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On the Use of Importance Sampling in Particle Transport Problems

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Abstract

The idea of importance sampling is applied to the problem of solving integral equations of Fredholm's type. Especially Bolzmann's neutron transport equation is taken into consideration. For the solution of the latter equation, an importance sampling technique is derived from some simple transformations at the original transport equation into a similar equation. Examples of transformations are given, which have been used with great success in practice.

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1. Introduction

Calculation of the particle flux which emanates from a known particle source in a given medium by the Monte Carlo method, according to the probability distributions which form the basis for the physical particle transport, may be very time-consuming. For instance, if the particel flux in a small region of the medium is to be calculated, only a small part of the observation material will essentially contribute to the answer. The same is true when one wishes to calculate the flux in regions which are far from the particle source, or in regions which are near the outer boundary of the medium.

Methods for reducing such disadvantages will be discussed in this paper. These methods may be briefly described as follows. The original probability distributions are substituted by new ones such that they emphasize parts of the sample space which contribute more to the final result than other parts, at the same time as the basic estimating variable is changed in order to conserve its property of being unbiased.

The above procedure is called importance sampling.

2. Integral equations

Many particle transport problems consist in calculating an integral of the form

$$I = \int g(x)\, \chi(x)\, dx \tag{1}$$

where $g(x) \geq 0$ and where $\chi(x)$ satisfies an integral equation of Fredholm's type

$$\chi(x) = \int \chi(x')\, K(x|x')\, dx' + p_o(x) \tag{2}$$

with

$$\begin{cases} p_o(x) \geq 0 \quad , \quad \int p_o(x)\, dx = 1 \\ K(x|x') = k(x')\, p(x|x') \\ \int p(x|x')\, dx = 1 \end{cases} \tag{3}$$

The above problem may be solved by the Monte Carlo method, provided that the following decompositions are possible:

$$\begin{cases} \chi(x) = \chi_0(x) + \chi_1(x) + \chi_2(x) + \ldots. \\ \chi_0(x) = p_0(x) \\ \chi_\nu(x) = \int \chi_{\nu-1}(x')\, K(x|x')\, dx' \\ \qquad = \int\int \ldots \int p_0(x_0)\, K(x_1|x_0) \ldots K(x|x_{\nu-1})\, dx_0\, dx_1 \ldots dx_{\nu-1} \\ \qquad \nu = 1, 2, 3, \ldots \end{cases} \tag{4}$$

and

$$\begin{cases} I = I_0 + I_1 + I_2 + \ldots \\ I_\nu = \int g(x)\, \chi_\nu(x)\, dx \quad , \quad \nu = 0, 1, 2, \ldots \end{cases} \tag{5}$$

Sufficient conditions for these decompositions are that

$$|| K || = \max_x \int K(x'|x)\, dx' < 1$$

and that the integral (6)

$$\int g(x)\, dx$$

exists.

2.1 A "naive" Monte Carlo solution

Assuming (6), a straightforward (naive) Monte Carlo calculation of the Nth partial sum for the infinite series (5)

$$J_N = I_0 + I_1 + \ldots + I_N \tag{7}$$

is as follows:

Generate a random walk

$$\gamma_N = (x_0, x_1, \ldots, x_N) \tag{8}$$

according to the following sampling scheme.
Choose x_0 according to the frequency function

$$p_0(x) \tag{9}$$

and x_ν successively from the transition probabilities

$$p(x_\nu | x_{\nu-1}) \qquad \nu = 1, 2, \ldots, N \tag{10}$$

The probability of the sequence γ_N is

$$dP(\gamma_N) = p_o(x_o)\, p(x_1 | x_o) \ldots p(x_N | x_{N-1})\, dx_o\, dx_1 \ldots dx_N \tag{11}$$

Estimate J_N by

$$\hat{J}_N(\gamma_N) = \hat{I}_o(\gamma_N) + \hat{I}_1(\gamma_N) + \ldots + \hat{I}_N(\gamma_N) \tag{12}$$

where

$$\hat{I}_o(\gamma_N) = g(x_o)$$

and

$$\hat{I}_n(\gamma_N) = k(x_o)\, k(x_1) \ldots k(x_{n-1})\, g(x_n) \ , \quad n = 1, 2, 3, \ldots, N \tag{13}$$

