THE QUADRATIC COLLISION PROBABILITY METHOD AND THE IMPORTANCE SAMPLING METHOD IN MONTE CARLO CALCULATION FOR THE FLUX AT A POINT*

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Abstract

The unbounded estimate is one of the troublesome problems in Monte Carlo method. Particularly, in the calculation for the flux at a point, the estimate may approach infinite. In this paper, a collision probability method is proposed in Monte Carlo calculation for the flux at a point, and two kinds of methods with the bounded estimation are presented: the quadratic collision probability method and the importance sampling method. The former method is simple and easy to use, whereas the latter is suitable for calculation of flux at many different points simultaneously. The practical calculation indicates that the variance of the present methods can be reduced by about 50 percent and the efficiency can be increased by 2 to 4 time in comparison with the existing methods.

1. Introduction

The application of Monte Carlo method to the calculation for the flux at a point plays an important part in the particle transport problems. It is because, first of all, the calculation of the point flux is often encountered in the practical problems. Second, because the problem of any local flux calculation can be solved through the calculation for the flux at a point. Finally, there are some difficulties with numerical calculation. Particularly, the problem is more serious for those problems with complicated geometry and other factors.

Let $\varphi(\boldsymbol{r}^0)$ denote the flux at the point $\boldsymbol{r}^0$. In other words, $\varphi(\boldsymbol{r}^0)d\boldsymbol{r}^0$ is the average track length by the particle through the volume element $d\boldsymbol{r}^0$ near $\boldsymbol{r}^0$. Thus, in order to calculate the point flux $\varphi(\boldsymbol{r}^0)$ by the usual Monte Carlo method, it is necessary to choose such a geometric volume V containing $\boldsymbol{r}^0$ in it that the $\varphi(\boldsymbol{r}^0)$ can be approximately obtained as follows:

$$\varphi(\boldsymbol{r}^0)\approx\varphi(V)=\int_V \varphi(\boldsymbol{r})d\boldsymbol{r}/|V|,$$

where $|V|$ is the volume of the geometric region. In order to make the approximate equation $\varphi(\boldsymbol{r}^0)\approx\varphi(V)$ hold more exactly, the geometric region V is taken very small. Thus, the general Monte Carlo method becomes very difficult.

There are probably two different ways to overcome the difficulty mentioned above. One is to exchange the location between the particle source and the detector (the point flux response function) so that the original particle source is turned into

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the detector, while the original detector into the particle source. In this way, the problem with the point flux calculation can be changed into one with the non-point flux calculation as long as the original source is not a point source. In this aspect, there are the reciprocal Monte Carlo[1,2] and the adjoint Monte Carlo[3-5]. Another is to use the statistical estimation techniques to treat the variables analytically involved where possible, or to use the biased sampling techniques to treat the variables which can cause large fluctuations in the results. There are the directing probability method[6-8], biased location sampling method[7], the maximum cross section method[9] and the reselection method[10-13] and so on.

The reciprocal Monte Carlo method has two important disadvantages. One is that the particle source can not be a point source. Another, the application is extremely limited, because the condition under which the source and the detector can be exchanged is seldom satisfied. As for the adjoint Monte Carlo the situation is different. In this case, the reciprocity between the source and detector is done formally, and does not meet the condition which is needed in the real reciprocity. Therefore, it overcomes the second difficulty appearing in the reciprocal Monte Carlo method successfully. But the adjoint Monte Carlo does not remove the first disadvantage, neverthereless, and it creates some new problems, such as the complicated random walk, larger statistical error[14] and so on.

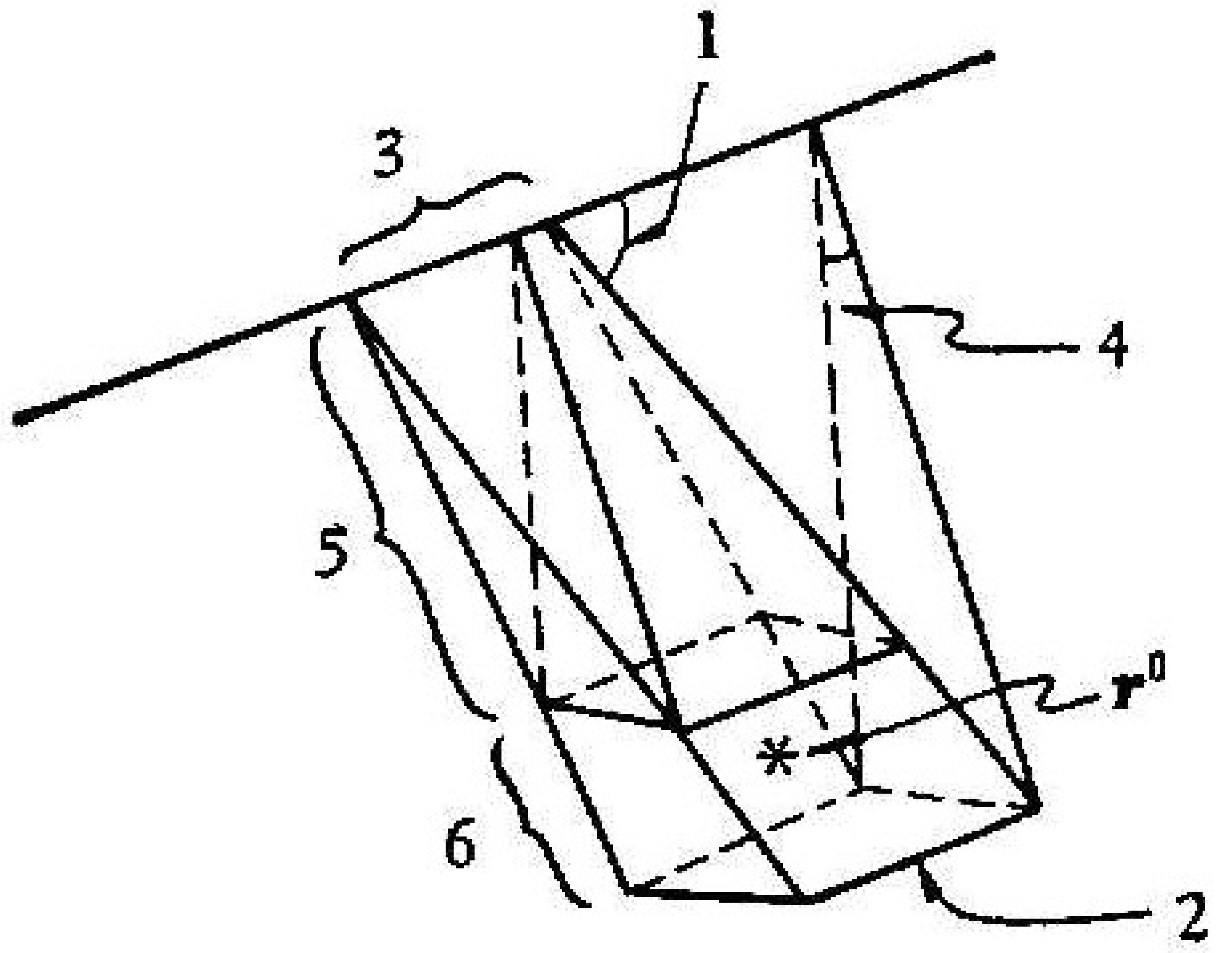
The directing probability method is a very simple and easy to use. But if there is scattering medium near point $\boldsymbol{r}_0$, the estimation of the directing probability is unbounded. For the homogeneous medium, Kalos proved that the estimation of the directing probability method is not only unbounded, but also its variance is divergent (for the heterogeneous medium, as long as there is some scattering medium near the point $\boldsymbol{r}^0$, the variance of the directing probability method is divergent as well). The boundlessness of the estimation often makes the statistical fluctuation of the Monte Carlo estimate become large. Meanwhile the divergence of the variance can directly affect the convergence rate.

