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MONTE CARLO ZERO-VARIANCE SCHEMES: THEORY, DEMONSTRATION AND PRACTICAL CONSEQUENCES

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ABSTRACT

Zero-variance Monte Carlo schemes are known for a wide class of estimators, among which the last-event, the collision, and the track-length estimator. For a special energy-dependent space-independent slowing-down model and a modified 1-D energy-independent transport model the scheme for the collision estimator is numerically demonstrated and some features are highlighted. It shows, amongst others, that the statistical particle weight does not behave inversely proportional to the importance function at the collision sites, but can have arbitrarily small values. Another proof is given for the existence of zero-variance schemes for two commonly used estimators: the surface-crossing estimator and the track-length estimator. It is shown that for these estimators biasing of the transport equation with an adjoint function different from the one commonly used is required. For these schemes also a numerical demonstration is given. Although zero-variance schemes can not be applied in practical applications, we can learn from them for devising effective variance reduction methods. Current automated variance reduction methods using weight windows are discussed in the light of zero-variance schemes. It is concluded that current methods, although successful, are not well founded and can be improved for the surface-crossing and track-length estimators.

Key Words: Monte Carlo, zero variance, variance reduction, weight window

1. INTRODUCTION

Monte Carlo calculations are very popular for accurate estimation of detector responses of any kind, as virtually no approximations are needed of the neutron or photon transport model and the system geometry. However, an inherent drawback of the Monte Carlo method is that one obtaines a statistical estimate of the requested quantity with a certain statistical imprecision. In this respect a zero-variance Monte Carlo calculation seems to be a contradictio in terminis. Nonetheless, it turns out to be possible to compose a sampling scheme that results in a zero variance, i.e. every particle history will result in the same score. As we will see later, this does not mean that every history must be identical.

A zero-variance calculation seems to be the ideal form of a Monte Carlo calculation, but it takes its price. To apply the zero-variance sampling scheme one has to have a lot of information of the problem in advance. This information includes the required answer itself and this makes a zero-variance scheme only a theoretical possibility. However, instead of solving the problem first before devising a zero-variance sampling scheme, one can try to approximate the zero-variance scheme in the hope of a considerable variance reduction compared to a straight-forward

sampling of the transport model for the problem at hand. This makes it worth to study zero-variance Monte Carlo games.

A zero-variance sampling scheme was already mentioned by Kahn [1]. He showed that biasing the transport equation with the importance function and using a last-event estimator, i.e. scoring takes place only when the particle history is terminated by absorption, a zero-variance is obtained. In later years the existence of a zero-variance scheme for the more commonly used collision estimator was proven [2-4]. This requires biasing by the same importance function, but also the use of a weight factor to account for the normalization of the biased transport kernel. Later on Dwivedi [5] showed the existence of zero-variance schemes for other estimators, including the track-length estimator, with a proof based on the use of the moments equations [6]. He also showed that there can exists more than one zero-variance scheme for the same estimator and that it is possible to apply separate biasing of the transition kernel for selecting a new collision site and the collision kernel for selecting a new energy and direction after scattering. Gupta [7] generalized this work to a whole class of zero-variance schemes including all current estimators. Finally Booth [8] proved that for any linear Monte Carlo process a zero-variance scheme exists, but then the random number distributions must be weighted instead of the transport kernel.

In this paper we shall briefly describe the derivation of the classical zero-variance collision estimator. To learn from these sampling schemes for practical situations it is important to see how they actually work out in a concrete situation. For application of the zero-variance scheme the adjoint function of the problem is needed in closed analytical form. Therefore, it is only possible to implement the zero-variance scheme for a few simplified cases. We will derive and apply the zero-variance scheme for the case of a slowing-down problem with a hydrogen-like material in an infinite, space-independent system and for a monoenergetic, one-dimensional problem with a slightly modified transport model to make the problem analytically tractable.

Nowadays, in general purpose Monte Carlo codes neither the last-event nor the collision estimators are available. Instead, the surface-crossing and/or track-length estimators are offered. Using the same theoretical framework as for the collision estimator we will show that for both the track-length and the surface-crossing estimators a zero-variance sampling scheme using biasing with the adjoint function can be derived and practical demonstrations will be given. However, this adjoint function differs in definition from that for the zero-variance collision estimator. Finally, some comments will be made about current variance reduction methods included in general purpose Monte Carlo codes and some lessons that can be learned in this respect from zero-variance schemes.

2. THEORY OF THE ZERO-VARIANCE COLLISION ESTIMATOR

Although there are many ways to reduce the variance of Monte Carlo calculation, we will concentrate here on transformations of the original problem in a specific way, which is called biasing. We first look at the mathematical description of the Monte Carlo calculation and biasing of the sampling process.

The collision density $\psi(P)$ of neutrons or photons at a point $P=(\boldsymbol{r},E,\boldsymbol{\Omega})$ in the phase space, with $\boldsymbol{r}$ the position coordinates, E energy and $\boldsymbol{\Omega}$ the particle direction, is given by the integral equation

$$\psi(P) = S_1(P) + \int K(P' \to P)\psi(P')dP', \tag{1}$$

with S_1 the source of first collisions (not to be confused with the actual particle source S) and K the transport kernel defined such that $K(P' \to P)dP$ is the probability of a particle going into a collision at P' to have its next collision in dP at P.

Suppose that the aim of the Monte Carlo calculation is to calculate the response of a (physical or hypothetical) detector according to

$$R = \int \eta(P)\psi(P)dP, \tag{2}$$

with η the detector response function with respect to the collision density ψ.

Looking for variance reduction, we can alter the Monte Carlo game and/or the estimator. Here we consider density biasing [9], i.e. changing the probability densities from which (first or) next collision points are sampled in such a way that the required detector response R is still correctly obtained. If the source function is multiplied by an everywhere positive function $I(P)$, normalized to

$$\int I(P)S_1(P)dP = 1, \tag{3}$$

we select a first-collision point P_1 from the probability density function (pdf) $\overline{S}_1(P_1) = I(P_1)S(P_1)$ and correct for not sampling the right pdf by introducing an initial particle weight

$$w(P_1) = \frac{S_1(P_1)}{\overline{S}_1(P_1)} = \frac{1}{I(P_1)}. \tag{4}$$

A next collision point is sampled from the biased transport kernel

$$\overline{K}(P' \to P) = \frac{I(P)K(P' \to P)}{I(P')}, \tag{5}$$

and we have to correct the particle weight for not sampling the right kernel by

$$w(P) = w(P')\frac{K(P' \to P)}{\overline{K}(P' \to P)} = w(P')\frac{I(P')}{I(P)}. \tag{6}$$

Together with Eq.(4) we see that at every collision point

$$w(P) = \frac{1}{I(P)}. \tag{7}$$

There is another way to interpret the biased Monte Carlo simulation. Multiplication of Eq.(1) by the biasing function $I(P)$ leads to a new transport equation for a particle density $\overline{\psi}(P) = I(P)\psi(P)$ with a source of first collisions $\overline{S}_1(P_1) = I(P_1)S(P_1)$ and particle transport properties defined by the kernel $\overline{K}(P)$ of Eq.(5). Then the required detector response R is obtained if the detector response function is taken as $\overline{\eta}(P) = \eta(P)/I(P)$. In this Monte Carlo game the statistical weight is unity at all collisions.