This estimator is unbiased because

$$E\, \hat{J}_N = E\, \hat{I}_o + E\, \hat{I}_1 + \ldots + E\, \hat{I}_N \tag{14}$$

and

$$E\, I_n(\gamma_N) = \int I_n(\gamma_N)\, dP(\gamma_N)$$

1) $$= \iint \ldots \int \left[\prod_{\nu=o}^{n-1} k(x_\nu)\, g(x_n)\, p_o(x_o) \right] \left[\prod_{\nu=1}^{N} p(x_\nu | x_{\nu-1}) \right] dx_o\, dx_1 \ldots dx_N$$

$$= \iint \ldots \int p_o(x_o) \left[\prod_{\nu=1}^{n} K(x_\nu | x_{\nu-1})\, g(x_n) \right] dx_o\, dx_1 \ldots dx_n \cdot$$

$$\cdot \iint \ldots \int \left[\prod_{\nu=n+1}^{N} p(x_\nu | x_{\nu-1}) \right] dx_{n+1} \ldots dx_n$$

$$= \int \chi_n(x_n)\, g(x_n)\, dx_n \cdot 1$$

$$= I_n \tag{15}$$

In the above calculations the relations (13), (11), (3) and (4) have been used in the stated order.

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1) Define $\prod_{\nu=o}^{-1} k(x_\nu) = 1$ and $K(x_o | x_{-1}) = 1$, then the calculations (15) are true also for $n = 0$.

Hence

$$E\,\hat{J}_N = I_o + I_1 + \ldots + I_N = J_N \tag{16}$$

2.2 Importance sampling

Instead of sampling random walk histories according to the "natural" probability densities $p_o(x)$ and $p(x|x')$, we may sample according to some other densities

$$p_o^*(x) \text{ and } p^*(x|x') \tag{17}$$

with $\int p_o^*(x)\,dx = 1$, $\int p^*(x|x')\,dx = 1$

at the same time as we change the estimating variable $\hat{J}_N(\gamma_N)$ to a new one, $\hat{J}_N^*$, in such a way that their mean values are the same.

We assume that the transition probabilities (17) are such that

2) $$p_o(x_o)\left[\prod_{\nu=1}^{n} K(x_\nu|x_{\nu-1})\right] g(x_n) > 0$$

implies

2) $$p_o^*(x) \prod_{\nu=1}^{n} p^*(x_\nu|x_{\nu-1}) > 0 \tag{18}$$

for $n = 0, 1, 2 \ldots.$

Let

$$\gamma_N = (x_o, x_1, \ldots, x_N)$$

be a random walk where x_o has been chosen according to $p_o^*(x_o)$ and the successive x_ν according to the transition probabilities $p^*(x_\nu|x_{\nu-1})$, $\nu = 1, 2, \ldots, N$.

Estimate the partial sum (7) by

$$\hat{J}_N^*(\gamma_N) = \hat{I}_o^*(\gamma_N) + \hat{I}_1^*(\gamma_N) + \ldots + \hat{I}_N^*(\gamma_N) \tag{19}$$

where

---

2) Define $\prod_{\nu=1}^{0} a_\nu = 1$

2) $$\hat{I}_n^* (\gamma_N) = \frac{p_o(x_o) \prod_{\nu=1}^{n} K(x_\nu | x_{\nu-1})}{p_o^*(x_o) \prod_{\nu=1}^{n} p^*(x_\nu | x_{\nu-1})} \cdot g(x_n) \qquad (20)$$