The location biased sampling method which was given by Kalos in 1963 is the first method with finite variance to overcome the divergence of the directing probability method. But his conclusion is based on the assumption of homogeneous medium, monoenergetic particle and isotropic scattering. On the other hand, not only is the method approximate, also it is complicated to apply to the calculation for the flux at a point, hence the method has not been widely used. The maximum cross section method given by Михайлов is another one to solve the variance divergence problem. It does not need any condition which must be satisfied by the location biased sampling method. As the location biased sampling method, although they have solved the problem about the variance divergence, they can not overcome the problem about the unbounded estimate at last.

The reselection method which was developed by Steinberg and Kalos in 1971 is the first one to solve the problem about the boundlessness of the estimate in Monte Carlo calculation for the flux at a point. Later, it was improved further by Steinberg, Lichtenstein, Kalli and Cashwell, but it is still complicated. And it is not able to calculate the flux at many different points simultaneously. In this paper, we present a collision probability method in Monte Carlo calculation for the flux at a point. Based on this, two kinds of the bounded estimate methods are given, namely, quadratic collision probability method and importance sampling method. In this way, two disadvantages of the reselection method mentioned above are overcome.

2. Collision Probability Method

Collision probability method is very similar to the directing probability method in Monte Carlo calculation for the flux at a point. Its basic principle is that (see the Fig. 1) a collision point $\boldsymbol{r}^*$ and a scattering azimuth angle are found so that the particle can pass through the unit cube containing the point $\boldsymbol{r}^0$ in it for the fixed scattering angle. The particle starting at point $\boldsymbol{r}$ and further undergoing collision contributes to the point flux $\varphi(\boldsymbol{r}^0)$, which is equal to the product of the following four factors: the probability with which the collision takes place at the point $\boldsymbol{r}^*$, the probability with which the particle scatters into the azimuth given, the probability without further collision by the particle from $\boldsymbol{r}^*$ to $\boldsymbol{r}^0$, and the track length by the particle through the unit cube.



1—the fixed scattering angle;
2—the unit cube;
3—the collision points $\boldsymbol{r}^*$ contributing possibly to the unit cube;
4—the azimuth angles contributing possibly to the unit cube;
5—without any collision from $\boldsymbol{r}^*$ to $\boldsymbol{r}^0$;
6—the track length through the unit cube

Fig. 1 The illustration of collision probability method

Now, the point flux $\varphi(\boldsymbol{r}^0)$ is expressed in the form of the sum of the successive scattering contribution: $\varphi(\boldsymbol{r}^0)=\varphi_0(\boldsymbol{r}^0)+\varphi_1(\boldsymbol{r}^0)+\cdots$. Let $\boldsymbol{r}_n$, E_n, $\boldsymbol{\Omega}_n$ and W_n stand for the location, energy, flight direction and weight for the particle to leave the n-th scattering, respectively. Thus, the particle's random walk history can be expressed by the sequence $\{\boldsymbol{r}_n,\ E_n,\ \boldsymbol{\Omega}_n,\ W_n\}_{n=0}^{\infty}$. Therefore, according to the basic principle of collision probability method, the unbiased estimate to the point flux with the method is obtained as follows:

$$\hat{\varphi}_n(\boldsymbol{r}^0)=W_{n-1}\Sigma_s(\boldsymbol{r}^*,\ E_{n-1})\frac{\int_F f(E_{n-1}\to E,\ \boldsymbol{\Omega}_{n-1}\to\boldsymbol{\Omega}_n^*|\boldsymbol{r}^*)dE}{\int_E f(E_{n-1}\to E,\ \boldsymbol{\Omega}_{n-1}\to\boldsymbol{\Omega}_n^*|\boldsymbol{r}_n)dE}\exp\left\{-\int_0^l\Sigma_t(\boldsymbol{r}_{n-1}+t\boldsymbol{\Omega}_{n-1},\ E_{n-1})dt-\int_0^{l'}\Sigma_t(r^*+t\Omega_n^*,\ E_n')\,dt\right\}\frac{\eta(\boldsymbol{\Omega}_{n-1}^{\wedge}\boldsymbol{\Omega}_n\geqslant\boldsymbol{\Omega}_{n-1}^{\wedge}\boldsymbol{\Omega}_{n-1}^0)}{2\pi l'|\boldsymbol{\Omega}_{n-1}\times\boldsymbol{\Omega}_n|^2},\tag{1}$$

where, $n\geqslant1$, $f(E'\to E,\ \boldsymbol{\Omega}'\to\boldsymbol{\Omega}|\boldsymbol{r})dE\,d\boldsymbol{\Omega}$ denotes the probability with which having a scattering at the point $\boldsymbol{r}$, the particle changes its energy E' and flight direction $\boldsymbol{\Omega}'$ into $dE\,d\boldsymbol{\Omega}$ near E and $\boldsymbol{\Omega}$; $\Sigma_s(\boldsymbol{r},\ E)$ and $\Sigma_t(\boldsymbol{r},\ E)$ denote the scattering cross section and the total cross section at the point $\boldsymbol{r}$ and energy E; E_n' is sampled from the density distribution $f(E_{n-1}\to E_n',\ \ \boldsymbol{\Omega}_{n-1}\to\boldsymbol{\Omega}_n^*|\boldsymbol{r}^*)\Big/\int_E f(E_{n-1}\to E,\ \boldsymbol{\Omega}_{n-1}\to\boldsymbol{\Omega}_n^*|\boldsymbol{r}^*)dE$; $\eta(\cdot)$ is a conditional function, if the condition is satisfied, its value is 1, otherwise

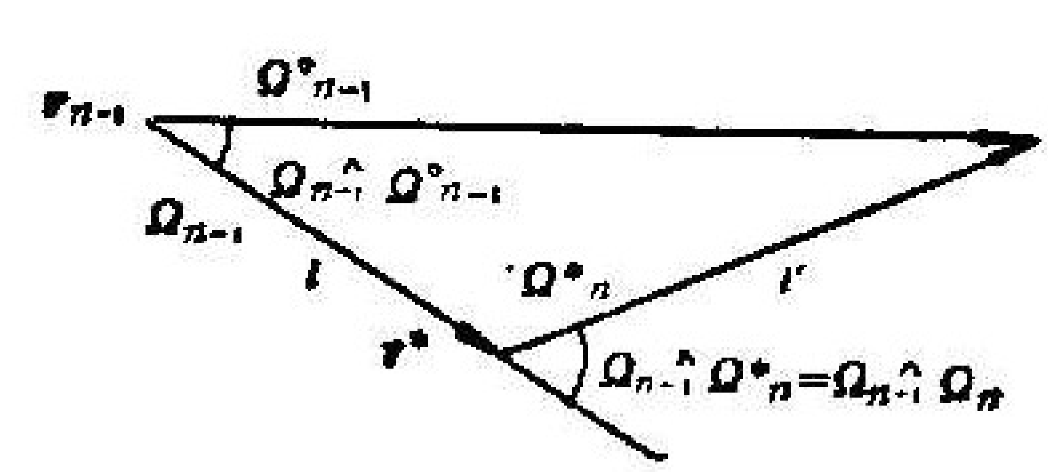


Fig. 2 The relationship between the collision point and the scattering direction

it is 0; the other quantities are defined in the Fig. 2.