As the altered transport kernel $\overline{K}(P' \rightarrow P)$ is, in general, not normalized to unity, we have to account for the normalization factor $\overline{\kappa}(P')$

$$\overline{\kappa}(P') = \int \overline{K}(P' \rightarrow P) dP. \tag{8}$$

This factor can be seen as a fictitious non-absorption probability and with probability $\overline{\mu}(P) = 1 - \overline{\kappa}(P)$ the history will be terminated. Another possibility is taking this factor into account by using it as a multiplication factor for the statistical weight of the particle and a next collision site is sampled from the normalized altered transport kernel $\overline{K}(P' \rightarrow P)/\overline{\kappa}(P')$.

It has been shown before [1-4] both for the last-event estimator and the collision estimator that the optimum choice for the biasing function is

$$I_{opt}(P) = \frac{\psi^+(P)}{R}, \tag{9}$$

with $\psi^+(P)$ the solution of the equation adjoint to Eqs.(1) and (2)

$$\psi^+(P) = \eta(P) + \int K(P \rightarrow P')\psi^+(P')dP'. \tag{10}$$

For a zero-variance collision estimator a necessary additional condition is to use the normalization factor $\overline{\kappa}(P')$ of the biased kernel as an additional weight factor. Then the particle weight at collision i also depends on all previous collision points:

$$\overline{w}_i = \overline{w}(P_1, P_2, ..., P_i) = \overline{\kappa}(P_1)\overline{\kappa}(P_2)...\overline{\kappa}(P_{i-1})\frac{R}{\psi^+(P_i)}. \tag{11}$$

As a history will never terminate the collision estimator becomes

$$\widehat{R}_{col} = \sum_{i=1}^{\infty} \overline{\kappa}(P_1)\overline{\kappa}(P_2)...\overline{\kappa}(P_{i-1})\frac{\eta(P_i)}{\psi^+(P_i)}R. \tag{12}$$

With the optimum choice of the biasing function according to Eq.(9) we have with Eq.(10)

$$\bar{\kappa}(P') = \int \overline{K}(P' \to P)dP' = \frac{1}{\psi^+(P)} \int K(P' \to P)\psi^+(P')dP' = 1 - \frac{\eta(P)}{\psi^+(P)}. \tag{13}$$

If we calculate $1 - \hat{R}_{col} / R$ we find

$$\begin{aligned} 1 - \hat{R}_{col} / R &= 1 - \frac{\eta(P_1)}{\psi^+(P_1)} - \bar{\kappa}(P_1)\frac{\eta(P_2)}{\psi^+(P_2)} - \bar{\kappa}(P_1)\bar{\kappa}(P_2)\frac{\eta(P_3)}{\psi^+(P_3)} - \ldots \\ &= \bar{\kappa}(P_1)\left[1 - \frac{\eta(P_2)}{\psi^+(P_2)} - \bar{\kappa}(P_2)\frac{\eta(P_3)}{\psi^+(P_3)} - \ldots\right] = \bar{\kappa}(P_1)\bar{\kappa}(P_2)\bar{\kappa}(P_3)\ldots = 0, \end{aligned} \tag{14}$$

as for an infinite number of collision points $\bar{\kappa} < 1$. Hence, $\hat{R}_{col} = R$ for each history, which proves the existence of a zero-variance collision estimator. As infinitely long histories are impractical, we have to apply a Russian roulette to terminate a history below a certain weight boundary. As this weight boundary can be made arbitrarily small it will no longer affect the variance of the calculation within the computer word length accuracy.

3 DEMONSTRATION OF THE ZERO-VARIANCE SCHEME

As the zero-variance sampling scheme requires, amongst others, manipulation of the transport kernel with the adjoint function, the adjoint function must be known analytically and it must be possible to sample the resulting biased kernel. Therefore the cases where this applies are very limited. We treat here two different cases. First, a space-independent slowing-down problem and second, an energy-independent one-dimensional modified transport problem.

3.1. Slowing-Down Example

We consider a space-independent neutron slowing-down problem in a hydrogen-like material with constant scattering and absorption cross sections Σ_s and Σ_a, respectively. The mass of the scattering nuclide must be equal to that of a neutron to avoid the well-known Placzek oscillations [10] in the energy dependence of the slowing-down spectrum, which would complicate the analytical work enormously. For a hydrogen-like material the scattering kernel with isotropic scattering is $K(P' \to P) = K(E' \to E) = \Sigma_s / (E'\Sigma_t)$ for $E < E'$ and zero else. If we take for simplicity a monoenergetic source $S(E) = S\delta(E - E_0)$ the slowing-down equation reads

$$\psi(E) = S\delta(E - E_0) + \frac{\Sigma_s}{\Sigma_t} \int_E^{E_0} \psi(E')\frac{dE'}{E'}. \tag{15}$$

By differentiating with respect to E and solving the resulting differential equation we find the following solution

$$\psi(E) = S\left\{\frac{\Sigma_s}{\Sigma_t}\frac{1}{E_0}\left(\frac{E_0}{E}\right)^{\frac{\Sigma_s}{\Sigma_t}} + \delta(E - E_0)\right\}. \tag{16}$$

Suppose we are interested in the neutron flux over the energy range from E_- to E_+. Then the detector response function is $\eta(E)=1/\Sigma_t$ for the energy range $E_-\leq E\leq E_+$ and zero else. The adjoint equation is given by

$$\psi^+(E) = \eta(E) + \frac{\Sigma_s}{\Sigma_t}\frac{1}{E}\int_{E_-}^{E}\psi^+(E')dE'. \tag{17}$$

Multiplication by E and differentiation with respect to E leads to a differential equation, from which we obtain the adjoint function for detecting the neutron flux over an energy range as

$$\psi^+(E) = \begin{cases} \dfrac{\Sigma_s}{\Sigma_a\Sigma_t}\left\{1-\left(\dfrac{E_-}{E}\right)^{\frac{\Sigma_a}{\Sigma_t}}\right\} + \dfrac{1}{\Sigma_t} & E_- \leq E \leq E_+ \\ \dfrac{\Sigma_s}{\Sigma_a\Sigma_t}\left\{\left(\dfrac{E_+}{E}\right)^{\frac{\Sigma_a}{\Sigma_t}} - \left(\dfrac{E_-}{E}\right)^{\frac{\Sigma_a}{\Sigma_t}}\right\} & E > E_+. \end{cases} \tag{18}$$

