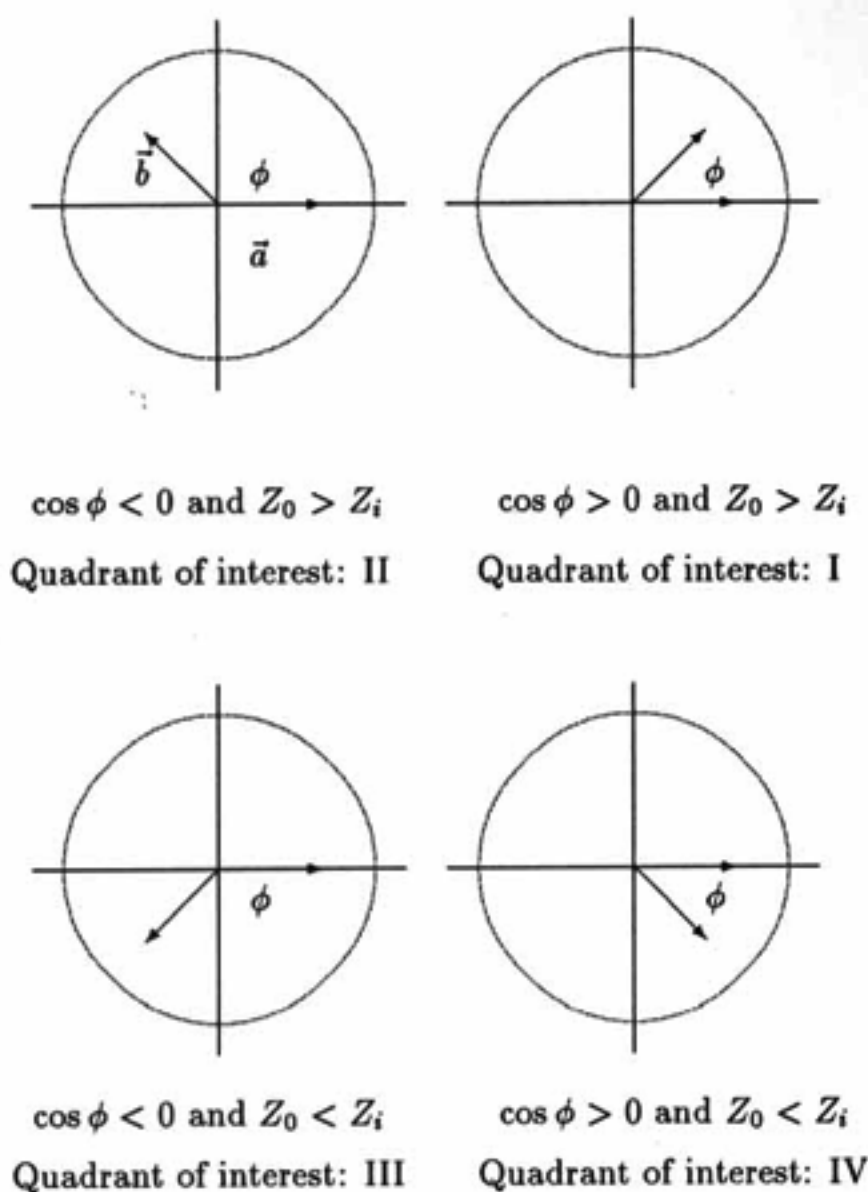


Figure 2: Determination of the Quadrant of Interest.

$$Z - Z_c = 0, \quad (11)$$

one can determine the angle formed by the vector given by the intersection of the planes defined by Eqs. 10 and 11 and the vector formed by the collision and intersection points both belonging to the plane given by Eq. 6, as can be seen in Figure 1. To determine in which quadrant is the intersection point we must know if it is above (I or II) or below (III or IV) the plane given by Eq. 11. This is accomplished comparing the z -coordinates of the collision and intersection points. Now, we need to define the cartesian axes for the sampling of the azimuthal angle in the quadrant of interest. One axis is contained in the plane $Z = Z_c$ and its direction is given by the vector product of Eq. 10 and Eq. 11. The other axis is assumed perpendicular with the former and belonging to the plane given by Eq. 6 and with positive Z direction. Then, the signal between the vectors.

$$\vec{a} = (vZ_c, -uZ_c, 0), \quad (12)$$

$$\vec{b} = (X_i - X_c, Y_i - Y_c, Z_i - Z_c), \quad (13)$$

will define if it is on the left (I or III) or on the right (I or IV) side. Therefore, the quadrant of interest is consequently defined. Now, one can play a fair russian roulette game to select more particles in this quadrant.