Owing to $\lim_{l'\to 0} l'/|\boldsymbol{\Omega}_{n-1}\times(\boldsymbol{r}^0-\boldsymbol{r}_{n-1})|=1$, it follows that

$$\frac{1}{2\pi l'|\boldsymbol{\Omega}_{n-1}\times\boldsymbol{\Omega}_n|^2}=\frac{l'}{2\pi|\boldsymbol{\Omega}_{n-1}\times(\boldsymbol{r}^0-\boldsymbol{r}_{n-1})|^2}=O\left(\frac{1}{l'}\right). \tag{2}$$

This result indicates that the variance of the collision probability method is definite. In other words, the method is a finite variance method for calculating the point flux.

3. Quadratic Collision Probability Method

In fact, the quadratic collision probability method is derived from the collision probability method in Monte Carlo calculation for the flux at a point. Its basic principle is to find such two collision points $\boldsymbol{r}^*_{n-1}$ and $\boldsymbol{r}^*_n$ that the particle is able to pass through the unit cube containing $\boldsymbol{r}^0$ for the fixed scattering direction (cf. Fig. 3). The point flux contribution $\varphi_n(\boldsymbol{r}^0)$ $(n\geqslant 2)$ which results from the particle starting at $\boldsymbol{r}_{n-2}$ and undergoing two successive collisions is equal to the product of four quantities as follows: the probability with which the particle starting at $\boldsymbol{r}_{n-2}$ made a collision at the point $\boldsymbol{r}_{n-1}$ satisfying the above conditions, the probability with which the particle starting at $\boldsymbol{r}_{n-1}$ made a collision at the point $\boldsymbol{r}^*_n$ satisfying the above conditions, the probability without any further collision from $\boldsymbol{r}^*_n$ to $\boldsymbol{r}^0$, and the track length by the particle through the unit hexahedron V.

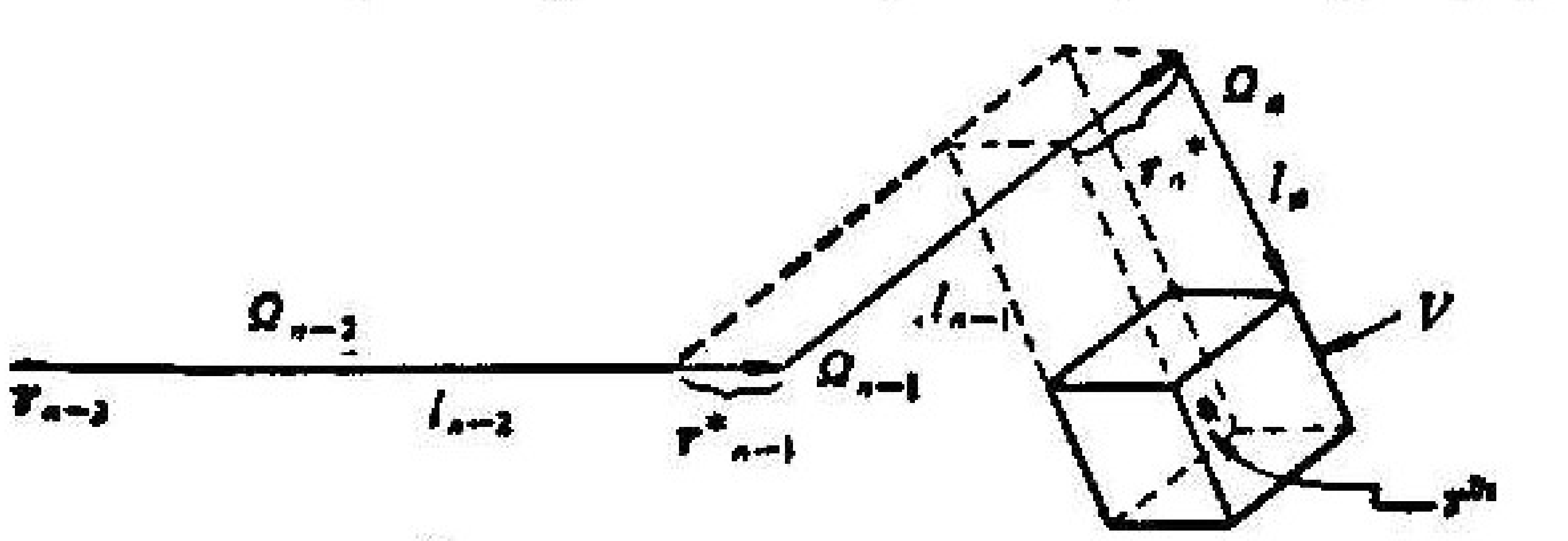


Fig. 3 The illustration of quadratic collision probability method

Suppose the random walk history of a particle is $\{\boldsymbol{r}_n, E_n, \boldsymbol{\Omega}_n, W_n\}_{n=0}^{\infty}$. Thus, according to the basic principle of quadratic collision probability method, we have the unbiased estimate of the point flux $\varphi_n(\boldsymbol{r}^0)$ with quadratic collision probability method as follows:

$$\begin{aligned}\hat{\varphi}_n(\boldsymbol{r}^0)=&W_{n-2}\Sigma_s(\boldsymbol{r}^*_{n-1}, E_{n-2})\frac{f(E_{n-2}\to E_{n-1}, \boldsymbol{\Omega}_{n-2}\to\boldsymbol{\Omega}_{n-1}|\boldsymbol{r}^*_{n-1})}{f(E_{n-2}\to E_{n-1}, \boldsymbol{\Omega}_{n-2}\to\boldsymbol{\Omega}_{n-1}|\boldsymbol{r}_{n-1})}\Sigma_s(\boldsymbol{r}^*_n, E_{n-1})\\&\times\frac{f(E_{n-1}\to E_n, \boldsymbol{\Omega}_{n-1}\to\boldsymbol{\Omega}_n|\boldsymbol{r}^*_n)}{f(E_{n-1}\to E_n, \boldsymbol{\Omega}_{n-1}\to\boldsymbol{\Omega}_n|\boldsymbol{r}_n)}\exp\left\{-\int_0^{l_{n-2}}\Sigma_t(\boldsymbol{r}_{n-2}+t\boldsymbol{\Omega}_{n-2}, E_{n-2})dt\right.\\&\left.-\int_0^{l_{n-1}}\Sigma_t(\boldsymbol{r}^*_{n-1}+t\boldsymbol{\Omega}_{n-1}, E_{n-1})dt-\int_0^{l_n}\Sigma_t(\boldsymbol{r}^*_n+t\boldsymbol{\Omega}_n, E_n)dt\right\}\\&\times\frac{\eta(l_{n-2}\geqslant 0)\eta(l_{n-1}\geqslant 0)\eta(l_n\geqslant 0)}{|(\boldsymbol{\Omega}_{n-2}\boldsymbol{\Omega}_{n-1}\boldsymbol{\Omega}_n)|},\end{aligned} \tag{3}$$