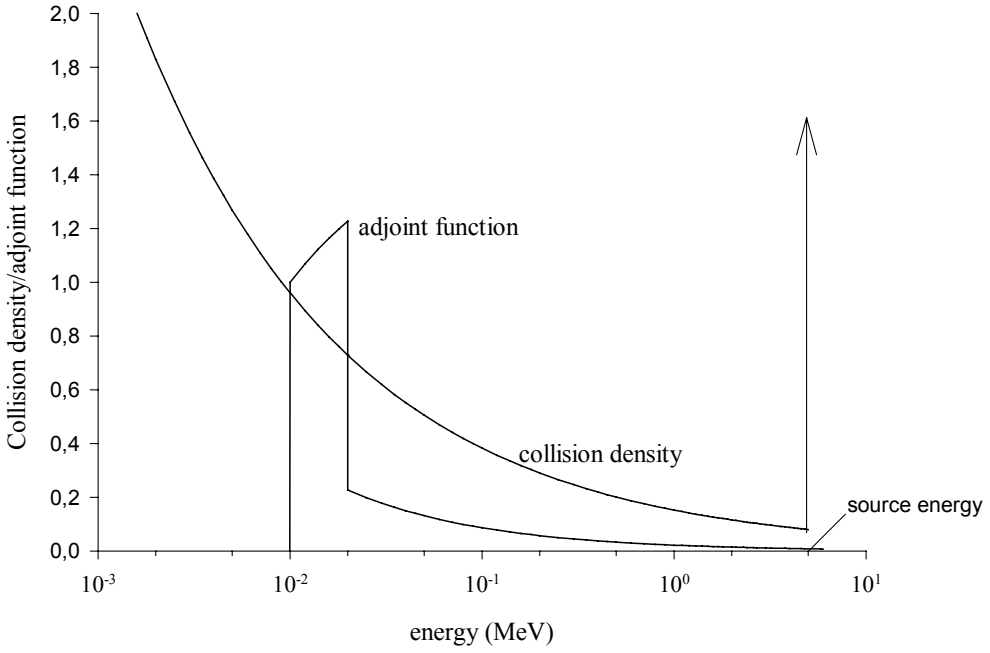

Figure 1. Collision density and adjoint function

Fig. 1 shows the energy dependence of the neutron collision density and the adjoint function. The detector response as obtained either by averaging the neutron collision density over the detector response function or averaging the adjoint function over the neutron source is for the case $E_0>E^+$

$$R = S\frac{\Sigma_s}{\Sigma_a\Sigma_t}\left\{\left(\frac{E_+}{E_0}\right)^{\frac{\Sigma_a}{\Sigma_t}} - \left(\frac{E_-}{E_0}\right)^{\frac{\Sigma_a}{\Sigma_t}}\right\}. \tag{19}$$

Because of the δ-function the source is not affected by biasing with the adjoint function. The biased kernel $\overline{K}(E'\to E) = K(E'\to E)\psi^+(E)/\psi^+(E')$ becomes for $E_-<E'<E_+$

$$\overline{K}(E'\to E) = \frac{\Sigma_s}{\Sigma_t}\frac{1}{E'}\frac{1+\frac{\Sigma_s}{\Sigma_a}\left[1-\left(\frac{E_-}{E}\right)^{\frac{\Sigma_a}{\Sigma_t}}\right]}{1+\frac{\Sigma_s}{\Sigma_a}\left[1-\left(\frac{E_-}{E'}\right)^{\frac{\Sigma_a}{\Sigma_t}}\right]} \qquad E_- < E < E'. \tag{20}$$

and for $E'>E_+$

$$\overline{K}(E'\to E) = \begin{cases} \dfrac{\Sigma_a}{\Sigma_t}\dfrac{1}{E'}\dfrac{1+\frac{\Sigma_s}{\Sigma_a}\left[1-\left(\frac{E_-}{E}\right)^{\frac{\Sigma_a}{\Sigma_t}}\right]}{\left(\frac{E_+}{E'}\right)^{\frac{\Sigma_a}{\Sigma_t}} - \left(\frac{E_-}{E'}\right)^{\frac{\Sigma_a}{\Sigma_t}}} & E_- < E < E_+ \\ \dfrac{\Sigma_s}{\Sigma_t}\dfrac{1}{E'}\dfrac{\left(\frac{E_+}{E}\right)^{\frac{\Sigma_a}{\Sigma_t}} - \left(\frac{E_-}{E}\right)^{\frac{\Sigma_a}{\Sigma_t}}}{\left(\frac{E_+}{E'}\right)^{\frac{\Sigma_a}{\Sigma_t}} - \left(\frac{E_-}{E'}\right)^{\frac{\Sigma_a}{\Sigma_t}}} & E_+ < E < E' \end{cases} \tag{21}$$

The weight factor at each collision becomes

$$\overline{\kappa}(E') = 1-\frac{\eta(E')}{\psi^+(E')} = 1-\frac{1}{1+\frac{\Sigma_s}{\Sigma_a}\left[1-\left(\frac{E_-}{E'}\right)^{\frac{\Sigma_a}{\Sigma_t}}\right]} \qquad E_- \le E' \le E_+ \tag{22}$$

and equal to 1 for $E'>E_+$. To sample a new energy E from $\overline{K}(E'\to E)$ we have to calculate the cumulative distribution function and solve E from

$$\rho = \int_{E'}^{E} \overline{K}(E' \rightarrow E'')dE'', \tag{23}$$

with ρ a random number with a uniform distribution between 0 and 1. The integral in Eq.(23) can be calculated analytically and the energy E solved explicitly. For the case $E'>E_+$ and $E_+<E<E'$ it must be solved by iteration.

For a numerical simulation a source energy of E_0=5 MeV was taken and the detector energy range to calculate the adjoint is from 0.01 to 0.02 MeV. Further, Σ_s=0.4 cm^{-1} and Σ_a=0.6 cm^{-1}. Then the detector response from Eq.(19) is R=0.00825919640 per source neutron.

Table I. Flux estimates for various values of the lower bound of Russian roulette

weight lower bound	Flux (cm^{-1})	standard deviation (%)
10^{-1}	8.242 10^{-3}	0.096
10^{-2}	8.2597 10^{-3}	0.010
10^{-3}	8.25923 10^{-3}	0.00093
10^{-4}	8.259195 10^{-3}	0.00009
10^{-5}	8.2591967 10^{-3}	0.000008
10^{-6}	8.25919628 10^{-3}	0.0000008
10^{-7}	8.25919641 10^{-3}	0.0000002
10^{-8}	8.25919640 10^{-3}	0.00000009

To terminate each history a Russian roulette was used. As the lower bound for the particle weight influences the variance of the calculation, we used various bounds to demonstrate the asymptotic behavior for low values of the lower bound. The upper bound of the weight window was always twice as large. It is not our intention to discuss the value of the standard deviation for a given value of the Russian roulette parameters. The Russian roulette is used only to show the limit behavior for very low weight boundaries. Table I shows the results of Monte Carlo simulations with 1000 particle histories for the estimation of the particle flux between 0.01 and 0.02 MeV. The table clearly shows that the resulting standard deviation is due to the Russian roulette used to terminate histories and that the standard deviation can be made as small as the computer word length accuracy allows.
Table II shows the flux estimates for various energy ranges, first without any biasing of the collision kernel and next with optimum biasing for the flux in the energy range from 0.01 to 0.02 MeV. For both calculations the lower bound of the weight window was chosen as 10^{-5}. From this table one can see that optimum biasing for the range from 0.01 to 0.02 MeV also helps for energy ranges just above, but that the variance becomes larger than for the standard case for energy ranges much above 0.02 MeV. As biasing of the collision kernel with the adjoint function $\psi^+(E)$ prohibits selection of energies after scattering where the adjoint function is zero, in the biased kernel calculation we can not estimate fluxes below 0.01 MeV.

