CONF-810606--78

A BOUNDED LIMIT FOR THE MONTE CARLO POINT-FLUX-ESTIMATOR

R. A. Grimesey (EG&G Idaho)

Kalos[1] has analyzed the so-called Next-Event-Estimator (NEE) for flux-at-a-point by Monte Carlo and proposed the OMCFE to avoid the singularity. Kalli and Cashwell[2] and Steinberg[3] and Kalos have developed a number of ingenious schemes along similar lines with bounded variance. Recently Iida and Seki[4] proposed the Void Detector technique as an approximation to avoid the NEE singularity.

The NEE estimator for the collided flux-at-a-point is derived from the integral form of the time-independent transport equation[5].

MASTER

$$\phi_c(\vec{r},E) = \int_{V'} K(R,E)q(\vec{r}',\vec{\Omega}_R,E)dv' \qquad (1)$$

where

$$K(R,E) = \frac{e^{-\Sigma(E)R}}{4\pi R^2}, \qquad (2)$$

for isotropic scattering in a homogeneous system; $R = |\vec{r}' - \vec{r}|$ is the distance to the detector point located at $\vec{r}$ from each collision point at $\vec{r}'$. $q(\vec{r}', \vec{\Omega}_R, E)$ is the isotropic scattering integral over all incident $\vec{\Omega}', E'$ at $\vec{r}'$ to $\vec{\Omega}_R$ in the direction of the detector at energy E.

In a Monte Carlo random walk, the kernel K(R,E) is used as an expected value estimator at every collision for the collided flux $\phi_c(\vec{r},E)$ at the detector point.

$$\phi_c(\vec{r},E) = \sum_i \phi_i = \sum_i W_i \frac{\Sigma_s(E')}{\Sigma(E')} P(\vec{\Omega}_{Ri},E'\to E)K(R_i,E) \qquad (3)$$

where W_i is the neutron weight entering the i^{th} collision and $P(\vec{\Omega}_{Ri},E'\to E)$ is the probability of a neutron isotropically scattering toward $\vec{r}$ at energy E. It is a well-known fact[1] that Equation (3) posesses infinite theoretical

Prepared under
E... No. DE-AC07-76ID...

variance because it is possible in a random walk for a collision to occur infinitesimally close to the detector at $\vec{r}$ with finite weight W_1.

In this paper, a limiting value for Equation (2) is derived from a diffusion approximation for the probability current at a radius R_1 from the detector point. The variance of Equation (3) is thus bounded using this asymptotic form for K(R,E). The NEE kernel for the monoenergetic case is:

$$K(R) = \frac{e^{-\Sigma R}}{4\pi R^2} \quad . \tag{4}$$

This kernel is proportional to the probability that a neutron entering collision at $\vec{r}'$ will reach the detector at $\vec{r}$ without another collision. It is now assumed that the corresponding probability current J(R) can be given by a diffusion approximation,

$$J(R) = -D\,\vec{\Omega}_R \cdot \vec{\nabla}_R K(R) = -D \frac{dK}{dR} \tag{5}$$

where D is the diffusion coefficient. The probability current J(R) flows only in a direction toward the detector at $\vec{r}$; i.e. the probability flow in the opposite direction from the detector is zero due to the definition of the kernel K(R). Thus $J(R_1)$ can be represented as:

$$J(R_1) = \frac{K(R_1)}{2} = \left.\frac{dK}{dR}\right|_{R_1} \tag{6}$$

Inside the radius R_1, the scalar K(R) is approximated by a linear function $\Psi(R)$ consistent with the diffusion approximation at the surface of a blackbody.

$$K(R < R_1) = \Psi(R) = \Psi_0 + R \frac{dK}{dR} \tag{7}$$

Combining Equations (6) and (7)

$$\Psi_0 + R_1 \left.\frac{dK}{dR}\right|_{R_1} = -2D \left.\frac{dK}{dR}\right|_{R_1} \quad . \tag{8}$$

Equation (8) represents a forward extrapolation of the function K(R) to the detector point.

$$\Psi_0 = -(2D + R_1) \left.\frac{dK}{dR}\right|_{R_1} \tag{9}$$

$$\text{where} \quad \left.\frac{dK}{dR}\right|_{R_1} = -\frac{(\Sigma R_1 + 2)}{R_1} K(R_1) \;. \tag{10}$$

$$\Psi_0 = (2D+R_1)(\Sigma R_1+2) \frac{\ell^{-\Sigma R_1}}{4\pi R_1^3} \tag{11}$$