It is easily seen that the above estimator is unbiased. The probability for γ_N is

$$dP^*(\gamma_N) = p_o^*(x_o) \left[\prod_{\nu=1}^{N} p^*(x_\nu | x_{\nu-1}) \right] dx_o \, dx_1 \ldots dx_N$$

and the mean value of $\hat{I}_n^*$ is as follows

$$E \hat{I}_n^* (\gamma_N) = \int I_n^* (\gamma_N) \, dP^* (\gamma_N)$$

$$= \iint \ldots \int \frac{p_o(x_o) \prod_{\nu=1}^{n} K(x_\nu | x_{\nu-1})}{p_o^*(x_o) \prod_{\nu=1}^{n} p^*(x_\nu | x_{\nu-1})} \cdot g(x_n) \cdot p_o^*(x_o) \cdot$$

$$\cdot \left[\prod_{\nu=1}^{N} p^*(x_\nu | x_{\nu-1}) \right] dx_o \, dx_1 \ldots dx_N$$

$$= \iint \ldots \int p_o(x_o) \left[\prod_{\nu=1}^{n} K(x_\nu | x_{\nu-1}) \, g(x_n) \right] dx_o \, dx_1 \ldots dx_n \cdot$$

$$\cdot \iint \ldots \int \left[\prod_{\nu=n+1}^{N} p^*(x_\nu | x_{\nu-1}) \right] dx_{n+1} \ldots dx_N$$

$$= I_n \cdot 1 = I_n$$

(Assumption (18) is used in the above calculations). A similar sampling technique is found in [5] p. 89.

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2) Define $\prod_{\nu=1}^{0} a_\nu = 1$

2.2.1 The variance

The only assumption about the transition probabilities (17) which up to now has been made, is (18), and this assumption was necessary for that the estimator (19) should be unbiased. In order to compare different importance sampling techniques, we need a measure for the precision of this estimator. As such a measure we choose the variance

$$D_N^{*\,2} = E\,(\hat{J}_N^{*}(\gamma_N))^2 - J_N^2 ,$$

thus only such transition probabilities (17) for which the above variance exists, are capable of being used for the estimate at J_N (provided that they satisfy (18) too).

The problem of calculating the above variance is of least the same degree of difficulty as the problem of calculating the unknown I itself. Therefore, beside every practical Monte Carlo calculating of I, an estimation of the variance should be made.

2.2.2 A zero variance sampling scheme for I_n

Consider the following importances sampling scheme. Calculate first the following functions recursively

$$\psi_n(x) = g(x) \tag{21}$$

$$\psi_{\nu-1}(x) = \int K(x'|x)\,\psi_\nu(x')\,dx' , \quad \nu = n, n-1, \ldots, 2, 1$$

and generate

$$\gamma_n = (x_0, x_1, \ldots x_n)$$

according to

$$p^*(x_0) = \frac{p_0(x_0)\ \psi_0(x_0)}{\int p_0(x_0)\ \psi_0(x_0)\,dx_0} \tag{22}$$

and

$$p_\nu^*(x_\nu|x_{\nu-1}) = K(x_\nu|x_{\nu-1})\ \frac{\psi_\nu(x_\nu)}{\psi_{\nu-1}(x_{\nu-1})} , \quad \nu = 1, 2, \ldots, n \tag{23}$$

The construction (21) of the functions $\psi_0(x)$, $\psi_1(x)$, ... , $\psi_n(x)$ implies that

$$\int p_\nu^*(x_\nu | x_{\nu-1})\, dx_\nu = 1 \tag{24}$$

and that

$$\int p_o(x_o)\ \psi(x_o)\ dx_o = \int\int\ldots\int p_o(x_o) \left[\prod_{\nu=1}^{n} K(x_\nu | x_{\nu-1}) \right] g(x_n) \cdot$$

$$\cdot\, dx_o\ dx_1\ \ldots\ dx_n = I_n \tag{25}$$

The estimator (20) now takes the form

$$I_n^*(\gamma_n) = \frac{p_o(x_o) \left[\prod_{\nu=1}^{n} K(x_\nu | x_{\nu-1}) \right] g(x_n)}{\frac{p_o(x_o)\ \psi_o(x_o)}{I_n} \left[\prod_{\nu=1}^{n} K(x_\nu | x_{\nu-1}) \frac{\psi_\nu(x_\nu)}{\psi_{\nu-1}(x_{\nu-1})} \right]}$$

$$= I_n \cdot \frac{g(x_n)}{\psi_n(x_n)}$$

$$= I_n \tag{26}$$

This estimator is no longer a random variable and thus has the varaince zero.