Table II. Flux estimates for various energy ranges without biasing and with optimum biasing for the range 0.01-0.02 MeV

energy range (MeV)	theoretical	no biasing		optimum biasing	
	flux (cm^{-1})	flux (cm^{-1})	st. deviation (%)	flux (cm^{-1})	st. deviation (%)
2.0 - 1.5	0.060991	0.06101	0.68	0.06085	0.93
1.0 - 1.5	0.069908	0.07008	0.61	0.07053	0.78
0.5 – 1.0	0.086361	0.08671	0.52	0.08640	0.60
0.2 - 0.5	0.070822	0.07066	0.54	0.07048	0.53
0.1 - 0.2	0.032880	0.03292	0.75	0.03309	0.60
0.05 – 0.1	0.021693	0.02157	0.86	0.02158	0.61
0.02 – 0.05	0.017790	0.01784	0.89	0.01789	0.53
0.01 – 0.02	0.0082592	0.008401	1.18	0.0082592	0.00
0.005 – 0.01	0.0054490	0.005436	1.36		
0.002 – 0.005	0.0044686	0.004476	1.41		
0.001 – 0.002	0.0020746	0.002074	1.84		

3.2. Slowing-Down Example

Even for a monoenergetic one-dimensional plane geometry transport case the solution is too complicated to handle for biasing the transport kernel. We therefore chose the following modification of the transport process. A particle can only move into the $+X$ and $-X$ direction. In that case equations can be derived from the integro-differential transport equation for the fluxes in the $+X$ and $-X$ direction. If both directions are equally probable in a collision or a source event, these equation can be added up to give the total flux $\phi(x)$ by

$$-\frac{d}{dx}\frac{1}{\Sigma_t(x)}\frac{d\phi(x)}{dx}+\Sigma_a(x)\phi(x)=S(x). \tag{24}$$

This transport model has the advantage that is described by a diffusion equation, which can be solved for many cases. The model was already used by Hoogenboom [11] for demonstration of a zero-variance sampling scheme for the adjoint equation. It is also mentioned by Cramer [12] in his recent overview of analytically solvable cases of particle transport.

For our numerical demonstration of the existence of the zero-variance collision estimator we will adopt an infinite system with constant cross sections and a source of the form

$$S(x)=\frac{1}{2}\alpha e^{-\alpha|x|}, \tag{25}$$

with α a parameter. The solution of the collision density $\psi(x)=\Sigma_t\phi(x)$ is

$$\psi(x) = \frac{1}{2}\frac{\alpha\Sigma_t^2}{\Sigma_a\Sigma_t - \alpha^2}\left\{e^{-\alpha|x|} - \frac{\alpha}{\sqrt{\Sigma_a\Sigma_t}}e^{-\sqrt{\Sigma_a\Sigma_t}|x|}\right\}. \quad (26)$$

Suppose the aim of our calculation is to calculate the averaged particle flux for the region $|x| \le a$. Then the detector response function $\eta(x)$ is equal to $1/(2a\Sigma_t)$ for $-a \le x \le a$, leading to the detector response

$$R = \frac{1}{2a\Sigma_a}\left\{1 + \frac{\alpha^2}{\Sigma_a\Sigma_t - \alpha^2}e^{-\sqrt{\Sigma_a\Sigma_t}a} - \frac{\Sigma_a\Sigma_t}{\Sigma_a\Sigma_t - \alpha^2}e^{-\alpha a}\right\}. \quad (27)$$

For the integral description of the problem the transport kernel K becomes

$$K(x' \to x) = \frac{\Sigma_s}{\Sigma_t}T(x' \to x) = \frac{1}{2}\Sigma_s e^{-\Sigma_t|x-x'|}, \quad (28)$$

with $T(x' \to x)$ the transition kernel and the collision kernel reduced to the scattering probability Σ_s/Σ_t. The factor ½ shows up because of equal probabilities for the particle going into the positive or negative direction. The source of first collisions $S_1(x)$ is

$$S_1(x) = \frac{1}{2}\frac{\alpha\Sigma_t}{\Sigma_t^2 - \alpha^2}\left\{\Sigma_t e^{-\alpha|x|} - \frac{\alpha}{\sqrt{\Sigma_a\Sigma_t}}e^{-\sqrt{\Sigma_a\Sigma_t}|x|}\right\}. \quad (29)$$

Now the solution of the collision density from the integral equation

$$\psi(x) = S_1(x) + \int K(x' \to x)\psi(x')dx' \quad (30)$$

can be verified.
For the choices α=0.25 cm^{-1}, Σ_t=1 cm^{-1} and Σ_s=0.4 cm^{-1} Table III shows the results of a standard Monte Carlo calculation with a collision estimator for calculating the average flux per source

Table III. Flux values averaged over a region with capture treated analog or implicitly

half width a of flux detector region (cm)	theoretical flux	analog capture		implicit capture	
		flux	st. dev. (%)	flux	st. dev. (%)
0.1	0.15745	0.1495	1.88	0.1578	1.57
0.5	0.15638	0.1521	0.91	0.1561	0.75
1.0	0.15353	0.1505	0.67	0.1538	0.55
2.0	0.14485	0.1442	0.48	0.1449	0.38
4.0	0.12387	0.1240	0.34	0.1237	0.24
6.0	0.10445	0.1046	0.28	0.1044	0.17
8.0	0.088455	0.0887	0.25	0.0885	0.12
10.0	0.075702	0.0758	0.23	0.0757	0.09

neutron for the region $|x|<a$ for increasing values of a. In one calculation capture is treated in an analog way. In the other calculation implicit capture is used, combined with Russian roulette to terminate histories, but with a very low lower bound for the statistical weight, in order to exclude the effect of the Russian roulette to the variance.

The equation adjoint to Eq.(30) for the detector response function $\eta(x)$ reads

$$\psi^+(x) = \eta(x) + \int K(x \to x')\psi^+(x')dx', \tag{31}$$

where we note that the transport kernel is self-adjoint for this case. The solution of the adjoint equation is

$$\psi^+(x) = \begin{array}{ll} \dfrac{1}{2a\Sigma_a}\left\{1 - \dfrac{\Sigma_s}{\Sigma_t} e^{-\sqrt{\Sigma_a\Sigma_t}a} \cosh\sqrt{\Sigma_a\Sigma_t}x\right\} & |x| \le a \\ \dfrac{1}{2a\Sigma_a}\dfrac{\Sigma_s}{\Sigma_t}\sinh\sqrt{\Sigma_a\Sigma_t}a \; e^{-\sqrt{\Sigma_a\Sigma_t}|x|} & |x| > a. \end{array} \tag{32}$$

Figure 2 shows the collision density and the adjoint function for this case.