A bounded non-linear representation for $\Psi(R<R_1)$ which is similar to K(R) is

$$\Psi(R<R_1) = \frac{\ell^{-\Sigma R}}{4\pi(R^2+\varepsilon^2)} \;. \tag{12}$$

Combining Equations (11) and (12) and solving for ε^2 as $R \to 0$,

$$\varepsilon^2 = \frac{1}{4\pi\Psi_0} \tag{13}$$

where Ψ_0 is given by Equation (11). Equation (12) is discontinuous to K(R) at the radius R_1 where the probability current J(R) was evaluated. A normalization factor β will force continuity.

$$\Psi(R<R_1) = \frac{\beta \; \ell^{-\Sigma R}}{4\pi(R^2+\varepsilon^2)} \tag{14}$$

where

$$\beta = \frac{R_1^2 + \varepsilon^2}{R_1^2} \;. \tag{15}$$

In the energy dependent case, the cross sections in Equations (11) and (14) are evaluated at the exit energy E from the collision. The bounded point flux estimator from Equation (4) corresponding to the i^{th} collision in Equation (3) is

$$\phi_i\big|_{R<R_1} = W_i \frac{\Sigma_s(E')}{\Sigma(E')} \quad P(\vec{\Omega}_{Ri}, E' \to E) \quad \frac{\beta \quad e^{-\Sigma(E)R_i}}{4\pi(R_i^{\,2}+\varepsilon^2)} \tag{16}$$

$$\phi_i\big|_{R\geq R_1} = W_i \frac{\Sigma_s(E')}{\Sigma(E')} \quad P(\vec{\Omega}_{Ri}, E' \to E) \quad \frac{e^{-\Sigma(E)R_i}}{4\pi R_i^{\,2}} \quad . \tag{17}$$

The radius R_1 at which Equation (11) is evaluated has not been specified. A simplified Monte Carlo program for a monoenergetic point source in a two-region spherical geometry with isotropic scattering was written to test the effectiveness of Equation (16) and (17). The point detector was located at a radius ρ from the source on the boundary between the two regions. A dimensionless parameter $\alpha = \Sigma R_1$ was defined, then $R_1 = \alpha/\Sigma$. Problems were run for 4 x 10^4 source histories and a wide variety of absorption to scatter ratios in the two regions indicate that the most consistent results are obtained for $\alpha < 0.1$. For $\alpha = 0.1$ and $\Sigma = 1.0$, $R_1 = 0.1$ cm. For these parameters, Ψ_0 is 116.0/cm^2-sec and $\beta = 1.069$. Typical results for the collided plus uncollided flux are presented in Table 1. An analytic solution[6] as well as results for the NEE estimator are also presented in Table 1. Since α is so small, it is difficult to obtain random collisions within the radius of 0.1 cm where Equation (16) is effective. The detector was deliberately moved to the vicinity of a collision point in several repeated problems to demonstrate the effectiveness of Equation (16). The very high flux from the NEE estimator for the second case in Table 1 is such a result. The total number of "hits" within the radius R_1 is also given in Table 1.

REFERENCES

1. M. H. Kalos, Nucl. Sci. Eng., 16, 111 (1963).

2. H. J. Kalli and E. D. Cashwell, "Evaluation of Three Monte Carlo Estimation Schemes for Flux at a Point", LA-6865-MS, LASL (1977).

3. H. A. Steinberg and M. H. Kalos, Nucl. Sci. Eng., 44, 406 (1971).

4. H. Iida and Y. Seki, Nucl. Sci. Tech. 17, 4 (1980).

5. G. I. Bell and S. Glasstone, "Nuclear Reactor Theory", Chapt 1, p. 25, Van Nostrand Reinhold Company, New York (1970).

6. A. M. Weinberg and E. P. Wigner, "The Physical Theory of Neutron Chain Reactors", Chapt. 8, p. 200, University of Chicago Press, Chicago (1958).

TABLE 1. MONTE CARLO RESULTS FOR POINT SOURCE AND α = 0.1

ρ (cm)	Σ_{a1}	Σ_{s1}	Σ_{a2}	Σ_{s2}	Hits	ϕ EXACT	ϕ NEE	ϕ NEED*
.71064	.2	.8	.5	.5	40	0.17668	0.1707±1.1%	.1704±1.1%
.71064	.2	.8	.2	.8	59	0.20878	2.5×10^9	.20793±1.46%
1.2	.1	.9	.1	.9	23	0.10208	0.10016±1.97%	0.098966±1.56%
2.0	.1	.9	.1	.9	7	0.03699	0.03793±4.67%	0.03631±3.06%

* ϕ NEED is the estimator by Equations (16) and (17).