where

$$\begin{aligned}l_{n-2}&=|\boldsymbol{r}^0-\boldsymbol{r}_{n-2}|\frac{(\boldsymbol{\Omega}^0_{n-2}\boldsymbol{\Omega}_{n-1}\boldsymbol{\Omega}_n)}{(\boldsymbol{\Omega}_{n-2}\boldsymbol{\Omega}_{n-1}\boldsymbol{\Omega}_n)},\\ l_{n-1}&=|\boldsymbol{r}^0-\boldsymbol{r}_{n-2}|\frac{(\boldsymbol{\Omega}_{n-2}\boldsymbol{\Omega}^0_{n-2}\boldsymbol{\Omega}_n)}{(\boldsymbol{\Omega}_{n-2}\boldsymbol{\Omega}_{n-1}\boldsymbol{\Omega}_n)},\\ l_n&=|\boldsymbol{r}^0-\boldsymbol{r}_{n-2}|\frac{(\boldsymbol{\Omega}_{n-2}\boldsymbol{\Omega}_{n-1}\boldsymbol{\Omega}^0_{n-2})}{(\boldsymbol{\Omega}_{n-2}\boldsymbol{\Omega}_{n-1}\boldsymbol{\Omega}_n)},\\ \boldsymbol{r}^*_{n-1}&=\boldsymbol{r}_{n-2}+l_{n-2}\boldsymbol{\Omega}_{n-2},\qquad \boldsymbol{r}^*_n=\boldsymbol{r}^*_{n-1}+l_{n-1}\boldsymbol{\Omega}_{n-1}.\end{aligned} \tag{4}$$

Obviously, the estimate (3) is still unbounded. But, it is not difficult to solve this problem. In order to do so, first introduce the biased density distributions for $\boldsymbol{\Omega}_{n-2}$, $\boldsymbol{\Omega}_{n-1}$ and $\boldsymbol{\Omega}_n$ as follows:

$$
\begin{aligned}
f_{n-2}(\boldsymbol{\Omega}_{n-2}) &= \frac{1}{\pi\cdot|\boldsymbol{\Omega}^0_{n-2}\times\boldsymbol{\Omega}_{n-2}|}\frac{1}{2\pi},\\
f_{n-1}(\boldsymbol{\Omega}_{n-2}\to\boldsymbol{\Omega}_{n-1}) &= \frac{|\boldsymbol{\Omega}^0_{n-2}\times\boldsymbol{\Omega}_{n-2}|^{1/2}}{4|(\boldsymbol{\Omega}_{n-2}\boldsymbol{\Omega}_{n-1}\boldsymbol{\Omega}^0_{n-2})|^{1/2}}\frac{1}{2\pi},\\
f_n(\boldsymbol{\Omega}_{n-2}\to\boldsymbol{\Omega}_n) &= \frac{|\boldsymbol{\Omega}^0_{n-2}\times\boldsymbol{\Omega}_{n-2}|^{1/2}}{4|(\boldsymbol{\Omega}_{n-2}\boldsymbol{\Omega}^0_{n-2}\boldsymbol{\Omega}_n)|^{1/2}}\frac{1}{2\pi}.
\end{aligned}
\tag{5}
$$

Because of the symmetry of distributions (5), that is, $-\boldsymbol{\Omega}_{n-2}$ and $\boldsymbol{\Omega}_{n-2}$ have the same distribution $f_{n-2}(\boldsymbol{\Omega}_{n-2})$, $-\boldsymbol{\Omega}_{n-1}$ and $\boldsymbol{\Omega}_{n-1}$ have the same distribution $f_{n-1}(\boldsymbol{\Omega}_{n-2}\to\boldsymbol{\Omega}_{n-1})$, and so do the $-\boldsymbol{\Omega}_n$ and $\boldsymbol{\Omega}_n$ the same distribution $f_n(\boldsymbol{\Omega}_{n-2}\to\boldsymbol{\Omega}_n)$. If $\boldsymbol{\Omega}_{n-2}$, $\boldsymbol{\Omega}_{n-1}$ and $\boldsymbol{\Omega}_n$ are sampled from the distribution $f_{n-2}(\boldsymbol{\Omega}_{n-2})$, $f_{n-1}(\boldsymbol{\Omega}_{n-2}\to\boldsymbol{\Omega}_{-1})$ and $f_n(\boldsymbol{\Omega}_{n-2}\to\boldsymbol{\Omega}_n)$, respectively, then it follows that (cf. Appendix)

$$
\left\{
\begin{aligned}
\boldsymbol{\Omega}'_{n-2} &= \frac{l_{n-2}}{|l_{n-2}|}\boldsymbol{\Omega}_{n-2},\\
\boldsymbol{\Omega}'_{n-1} &= \frac{l_{n-1}}{|l_{n-1}|}\boldsymbol{\Omega}_{n-1},\\
\boldsymbol{\Omega}'_{n} &= \frac{l_{n}}{|l_{n}|}\boldsymbol{\Omega}_{n},
\end{aligned}
\right.
\tag{6}
$$

and $\boldsymbol{\Omega}'_{n-2}$, $\boldsymbol{\Omega}'_{n-1}$ and $\boldsymbol{\Omega}'_n$ obey the same distribution $f_{n-2}(\boldsymbol{\Omega}'_{n-2})$, $f_{n-1}(\boldsymbol{\Omega}'_{n-2}\to\boldsymbol{\Omega}'_{n-1})$ and $f_n(\boldsymbol{\Omega}'_{n-2}\to\boldsymbol{\Omega}_n)$, respectively. Further, suppose the energy E'_{n-2}, E'_{n-1} and E'_n are sampled from the distributions $f(E'_{n-3}\to E'_{n-2},\ \boldsymbol{\Omega}_{n-3}\to\boldsymbol{\Omega}'_{n-2}|\boldsymbol{r}_{n-2})\Big/\int_E f(E_{n-3}\to E,\ \boldsymbol{\Omega}_{n-3}\to\boldsymbol{\Omega}'_{n-2}|\boldsymbol{r}_{n-2})\,dE$, $f(E'_{n-2}\to E'_{n-1},\ \boldsymbol{\Omega}_{n-2}\to\boldsymbol{\Omega}'_{n-1}|\boldsymbol{r}^*_{n-1})\Big/\int_E f(E'_{n-2}\to E,\ \boldsymbol{\Omega}'_{n-2}\to\boldsymbol{\Omega}'_{n-1}|\boldsymbol{r}^*_{n-1})dE$ and $f(E'_{n-1}\to E'_n,\ \boldsymbol{\Omega}'_{n-1}\to\boldsymbol{\Omega}'_n|\boldsymbol{r}^*_n)\Big/\int_E f(E'_{n-1}\to E,\ \boldsymbol{\Omega}'_{n-1}\to\boldsymbol{\Omega}'_n|\boldsymbol{r}^*_n)\,dE$ sequentially. Then, the estimate (3) is changed into