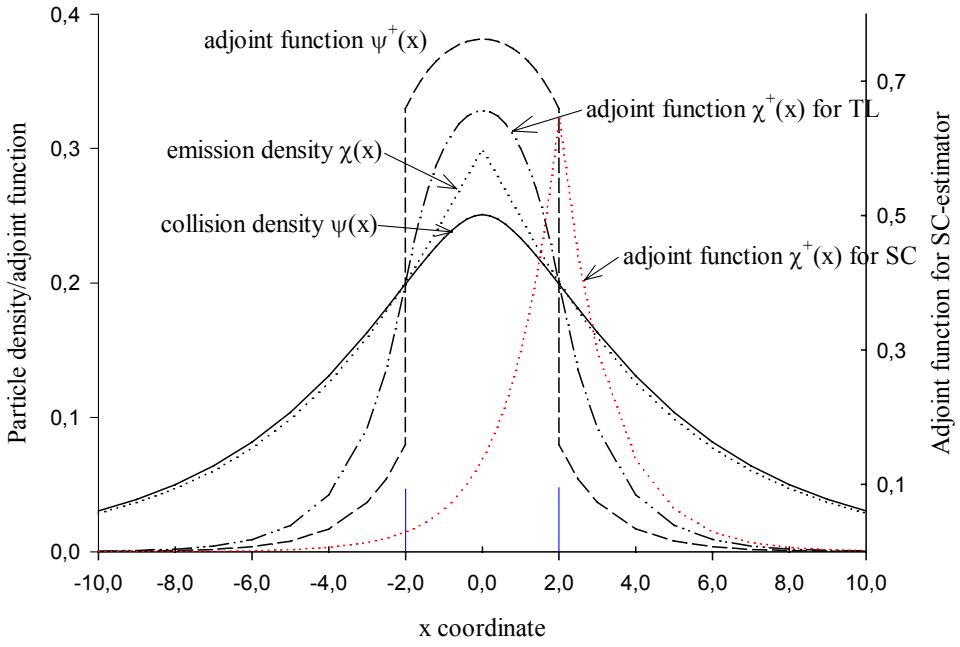

Figure 2. Various functions for the 1-D transport example

For the zero-variance collision estimator we have to bias the source of first collisions $S_1(x)$ and the transport kernel $K(x' \rightarrow x)$ with $\psi^+(x)/R$. For sampling the biased first-collision source $\overline{S}_1(x) = S_1(x)\psi^+(x)/R$ we see that this function is symmetric with respect to x=0 and we can select a value of x in the range $0<x<\infty$ and then with probability ½ accept $-x$ as the starting position. As the analytic expression of $\overline{S}_1(x)$ differs for $0<x<a$ and $x>a$ the probability for having a value of x in the range $0<x<a$ must be calculated from

$$P_{0<x<a} = 2\int_0^a \overline{S}_1(x)dx, \tag{33}$$

and then solve the equation

$$\rho = \frac{2}{P_{0<x<a}} \int_0^x \overline{S}_1(x')dx', \tag{34}$$

with ρ a random number uniformly distributed between 0 and 1. Because several exponential terms show up in the integral, this equation must be solved iteratively. The same holds for the range $x>a$. Use of a formula manipulating program like MAPLE [13] was found a great help in working out the analytical formulas.

To sample the biased transport kernel the situation is even more complicated. Suppose $x'>0$. Then we have to distinguish three ranges for x: $-\infty<x<-a$, $-a<x<a$ and $x>a$. Depending on the value of x' we must further split up the last two regions. If $0<x'<a$ we have to consider the regions $-a<x<x'$ and $x'<x<a$, and if $x'>a$ we have to split up the last region into $a<x<x'$ and $x'<x<\infty$. For all these regions the probability of selecting that region must be calculated. When a region is selected with the proper probability the value of x must be sampled from an equation analogous to Eq.(34). As the formulas concerned are rather lengthy they are not given here, but can be found in a separate report [14].

Table IV shows the results for the averaged flux for the region up to a=2 cm for various values of the lower bound of the Russian roulette. This clearly demonstrates the zero-variance character of biasing scheme.

Table IV. Collision estimator results with decreasing lower bounds

weight lower bound	flux	st. dev. (%) N=1000
10^{-1}	0.1455	0.33
10^{-2}	0.14483	0.033
10^{-3}	0.144860	0.0035
10^{-4}	0.1448517	0.00036
10^{-5}	0.14485110	0.000037
10^{-6}	0.144851019	0.0000035
10^{-7}	0.144851015	0.00000037

4. THEORETICAL CALCULATION OF THE VARIANCE

In practice the variance (or standard deviation) of the result of a Monte Carlo calculation will be estimated from the scores of all particle histories contributing to the desired quantity. However, Coveyou et al. [9] introduced a simple and elegant way to calculate the variance theoretically. This requires the solution of an equation probably more complicated than the one to be solved originally, but for theoretical purposes it is very useful. We will apply this method for showing that other estimators and sampling schemes exists with a zero variance.

We therefore restrict ourselves to the case of sampling a first collision point from the biased source distribution $\overline{S}_1(P) = S_1(P)I(P)$ and sampling a next collision point from the normalized biased transport kernel $\overline{K}_n(P' \to P) = \overline{K}(P' \to P)/\overline{\kappa}(P')$. For a fair game the initial weight of the source particle is set to $1/I(P)$ and at every collision the particle weight is multiplied by the normalization factor $\overline{\kappa}(P')$ of the biased kernel and a factor $I(P')/I(P)$ to account for not sampling the original kernel $K(P' \to P)$.

Following Coveyou et al. [9] we define $\overline{\xi}(P)$ as the present and future contribution of a particle having a collision at P to the estimator considered. Then we have

$$\overline{\xi}(P) \overset{distr}{=} \eta(P) + \overline{\kappa}(P)\frac{I(P)}{I(P')}\overline{\xi}(P'), \tag{35}$$

with P' the next collision point and *distr* meaning equality in the sense of equal distributions. The expected value of $\overline{\xi}(P)$ is

$$\begin{aligned} W(P) &= \left\langle \overline{\xi}(P) \right\rangle = \int \overline{K}_n(P \to P') \left\langle \eta(P) + \overline{\kappa}(P)\frac{I(P)}{I(P')}\overline{\xi}(P') \right\rangle dP' \\ &= \eta(P) + \int \overline{K}(P \to P')\frac{I(P)}{I(P')}W(P')dP' = \eta(P) + \int K(P \to P')W(P')dP'. \end{aligned} \tag{36}$$

Comparison with Eq.(10) shows that $W(P)=\psi^+(P)$. The expected value of the estimator is

$$\left\langle \hat{R} \right\rangle = \int \left\langle \xi(P) \right\rangle \frac{1}{I(P)}\overline{S}_1(P)dP = \int \psi^+(P)S_1(P)dP = R. \tag{37}$$

Hence the estimator is indeed unbiased. The expected squared contribution at P is

$$\begin{aligned} Q(P) &= \left\langle \xi^2(P) \right\rangle = \int \overline{K}_n(P \to P') \left\langle \left\{ \eta(P) + \overline{\kappa}(P)\frac{I(P)}{I(P')}\xi(P') \right\}^2 \right\rangle dP' \\ &= \eta^2(P) + 2\eta(P)\int K(P \to P')W(P')dP' + \overline{\kappa}(P)\int \overline{K}(P \to P')\frac{I^2(P)}{I^2(P')}Q(P')dP'. \end{aligned} \tag{38}$$

After division by $I^2(P)$ we have

$$\frac{Q(P)}{I^2(P)} = \frac{\eta(P)}{I(P)}\left\{2\frac{W(P)}{I(P)} - \frac{\eta(P)}{I(P)}\right\} + \overline{\kappa}(P)\int \overline{K}(P \to P')\frac{Q(P')}{I^2(P')}dP'. \tag{39}$$

The mean square value of the estimator is

$$\left\langle \hat{R}^2 \right\rangle = \int Q(P)\frac{1}{I^2(P)}\overline{S}_1(P)dP. \tag{40}$$

For the optimum choice of the biasing function $I(P)$ according to Eq.(9) we can see by substitution that $Q(P)/I^2(P)=R^2$ is a solution of Eq.(39) and from Eq.(40) that the estimator has zero variance.