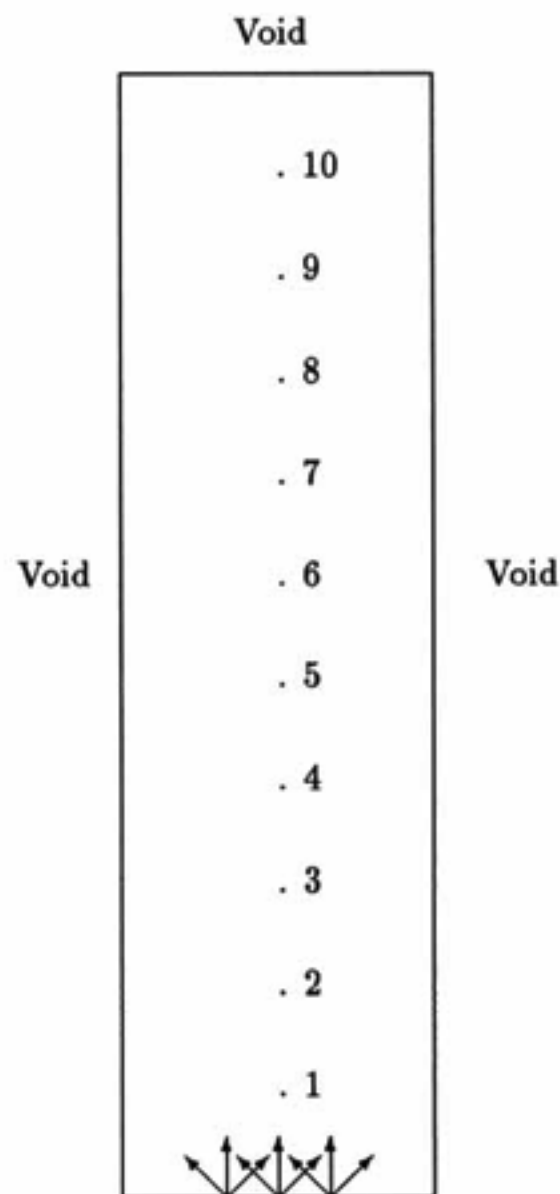


Figure 3: Sodium Cylinder Test Problem.

Figure 2 shows the four possible situations in the determination of the the quadrant of interest.

APPLICATION

The problem chosen to illustrate the variance reduction obtained with the azimuthal angle of scattering biasing is a sodium cylinder with 30 cm radius and 102 cm height, immersed in vacuum. The neutron source is located at the bottom of the cylinder with an upward cosine direction distribution. Energies from 15.0 down to $5.8E-04$ MeV were analyzed. The biasing consisted in selecting the quadrant of interest in seven out of ten trials, which is accomplished by a russian roulette game. Ten detectors are defined in the axis of the sodium cylinder 10 cm apart.

Table 1 shows the results for the test problem, which were labeled MORSE-Yes, with the biasing scheme, and MORSE-No, with no variance reduction. The calculations show the obtained results for the points shown in Figure 3. The net effect of the technique is to enhance the statistics of the outer detectors, i.e., more particles will get farther in the sodium cylinder, making important contributions to these detectors (closer collisions mean larger contributions).

The smaller fractional standard deviations for De-

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Table 1: Comparison of the Calculated Results — Sodium Deep Penetration Problem

Det	MORSE-Yes*	MORSE-No*
1	1.8846E-05 (0.01107)**	2.0563E-05 (0.05030)
2	5.4507E-06 (0.03851)	5.2307E-06 (0.01348)
3	1.5439E-06 (0.03368)	1.8663E-06 (0.07512)
4	5.7229E-07 (0.05981)	5.7013E-07 (0.03285)
5	1.8812E-07 (0.07744)	2.0927E-07 (0.07273)
6	6.4345E-08 (0.07277)	6.8288E-08 (0.04960)
7	2.0507E-08 (0.06385)	3.1967E-08 (0.14043)
8	7.6541E-09 (0.12895)	1.2827E-08 (0.15334)
9	2.5365E-09 (0.13356)	3.7621E-09 (0.14466)
10	8.9113E-10 (0.15191)	1.3314E-09 (0.25030)

*See text.

**Fractional standard deviation.

tectors 7, 8, 9, and 10 show that their solutions benefited from the enhanced collision density in their vicinity. The relative figure of merit between the two MORSE calculations ($1/\sigma^2T$) for Detector 10, was 2.54, which is a significant increase in efficiency. Also, there was only a 7% increase in computer time.

CONCLUSIONS

It is recognized that angular biasing schemes work better if used with space and energy biasing, which is due to its natural conditional dependency. Therefore, the full potential of the technique presented in this paper as well as its applicability in a variety of different problems must be more thoroughly assessed. On the other hand, based on the obtained results, we expect that this technique may be used in a routine basis without much effort as it is necessary for most of the other variance reduction techniques.

As future work, it is expected that the DXTRAN feature of the MCNP code[5] can be made more efficient if it is used to actually bias the collision kernel towards a point of interest in the same manner the angular biasing was accomplished in this paper. In this case, the polar angle of scattering would be also biased.