$$
\begin{aligned}
\hat{\varphi}_n(\boldsymbol{r}^0) = 16W_{n-2}\pi^4 &\int_E f(E_{n-3}\to E,\ \boldsymbol{\Omega}'_{n-3}\to\boldsymbol{\Omega}'_{n-2}|\boldsymbol{r}_{n-2})dE\\
&\times\Sigma_s(\boldsymbol{r}^*_{n-1},\ E'_{n-2})\int_E f(E'_{n-2}\to E,\ \boldsymbol{\Omega}'_{n-2}\to\boldsymbol{\Omega}'_{n-1}|\boldsymbol{r}^*_{n-1})dE\\
&\times\Sigma_s(\boldsymbol{r}^*_n,\ E'_{n-1})\int_E f(E'_{n-1}\to E,\ \boldsymbol{\Omega}'_{n-1}\to\boldsymbol{\Omega}'_n|\boldsymbol{r}^*_n)dE\\
&\times\exp\left\{-\int_0^{|l_{n-2}|}\Sigma_t(\boldsymbol{r}_{n-2}+t\boldsymbol{\Omega}'_{n-2},\ E'_{n-2})dt-\int_0^{|l_{n-1}|}\Sigma_t(\boldsymbol{r}^*_{n-1}\right.\\
&\left.+t\boldsymbol{\Omega}'_{n-1},\ E'_{n-1})\,dt-\int_0^{|l_n|}\Sigma_t(\boldsymbol{r}^*_n+t\boldsymbol{\Omega}'_n,\ E'_n)dt\right\}\\
&\times\frac{|(\boldsymbol{\Omega}'_{n-2}\boldsymbol{\Omega}'_{n-1}\boldsymbol{\Omega}^0_{n-2})|^{1/2}|(\boldsymbol{\Omega}'_{n-2}\boldsymbol{\Omega}^0_{n-2}\boldsymbol{\Omega}'_n)|^{1/2}}{|(\boldsymbol{\Omega}'_{n-2}\boldsymbol{\Omega}'_{n-1}\boldsymbol{\Omega}'_n)|}.
\end{aligned}
\tag{7}
$$

It is not difficult to see that the estimate (7) is bounded.

Comparing with the reselection method, we see that the quadratic collision probability method is more suitable for calculating the flux at many different points simultaneously. The reason is that the quadratic collision probability method is affected by the point $\boldsymbol{r}^0$ only locally the latest two collisions, while the reselection method is affected by the point $\boldsymbol{r}^0$ globally in the entire process from in the beginning to the end.

4. The Importance Sampling Method

The importance sampling method is one of the most important methods amongst the various Monte Carlc sampling techniques. If the importance function is chosen appropriately, importance sampling method is not only simple and easy to use, but also can reduce the variance of the estimate sharply.

Let $\chi(\boldsymbol{r}, E, \boldsymbol{\Omega})\, d\boldsymbol{r}dEd\boldsymbol{\Omega}$ be the average numbers of the particle which was emitted in $d\boldsymbol{r}$ near $\boldsymbol{r}$ and in $dEd\boldsymbol{\Omega}$ near E and $\boldsymbol{\Omega}$ starting from the source $S(\boldsymbol{r}, E, \boldsymbol{\Omega})$. Then $\chi(\boldsymbol{r}, E, \boldsymbol{\Omega})$ should satisfy the following equation:

$$\chi(\boldsymbol{r}, E, \boldsymbol{\Omega}) = \int_{4\pi}\int_{E'}\int_{r'} \chi(\boldsymbol{r}', E', \boldsymbol{\Omega}')T(\boldsymbol{r}'\to\boldsymbol{r}\,|\,E', \boldsymbol{\Omega}')$$
$$\times\frac{\Sigma_s(\boldsymbol{r}, E')}{\Sigma_t(\boldsymbol{r}, E')} f(E'\to E, \boldsymbol{\Omega}'\to\boldsymbol{\Omega}\,|\,\boldsymbol{r})d\boldsymbol{r}'dE'd\boldsymbol{\Omega}' + S(\boldsymbol{r}, E, \boldsymbol{\Omega}), \tag{8}$$

where $T(\boldsymbol{r}'\to\boldsymbol{r}\,|\,E', \boldsymbol{\Omega}')d\boldsymbol{r}$ is the average collision numbers per particle beginning at $\boldsymbol{r}'$ with energy E' along the direction $\boldsymbol{\Omega}'$ to the point $\boldsymbol{r}$ in $d\boldsymbol{r}$.

By introducing the transformation

$$\chi(\boldsymbol{r}, E, \boldsymbol{\Omega}) = |\boldsymbol{\Omega}\times(\boldsymbol{r}^0-\boldsymbol{r})|\cdot\bar{\chi}(\boldsymbol{r}, E, \boldsymbol{\Omega}). \tag{9}$$

It is easy to see that $\bar{\chi}(\boldsymbol{r}, E, \boldsymbol{\Omega})$ should meet the following equation:

$$\bar{\chi}(\boldsymbol{r}, E, \boldsymbol{\Omega}) = \int_{4\pi}\int_{E'}\int_{r'} \bar{\chi}(\boldsymbol{r}', E', \boldsymbol{\Omega}')$$
$$\times\frac{|\boldsymbol{\Omega}'\times(\boldsymbol{r}^0-\boldsymbol{r}')|}{|\boldsymbol{\Omega}\times(\boldsymbol{r}^0-\boldsymbol{r})|}\,T(\boldsymbol{r}'\to\boldsymbol{r}\,|\,E', \boldsymbol{\Omega}')\,\frac{\Sigma_s(\boldsymbol{r}, E')}{\Sigma_t(\boldsymbol{r}, E')}$$
$$\times f(E'\to E,\ \boldsymbol{\Omega}'\to\boldsymbol{\Omega}\,|\,\boldsymbol{r})\,d\boldsymbol{r}'dE'd\boldsymbol{\Omega}' + \frac{S(\boldsymbol{r}, E, \boldsymbol{\Omega})}{|\boldsymbol{\Omega}\times(\boldsymbol{r}^0-\boldsymbol{r})|}. \tag{10}$$

Due to Eq. (10), the particle's random walk history can be obtained for the importance sampling as follows. First, from the distribution

$$\frac{\dfrac{S(\boldsymbol{r}_0, E_0, \Omega_0)}{|\boldsymbol{r}^0-\boldsymbol{r}_0|}}{\displaystyle\int_E\int_r \frac{S(\boldsymbol{r}, E, \boldsymbol{\Omega}_0)}{|\boldsymbol{r}^0-\boldsymbol{r}|}\,d\boldsymbol{r}\,dE}\ \frac{1}{\pi|\boldsymbol{\Omega}_0\times\boldsymbol{\Omega}_0^0|}\ \frac{1}{2\pi}. \tag{11}$$

the particle's initial location $\boldsymbol{r}_0$, energy E_0, and flight direction $\boldsymbol{\Omega}_0$ can be defined, and the initial weight is

$$\overline{W}_0 = 2\pi^2\int_E\int_r \frac{S(\boldsymbol{r}, E, \boldsymbol{\Omega}_0)}{|\boldsymbol{r}^0-\boldsymbol{r}|}\,d\boldsymbol{r}\,dE. \tag{12}$$