A more general way to calculate the variance of a Monte Carlo calculation is developed by various authors based on the moments equations. This theory is treated in detail in the book of Lux and Koblinger [6].

5. ZERO-VARIANCE SURFACE-CROSSING AND TRACK-LENGTH ESTIMATORS

In modern general purpose Monte Carlo codes like MCNP [15] last-event and collision estimators are not available as they are inferior (at least for a complete analog Monte Carlo calculation) to the track-length estimator for estimating the flux averaged over a certain volume. Apart from the track-length estimator a surface-crossing estimator is normally available for estimating the flux at a surface. It is therefore interesting to see whether a zero-variance sampling scheme exists for these estimators also using the adjoint function for biasing the transport equation. As these estimators feature some basic differences with the collision estimator, the optimum biasing for the collision estimator can not be simply copied.

5.1. The Surface-Crossing Estimator

If in a simulated particle history a collision event happened at position $\boldsymbol{r}$ and the next collision event takes place at $\boldsymbol{r}_n$ and the particle crosses on its flight from $\boldsymbol{r}$ to $\boldsymbol{r}_n$ the surface (or a specific part of that surface) at which the particle current or flux must be calculated, a score is obtained. This estimator can never result in a zero variance, because it depends on the sampled path length whether a particle starting at $\boldsymbol{r}$ that can potentially reach the scoring surface will actually reach that surface. For a zero-variance estimator we need to use the expected value of reaching the scoring surface as the estimator. This leads to an expected-value estimator, i.e. irrespective of the track length actually sampled, the score is set equal to the probability to reach the surface (for a flux estimate this must be divided by the cosine of the angle between the particle flight direction and the normal to the surface). As this estimator assumes a particle leaving a collision (instead of going into a collision as before) the required detector response is given by $R=\int \eta_\chi(P)\chi(P)dP$, with $\chi(P)$ the emission density, i.e. the density of particles leaving a collision or the source and $\eta_\chi(P)$

the expected value of the detector response function with respect to the emission density. The transport equation for the emission density reads

$$\chi(P) = S(P) + \int L(P' \to P)\chi(P')dP', \tag{41}$$

with $L(P' \to P)dP$ the probability for a particle leaving the source or a collision at P' to have its next collision in dP at P. The transport kernel L differs from K because the transition kernel T now comes first and the collision kernel afterwards.

Now, the proposition is that a zero-variance scheme is obtained if we bias the transport equation (41) by the adjoint function and use implicit capture, which means application of a weight factor equal to the normalization of the biased transport kernel. The function adjoint to χ is given by

$$\chi^+(P) = \eta_\chi(P) + \int L(P \to P')\chi^+(P')dP'. \tag{42}$$

The prove that a zero-variance scheme exists if the transport equation (41) is biased by the adjoint function of Eq.(42) and implicit capture is used, is basically the same as for the collision estimator in Sect. 2. The difference is that the expected value of the squared contribution from a phase space point P is given by

$$\frac{Q_\chi(P)}{I^2(P)} = \frac{\eta_\chi(P)}{I(P)}\left\{2\frac{\chi^+(P)}{I(P)} - \frac{\eta_\chi(P)}{I(P)}\right\} + \overline{\kappa}_L(P)\int \overline{L}(P \to P')\frac{Q_\chi(P')}{I^2(P')}dP', \tag{43}$$

while the mean squared value of the estimator is given by

$$\left\langle \hat{R}^2 \right\rangle = \int \overline{Q}(P)\overline{S}(P)dP, \tag{44}$$

with the biased source $\overline{S}$ instead of $\overline{S}_1$. For the biasing function $I(P)$ chosen equal to $\chi^+(P)/R$ the normalization of the biased kernel becomes

$$\overline{\kappa}_L(P) = \int \overline{L}(P \to P')dP' = 1 - \frac{\eta_\chi(P)}{\psi^+(P)}, \tag{45}$$

and by substitution we see again that $Q_\chi(P)/I^2(P)=R^2$ is a solution of Eq.(43), which proves that the variance will be zero.

5.2. Demonstration of the Zero-Variance Scheme for the Surface-Crossing Estimator

The emission density for the case of two-direction 1-D transport can simply be calculated from $\chi(x)=S(x)+\Sigma_s/\Sigma_t\psi(x)$. The detector response function for the flux at a surface $x=a$ becomes

$$\eta_\chi(x) = \frac{1}{2}\mathrm{e}^{-\Sigma_t|x-a|}, \tag{46}$$

and the detector response

$$R = \frac{1}{2}\frac{\alpha\Sigma_t}{\Sigma_a\Sigma_t - \alpha^2}\left\{\mathrm{e}^{-\alpha a} - \frac{\alpha}{\sqrt{\Sigma_a\Sigma_t}}\mathrm{e}^{-\sqrt{\Sigma_a\Sigma_t}a}\right\}, \tag{47}$$

which is in agreement with Eq.(26), because $\phi(a)=\psi(a)/\Sigma_t$. The adjoint equation (42) has the solution

$$\chi^+(x) = \frac{1}{2}\sqrt{\frac{\Sigma_t}{\Sigma_a}}\mathrm{e}^{-\sqrt{\Sigma_a\Sigma_t}|x-a|}. \tag{48}$$

The adjoint function is also shown in Fig. 2. This function is used for biasing Eq.(41). Because of the monoenergetic transport model the transport kernel is self-adjoint and there is no difference between the kernels K and L. Sampling the biased source and kernel L requires analogous treatment as in Sect. 3.2.

Table V shows the results of Monte Carlo calculations for the flux at a=2 cm with the optimum biasing function and using various values of the lower bound for the Russian roulette. Again a zero-variance can be seen in the limit of zero Russian roulette lower bound. The theoretical flux value is R=0.125109917.

Table V. Surface-crossing estimator results with decreasing lower bounds

weight lower bound	flux	standard deviation (%)
10^{-1}	0.1250	0.37
10^{-2}	0.12517	0.040
10^{-3}	0.125107	0.0034
10^{-4}	0.1251107	0.00034
10^{-5}	0.12510989	0.000034
10^{-6}	0.125109913	0.0000033
10^{-7}	0.125109918	0.0000004

5.3. The Track-Length Estimator

The track-length estimator scores the track length covered by a particle within the volume for which the averaged flux must be determined. For a particle outside the volume and having the right direction to cross the volume, it depends on the distance sampled whether the detector volume will actually be entered. Therefore, again an expected value track-length estimator is needed for a zero variance. In this case the expected value of the track length through the detector volume must be calculated and used as the estimator. As for the surface-crossing estimator, this estimator is applied to a particle leaving a collision or the source and the detector response is obtained as an integral over the emission density. The adjoint function is the solution

of Eq.(42) but with a different detector response function than for the surface-crossing estimator. The proof that the variance is zero is exactly the same as for the surface-crossing estimator shown in Sect. 5.1.