Secondly, as soon as the location $\boldsymbol{r}_m$, energy E_m, flight direction $\boldsymbol{\Omega}_m$ and weight $\overline{W}_m$ leaving the m-th collision are defined, the collision location $\boldsymbol{r}_{m+1}$ is sampled from the following distribution:

$$T(\boldsymbol{r}_m\to\boldsymbol{r}_{m+1}\,|\,E_m, \Omega_m) = \frac{\Sigma_t(\boldsymbol{r}_{m+1}, E_m)}{|\boldsymbol{r}_{m+1}-\boldsymbol{r}_m|^2}$$
$$\times\exp\left\{-\int_0^{|\boldsymbol{r}_{m+1}-\boldsymbol{r}_m|}\Sigma_t(\boldsymbol{r}_m+t\boldsymbol{\Omega}_m, E_m)\,dt\right\}\delta\left(\boldsymbol{\Omega}_m-\frac{\boldsymbol{r}_{m+1}-\boldsymbol{r}_m}{|\boldsymbol{r}_{m+1}-\boldsymbol{r}_m|}\right); \tag{13}$$

while the energy E_{m+1} and the flight direction $\boldsymbol{\Omega}_{m+1}$ after the collision are sampled from the distribution

$$\frac{f(E_m \to E_{m+1},\ \boldsymbol{\Omega}_m \to \boldsymbol{\Omega}_{m+1} \mid \boldsymbol{r}_{m+1})}{\int_E f(E_m \to E,\ \boldsymbol{\Omega}_m \to \boldsymbol{\Omega}_{m+1} \mid \boldsymbol{r}_{m+1})\,dE}\ \frac{1}{\pi \mid \boldsymbol{\Omega}_{m+1} \times \boldsymbol{\Omega}^0_{m+1} \mid}\ \frac{1}{2\pi}; \tag{14}$$

the weight $\overline{W}_{m+1}$ is given by the following equation (cf. Fig. 4)

$$\overline{W}_{m+1} = \overline{W}_m \cdot 2\pi^2 \mid \boldsymbol{\Omega}_m \times \boldsymbol{\Omega}^0_{m+1} \mid \frac{\Sigma_s(\boldsymbol{r}_{m+1},\ E_m)}{\Sigma_t(\boldsymbol{r}_{m+1},\ E_m)} \times \int_E f(E_m \to E,\ \boldsymbol{\Omega}_m \to \boldsymbol{\Omega}_{m+1} \mid \boldsymbol{r}_{m+1})\,dE. \tag{15}$$

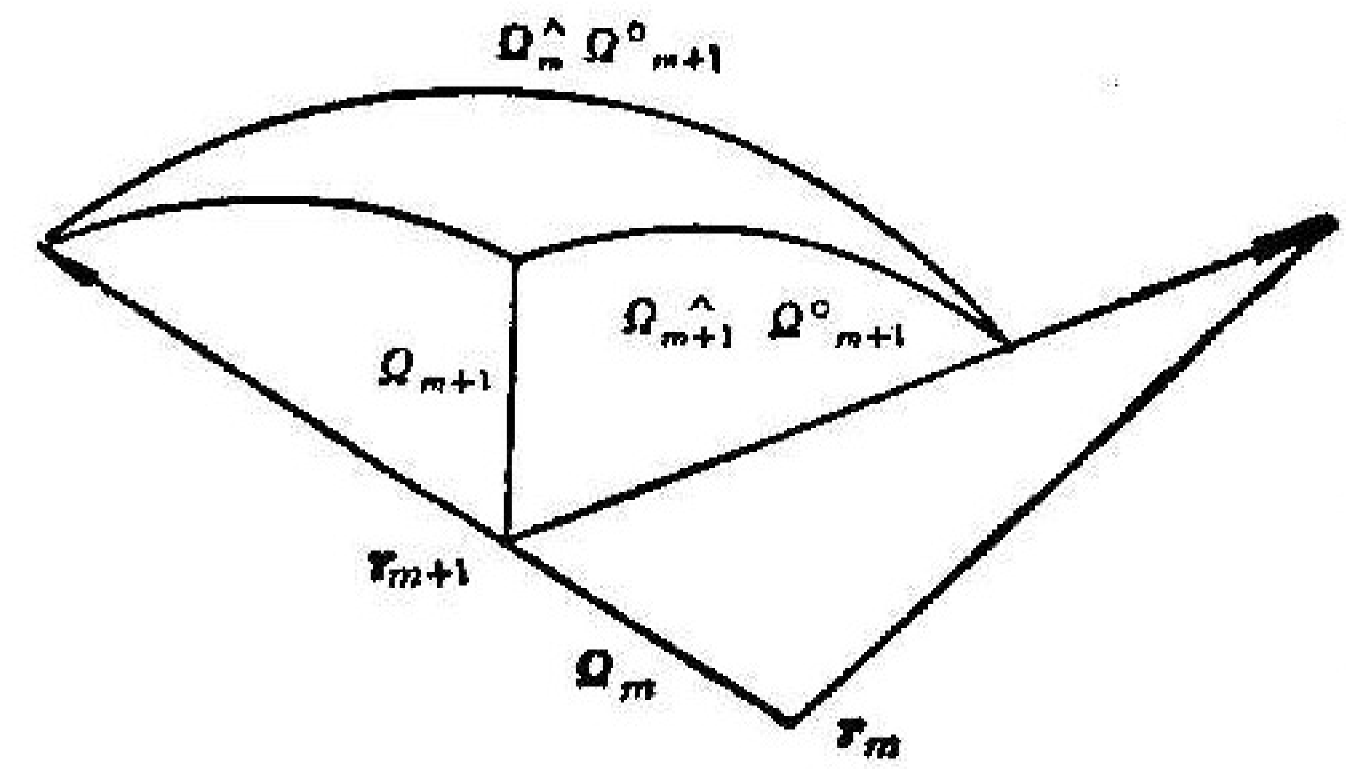


Fig. 4 The relationship between the particle's location and its flight direction

Owing to the transformation (9), it follows that $W_{n-1} = \overline{W}_{n-1} \cdot \mid \boldsymbol{\Omega}_{n-1} \times (\boldsymbol{r}^0 - \boldsymbol{r}_{n-1}) \mid$. For the collision probability method (1), $\boldsymbol{\Omega}_n$ is sampled from the distribution

$$\int_E f(E_{n-1} \to E,\ \boldsymbol{\Omega}_{n-1} \to \boldsymbol{\Omega}_n \mid \boldsymbol{r}_n)\,dE_n,$$

therefore, if $\boldsymbol{\Omega}_n$ is sampled from the distribution $(1/\pi \cdot \mid \boldsymbol{\Omega}_{n-1} \times \boldsymbol{\Omega}_n \mid) \cdot (1/2\pi)$ instead, then the result (1) with collision probability method is turned into

$$\hat{\varphi}_n(\boldsymbol{r}^0) = \overline{W}_{n-1}\pi\ \Sigma_s(\boldsymbol{r}^*,\ E_{n-1}) \int_E f(E_{n-1} \to E,\ \boldsymbol{\Omega}_{n-1} \to \boldsymbol{\Omega}_n \mid \boldsymbol{r}^*)\,dE \times \exp\left\{ -\int_0^l \Sigma_t(\boldsymbol{r}_{n-1} + t\boldsymbol{\Omega}_{n-1},\ E_{n-1})\,dt - \int_0^{l'} \Sigma_t(\boldsymbol{r}^* + t\boldsymbol{\Omega}^*_n,\ E'_n)\,dt \right\}. \tag{16}$$