5.4. Demonstration of the Zero-Variance Scheme for the Track-Length Estimator

Suppose we want again to calculate the particle flux averaged over the region $|x|<a$. The track-length estimator depends on the position of the emission point and the next collision point. The expected-value track-length estimator is obtained by averaging the various possible actual track lengths over the corresponding probability of occurrence given by the transition kernel T. This leads to

$$\eta_{evtl}(x) = \begin{cases} \dfrac{1}{2\Sigma_t}\left\{e^{\Sigma_t(a-|x|)} - e^{\Sigma_t(a+|x|)}\right\} & |x|>a \\ \dfrac{1}{2\Sigma_t}\left\{2\text{-}e^{-\Sigma_t(a-x)} - e^{-\Sigma_t(a+x)}\right\} & |x|<a \end{cases} . \tag{49}$$

The solution for the adjoint function for this detector response function is

$$\chi^{+}_{evtl}(x) = \begin{cases} \dfrac{1}{2a\Sigma_a}\left\{1 - e^{-\sqrt{\Sigma_a\Sigma_t}\,a}\cosh\sqrt{\Sigma_a\Sigma_t}\,x\right\} & |x|\le a \\ \dfrac{1}{2a\Sigma_a}\sinh\sqrt{\Sigma_a\Sigma_t}\,a\; e^{-\sqrt{\Sigma_a\Sigma_t}|x|} & |x|>a \end{cases} . \tag{50}$$

This function looks the same as the adjoint function from Eq.(32), but differs due to the absence of the factor Σ_s/Σ_t for $|x|<a$ (see also Fig. 2). This function is used for biasing the equation for the emission density. Table VI shows the results of Monte Carlo calculations for the average flux in the region $|x|<a$ with a=2 cm using the optimum biasing function and for various values of the lower bound for the Russian roulette. Here too, a zero-variance can be seen in the limit of zero Russian roulette lower bound. The theoretical flux value is R=0.144851015.

Table VI. Track-length estimator results with decreasing lower bounds

weight lower bound	flux	st. dev. (%) N=1000
10^{-1}	0.1452	0.32
10^{-2}	0.14481	0.033
10^{-3}	0.144847	0.0035
10^{-4}	0.1448496	0.00033
10^{-5}	0.14485095	0.000034
10^{-6}	0.144851009	0.0000032
10^{-7}	0.144851015	0.00000036

6. PRACTICAL CONSEQUENCES

Zero-variance estimators are not only of theoretical value. One can try to come close to the sampling scheme in order to get an appreciable variance reduction. To this aim several Monte Carlo codes calculate the adjoint function in a certain detail. MCNP [15] has an option that estimates the adjoint function from the Monte Carlo calculation itself. AVATAR [16] and A^{3}MCNP [17] apply a discrete ordinates calculation to obtain the space and energy group dependent adjoint function. MCBEND [18] applies a diffusion calculation to this end. However, none of these codes use the adjoint function for actually biasing the transport kernel. This is indeed a complicated task as it requires many calculations for each space interval and energy range for which the adjoint function is calculated. Instead the form most widely used is to apply the adjoint function to define so-called weight windows, regulating the splitting and Russian roulette techniques used throughout Monte Carlo calculations. If a particle weight turns out to be larger than the upper bound of the weight window when a particle has a collision or is crossing a surface set up for this application, the particle undergoes splitting. If its weight is below the lower bound of the weight window, Russian roulette is applied. Weight windows can be both space and energy dependent.

It is often stated, or implicitly assumed, that the bounds of the weight window should be inversely proportional to the importance function at the collision site or the surface-crossing point. Indeed it sounds plausible that a particle history should not be terminated if it is in a region with high importance. The effect of weight windows so designed is that the particle will always have a weight inversely proportional with the adjoint function (within the width of the window). The need for such a behavior of the particle weight seems to be supported by theory, especially Eq.(7). As it is assumed that the optimum biasing function is proportional to the adjoint function, and we saw from the zero-variance schemes that this assumption is correct, it seems obvious to set the weight window bounds inversely proportional to the adjoint function.

Although the method of a weight window determined from the adjoint function turns out to be effective in many cases, there are at least three reasons why the theory behind this assumption is weak or even wrong. The result of Eq.(7), stating that the particle weight after biasing the source function and the transport kernel is the inverse of the biasing function at each collision point only holds for the case of an analog form of dealing with capture, as this was a prerequisite in the derivation of Eq.(7). When implicit capture is used, as is required in all zero-variance schemes, the weight factor compensating for capture will continuously lower the particle weight with respect to Eq.(7) as more collisions have taken place. This is shown by Eq.(11). The statement that Eq.(7) is not relevant for setting the weight window is also supported by the alternative interpretation of the biased Monte Carlo scheme discussed in Sect. 2, where it is discussed that the particle weight remains unity (in case of analog treatment of capture) when the process is seen as solving a different transport equation.

A second reason is that introducing a weight window to apply Russian roulette if a particle weight drops below the lower bound, is not a way to reduce the variance of a calculation. Instead it increases the variance, but its benefit is that it saves computer time by not spending effort to particles that are unlikely to contribute to the detector response. Hence, it is (or can be) an efficiency improvement. However, for maximizing the efficiency improvement, which is actually

the goal of all deviations of a pure analog Monte Carlo game, the computer time per history is an important parameter, which is totally absent in the definition of the adjoint function.

A third reason is that, although in these zero-variance schemes the optimum biasing function is the adjoint function, the adjoint functions differ for each estimator due to the different detector response function driving the adjoint equation. Only for the last-event and the collision estimator they are identical. Hence, it is likely that codes calculating the adjoint function are not using the right source term in the adjoint equation.

It is instructive to study what happens with the particle weight during a history in a zero-variance sampling scheme. From the 1-D transport example given in Sect. 3 we selected one history and show the particle variables at successive collisions in Table VII. The histories terminate due to the Russian roulette with a lower bound set at 10^{-6}.

Table VII. Particle variables during a selected history

collision	x	weight	$\overline{\kappa}(x)$	importance	score	cumulative score
1	-1.1037	$1.0000\ 10^{+0}$	0.31976	0.36752	$9.8536\ 10^{-2}$	0.09853359839
2	-1.5656	$3.1976\ 10^{-1}$	0.28953	0.35188	$3.2907\ 10^{-2}$	0.13144070608
3	-3.0451	$9.2580\ 10^{-2}$	1.00000	0.03541	0	0.13144070608
4	-3.9251	$9.2580\ 10^{-2}$	1.00000	0.01791	0	0.13144070608
5	-4.1930	$9.2580\ 10^{-2}$	1.00000	0.01456	0	0.13144070608
6	-3.8208	$9.2580\ 10^{-2}$	1.00000	0.01942	0	0.13144070608
7	-3.1073	$9.2580\ 10^{-2}$	1.00000	0.03375	0	0.13144070608
8	-1.8455	$9.2580\ 10^{-2}$	0.26144	0.33850	$9.9043\ 10^{-2}$	0.14134500859
9	0.24931	$2.4204\ 10^{-2}$	0.34314	0.38060	$2.3029\ 10^{-3}$	0.14364974784
10	-1.2306	$8.3055\ 10^{-3}$	0.31279	0.36379	$8.2676\ 10^{-4}$	0.14474710629
11	-1.3897	$2.5979\ 10^{-3}$	0.30302	0.35869	$2.6228\ 10^{-4}$	0.14473698577
12	0.24098	$7.8721\ 10^{-4}$	0.34322	0.38064	$7.4892\ 10^{-5}$	0.14481187788
13	1.8099	$2.7019\ 10^{-4}$	0.26554	0.34039	$2.8745\ 10^{-5}$	0.14484062242
14	1.0336	$7.1746\ 10^{-5}$	0.32304	0.36930	$7.0353\ 10^{-6}$	0.14484765776
15	0.1543	$2.3177\ 10^{-5}$	0.34385	0.38101	$2.2028\ 10^{-6}$	0.14484986059
16	0.0616	$7.9694\ 10^{-6}$	0.34422	0.38122	$7.5702\ 10^{-7}$	0.14485061761
17	0.3658	2.743210^{-6}	0.34182	0.37983	$2.6153\ 10^{-7}$	0.14485087914
18	0.3337	$2.0000\ 10^{-6}$ [a]	0.34223	0.38007	$1.9056\ 10^{-7}$	0.14485106970

[a] due to Russian roulette survival

This example confirms that the particle weight can take on arbitrarily small values and does not follow the inverse importance function, as could be expected from Eq.(11). It also shows that although the total score of each history is the same and equal to the desired quantity R, each history will have a different course. From Table VII, we can see that if the particle has a collision outside the detector region and thus a zero contribution to the score, the particle weight does not

change, because the value of the normalization factor of the biased kernel is equal to 1. This also follows directly from Eq.(13), as $\eta(x)$ is zero outside the detector region. One could say that in these zero-variance scheme a collision event outside the detector sensitive range (both in space and energy) becomes irrelevant and one has to wait until the particle arrives again in the detector range before scoring can continue. This may become even more clear from the energy dependent example of Sect. 3.1 where all collisions in the energy range above the detector sensitive range could have been skipped. If a history was started just above the upper energy of the detector range E_+ instead of the source energy E_o (but still using the correct E_o in the adjoint function) the correct result is obtained, as the conditional probability of scattering to a certain energy within the detector range from an energy above that range is independent of the energy before scattering. The zero-variance sampling scheme prevents the particle weight to be affected by a collision in the range where no contribution to the score can be made. It does not provide the quickest way to arrive in the range where a non-zero contribution is made. Therefore, the zero-variance scheme is not optimal with respect to computer time. It is possible to further bias the sampling process for those parts of the phase space where no contribution is made to get quicker to the area where a non-zero contribution is made, thus saving computer time. Note that because of the expected-value character of the zero-variance surface-crossing and track-length estimators, at every position a non-zero contribution is made. This picture may change in a combined space-energy dependent problem with a non-zero detector response only for a limited energy range.

7. CONCLUSIONS AND DISCUSSION

Some examples are shown of actual application of zero-variance biasing schemes for the collision estimator, the surface-crossing estimator and the track-length estimator. All these schemes require biasing of the transport kernel with the appropriate adjoint function and application of a weight factor for the unnormalized kernel (“implicit capture”). The last two estimators require an expected value variant. It is emphasized that the appropriate adjoint function is different for both estimators and also differs from that in the zero-variance collision estimator. A numerical demonstration of the zero-variance schemes is given for a monoenergetic two-direction one-dimensional transport problem. Such examples are useful to understand how the zero-variance scheme work out in practice.

Dwivedi [5] showed that a zero-variance scheme is also obtained if the transition kernel is biased with the adjoint collision density from Eq.(10) and the collision kernel with the adjoint emission density from Eq.(42). Unfortunately, this can not be demonstrated with the numerical examples given in this paper. For the only-energy dependent example in Sect. 3.1 the collision and emission densities are identical and so are their adjoint functions. For the only-space dependent examples in Sect. 3.2 and Sect. 5 the collision kernel is reduced to the scattering probability and is not actually sampled. As it will be very difficult, if not impossible, to define a combined energy and space dependent transport problem that can be treated analytically, the best way for such a demonstration is an extension of the space-dependent problem used in this paper to a two-group model. However, the analytical treatment of such a case will be much more involved than in Sect. 3.2 and 5.

Although there exist many zero-variance schemes, one may wonder whether biasing of the transport equation with the adjoint function always leads to a zero-variance for any estimator. From the proof of the zero-variance surface-crossing estimator given in Sect. 5.1 it follows that a zero-variance scheme exists for any estimator if an expected-value form is used, if necessary, the transport kernel is biased by the appropriate adjoint function and a weight factor is used to account for the biased kernel normalization.

Both from the theory and the practical demonstrations the basis for variance reduction methods based on weight windows as generally offered in Monte Carlo codes is questioned. There are several reasons, as discussed in Sect. 6, why variance reduction (or better efficiency improvement) based on a weight window determined by the inverse adjoint function can not be optimal. It will therefore be useful to develop a better theory to guide the weight window parameters in practical cases. The analytically accessible cases demonstrated in this paper can be used to verify such a theory.

Although the theory of Coveyou et al. [9] used in this paper to calculate the variance of a Monte Carlo simulation can not be used for studying the effect of a Russian roulette (nor splitting) as it can not handle weight dependent decisions for particle history termination, there are more general theories for the theoretical calculation of the statistical error [6]. This may serve as a basis to derive well founded weight window parameters that minimizes the variance. Still the problem of maximum efficiency, taking into account the computer time, remains.

We tried to study the effect of using different adjoint functions for determining the weight window in MCNP for the case of the 1-D two-direction transport model. To this end a modification in a subroutine of MCNP was needed to force the particle direction in either the $+X$ or $-X$ direction. To sample the exponential source from Eq.(25) additional modifications were necessary. An adapted one-group cross section library was used to apply the desired cross sections. For a standard case without variance reduction the correct result and variance was obtained. However, use of the weight window parameters obtained from the weight window generator did not result in an efficiency improvement at all. This may be due to the high absorption probability in our example. Also the energy-dependent case was calculated by MCNP using a specially designed cross section library with an artificial Hydrogen isotope. Here the weight window generation neither worked, as the reference value for the estimated importance function can only be linked to a geometric source cell and not to the appropriate energy source range.

Another variance reduction method generally offered in Monte Carlo codes is path length stretching. This effectively modifies the total cross section when sampling a track length in order to favor those track lengths that will bring the particle closer to the detector. In fact, it biases the transition kernel T. This comes close to the optimum biasing required for a zero-variance scheme. In fact Dwivedi [19] has shown the connection with determining the optimum path length stretching parameter for a 1-D energy independent case. Ueki and Larsen [20] developed further extensions.

In general, it may be concluded that a lot of research can be done for further improvement of the efficiency of Monte Carlo calculations.

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