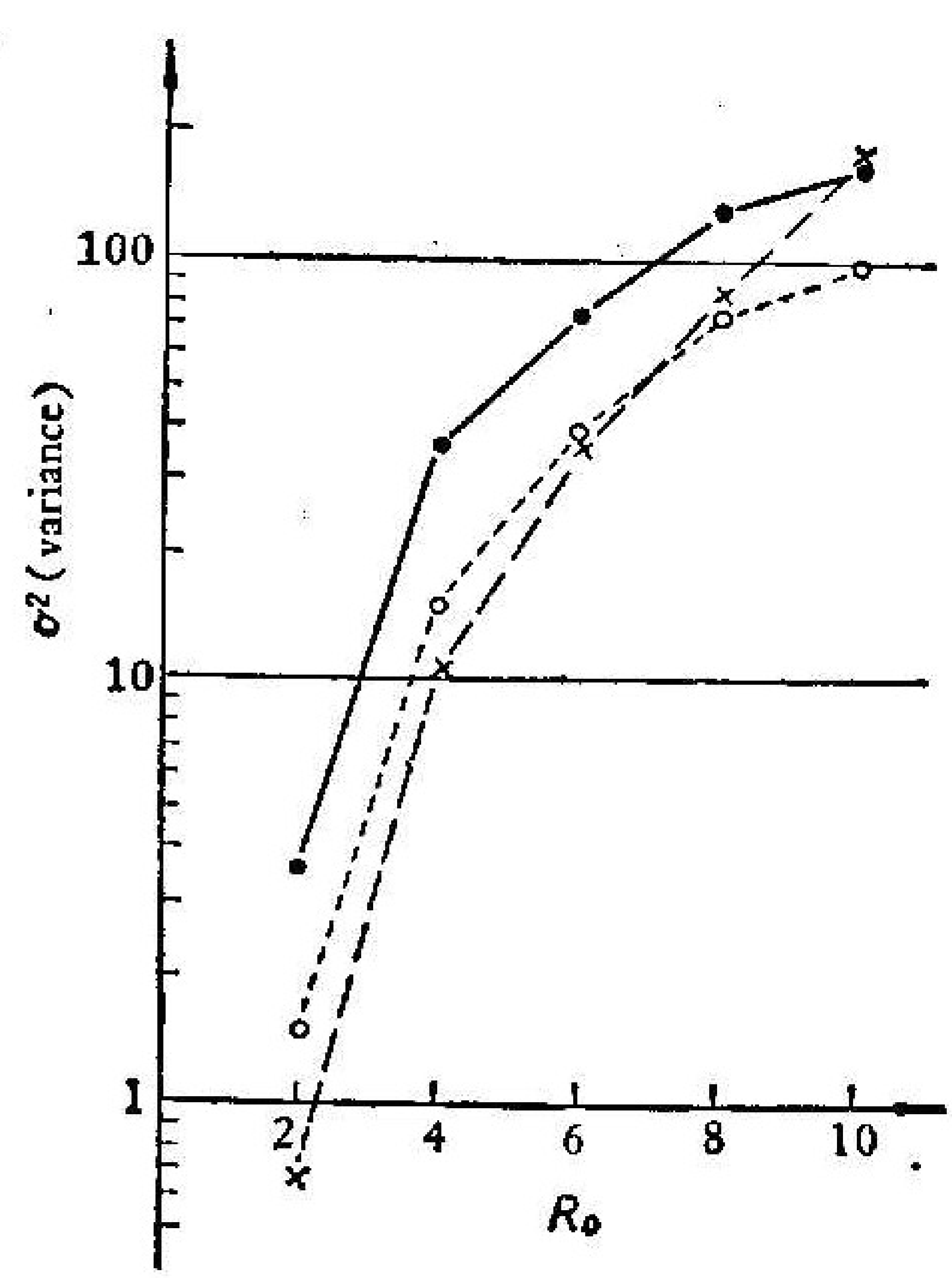
Obviously, the estimate (16) with importance sampling method mentioned above is bounded.

The importance sampling method is given for most general case, while the reselection method is based on the monoenergitic assumption. Moreover, it is also obvious that the importance sampling method not only is easy to sample and its random walk is simple and convenient, also its computational cost is less.

5. An Example

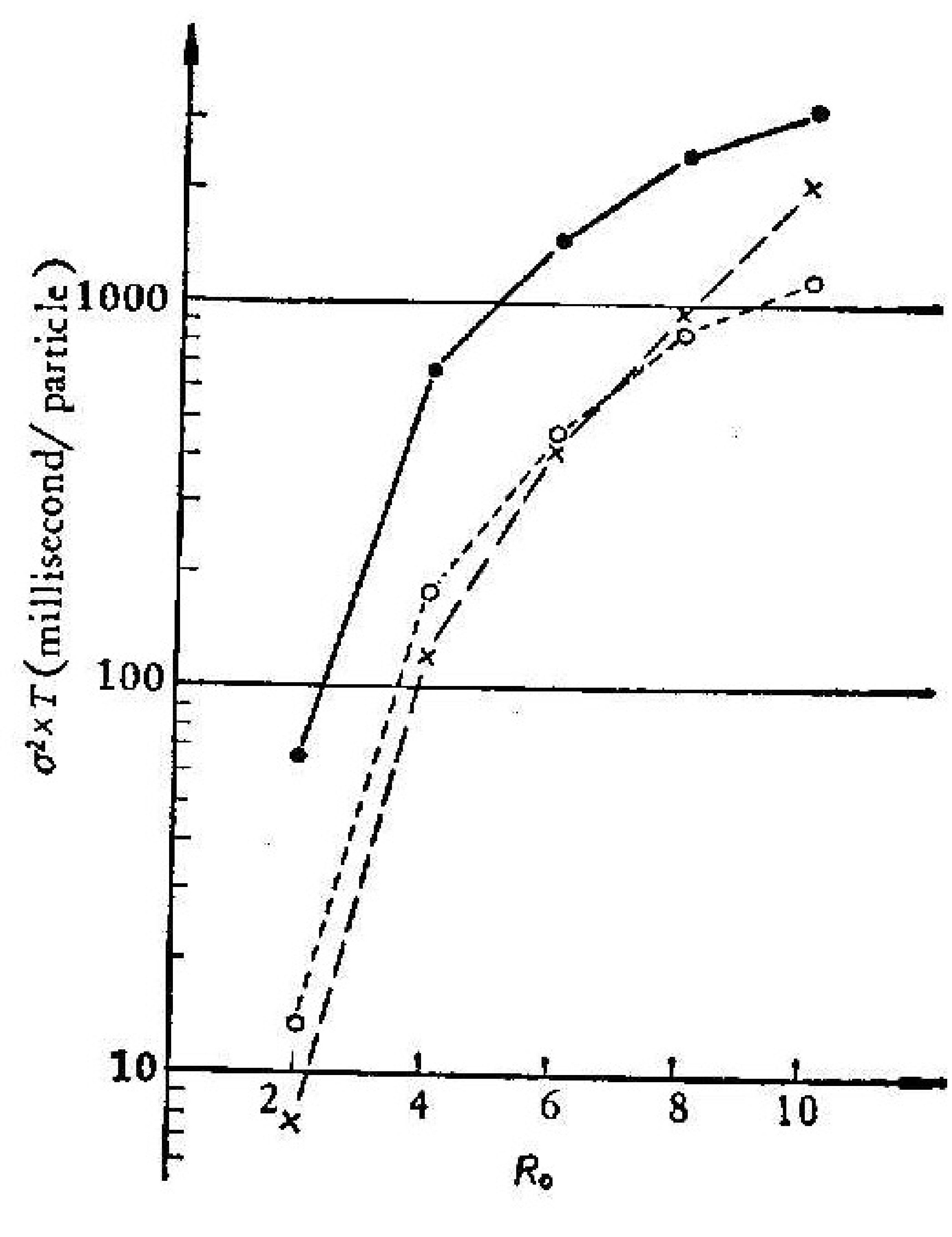
In order to examine roughly, the various calculation methods for the flux at a point we take the following problem as an example, and compute it on the NOVA-840 computer: there is a sphere with the radius R_0 in the infinite space filled with a single medium, the source with the isotropic emission is uniformly distributed everywhere in the sphere. The source intensity is 1, and the total cross section is identically 1, the collision is the isotropic scattering. It is desirable to compute the flux undergone at most five collisions at the centre of the sphere. The methods used are the directing probability method, the location biased sampling method (the flight direction biased sampling method), the maximum cross section method, the collision probability method, the reselection method, the quadratic collision probability method and the importance sampling method. Because the reciprocial condition is satified in this example (with the monoenergetic particle and the infinite homogeneous medium as well), the reciprocal Monte Carlo is also used to get the standard result.

The computation has been done for each case of $R_0=2$, 4, 6, 8 and 10. The computation results indicate that all results are in agreement with the standard result except the result with the directing probability method. In fact, when $R_0=4$, 6, 8, and 10, the results with the directing probability method are lower than the standard by 8%, 9%, 10% and 25% respectively. And the bounded estimate methods, such as the reselection method, the quadratic collision probability method and the importance sampling method, are better than the other unbounded estimate methods in variance and efficiency. Among them, some methods are quite good. The variance and efficiency of the reselection method, the quadratic collision probability method and the importance sampling method are shown in the Figs. 5—6. From these figures, it is clear that the variance of the quadratic collision probability method and the importance sampling method are always less than that of the reselection method, and their efficiency is higher than mat of the reselection method. In fact, their variance is reduced by 50%, and their efficiency is raised 2 and 4 times.



——·—— the reselection method;
---×--- quadratic collision probability method;
···○··· importance sampling method.

Fig. 5 The variance of various methods



——·—— the reselection method;
---×--- quadratic collision probability method;
···○··· importance sampling method.

Fig. 6 The efficiency of various methods

Appendix:

Let $\boldsymbol{i}=\boldsymbol{\Omega}^0_{n-2}$. $\boldsymbol{i}$, $\boldsymbol{j}$ and $\boldsymbol{k}$ together form a coordinate system. Then $\boldsymbol{\Omega}_{n-2}$ is sampled from the distribution $f_{n-2}(\boldsymbol{\Omega}_{n-2})$ below:

$$\boldsymbol{\Omega}_{n-2}=\cos\pi\xi\cdot\boldsymbol{i}+\sin\pi\xi\cdot\boldsymbol{j},$$

where ξ is a random number. While the sampling method from the distribution $f_{n-1}(\boldsymbol{\Omega}_{n-2}\rightarrow\boldsymbol{\Omega}_{n-1})$ is as follows:

$$\boldsymbol{\Omega}_{n-1}=\sin\alpha\cos 2\pi\xi_1\cdot\boldsymbol{i}+\sin\alpha\sin 2\pi\xi_1\cdot\boldsymbol{j}+\cos\alpha\cdot\boldsymbol{k},$$

where ξ_1 is a random number, too, α is the angle formed by $\boldsymbol{\Omega}_{n-1}$ and $\boldsymbol{\Omega}^0_{n-2}\times\boldsymbol{\Omega}_{n-2}$, it is defined from the following equation

$$\cos\alpha=(2\xi_2-1)\cdot|2\xi_2-1|,$$

ξ_2 is a random number like ξ_1. Sampling from the distribution $f_n(\boldsymbol{\Omega}_{n-2}\to\boldsymbol{\Omega}_n)$ is same as from the distribution $f_{n-1}(\boldsymbol{\Omega}_{n-2}\to\boldsymbol{\Omega}_{n-1})$.

References

[1] C. J. Everett, E. D. Cashwell, O. W. Rechard, LA-1583, 1953.
[2] C. W. Maynard, *Nucl. Sci. Eng.*, 10, 97, 1961.
[3] M. H. Kalos, *Nucl. Sci. Eng.*, 33, 284, 1968.
[4] B. Eriksson, C. Johansson, M. Leimdorfer, M. H. Kalos, *Nucl. Sci. Eng.*, 37, 410, 1969.
[5] Pei Lu-cheng, *Sciences and Techniques*, 1, 16, 1980. (in Chinese)
[6] Pei Lu-cheng, Dong Xiu-fang, *Sciences and Techniques*, 4, 236, 1963. (in Chinese)
[7] M. H. Kalos, *Nucl. Sci. Eng.*, 16, 111, 1963.
[8] J. Spanier, E. M. Gelbard, Monte Carlo principles and neutron transport problems, Addison-Wesley Reading, Massachusetts, 1969.
[9] Г. А. Михайлов, Некоторые вопросы теории методов Монте-Карло, Новосибирск, «Наука», 1974.
[10] H. A. Steinberg, M. H. Kalos, *Nucl. Sci. Eng.*, 44, 406, 1971.
[11] H. A. Steinberg, H. Lichtenstein, *Trans. Am. Nucl. Soc.*, 17, 259, 1973.
[12] H. A. Steinberg, ANL-75-2, 282, 1974.
[13] H. J. Kalli, E. D. Cashwell, LA-6865-MS, 1977.
[14] J. E. Hoogenboom, ANL-75-2, 243, 1974.
[15] Pei Lu-cheng, *Sciences and Techniques*, 6, 422, 1963. (in Chinese)
[16] Pei Lu-cheng and Zhang Xiao-ze, Monte Carlo method and its application to the particle transport problem, Sciences Press, 1980. (in Chinese)