Another zero variance sampling technique is found in [2] and [3].

3. A physical application

3.1 Definitions

Consider particles (neutrons) in a space

$$R = \{(\overline{r}, \overline{E})\} \tag{27}$$

where

$\bar{r}$	is the spatial vector	
$\bar{E} = E\bar{\Omega}$	is the directed energy, $E = \lvert\bar{E}\rvert$, and	(28)
$\bar{\Omega}$	is the unit direction vector	

The spatial part of R consists of a medium whose atoms are randomly distributed.

The particles are introduced into R according to a density function

$$p_o(\bar{r}, \bar{E})$$

$$p_o \geq 0 \ , \quad \iint p_o(\bar{r}, \bar{E}) \, d\bar{r} \, d\bar{E} = 1 \qquad (29)$$

These particles do not interact with one another, but they collide with the atoms in the medium and get new energies and moving directions. The particles move in straight lines and with unchanged energies between their collision points.

The motion of the particles is completely described in terms of <u>the flux, $\Phi(\bar{r}, \bar{E})$</u> , and <u>the density of particles leaving collisions</u> , <u>$\chi(\bar{r}, \bar{E})$</u>.

The function $\chi(\bar{r}, \bar{E})$ is defined through the <u>transport equation</u>

$$\chi(\bar{r}, \bar{E}) = \iint \chi(\bar{r}', \bar{E}') \ K(\bar{r}, \bar{E} \,|\, \bar{r}', \bar{E}') \, d\bar{r}' \, d\bar{E}' + p_o(\bar{r}, \bar{E}) \qquad (30)$$

The kernel K is so defined that the mean number of particles leaving a collision in the region V, provided that they have left the preceding collision at $(\bar{r}', \bar{E}')$, is given by

$$\iint_V K(\bar{r}, \bar{E} \,|\, \bar{r}', \bar{E}') \, d\bar{r}' \, d\bar{E}' \qquad (31)$$

We write the kernal K into the form

$$K(\bar{r}, \bar{E} \,|\, \bar{r}', \bar{E}') = c(\bar{E}') \, p(\bar{r}, \bar{E} \,|\, \bar{r}', \bar{E}') \qquad (32)$$

where $p(\bar{r}, \bar{E} \,|\, \bar{r}', \bar{E}')$ is the probability density for transition from the state $(\bar{r}', \bar{E}')$ to the state $(\bar{r}, \bar{E})$.

This transition probability can be factorized into a transport part p_T and a collision part p_c

$$p(\bar{r}, \bar{E} | \bar{r}', \bar{E}') = p_T(\bar{r} | \bar{r}', \bar{E}') \cdot p_c(\bar{E} | \bar{E}', \bar{r}) \tag{33}$$

Apart from the necessary delta functions that ensure that the next collision lies along a ray emanating from $\bar{r}$ with direction $\bar{\Omega}$, p_T has the form of a probability that the next collision takes place at a distance $(\ell, \ell + d\ell)$ along that ray

$$p_T(\bar{r} + \bar{\Omega} \cdot \ell | \bar{r}, E\bar{\Omega})\, d\ell = \Sigma(\bar{r} + \bar{\Omega}\ell, \bar{E}) \cdot \mathrm{EXP}\left[-\int_0^{\ell} \Sigma(\bar{r} + \bar{\Omega}\ell', \bar{E}) d\ell' \right] d\ell \tag{34}$$

where the function Σ is termed the total cross section and depends on the energy E of the particle and of the medium. The corresponding distribution function is

$$P_T(\bar{r} + \bar{\Omega}\ell | \bar{r}, E\bar{\Omega}) = \int_0^{\ell} p_T(\bar{r} + \Omega\ell' | \bar{r}, E\bar{\Omega})\, d\ell'$$

$$= 1 - \mathrm{EXP}\left[-\int_0^{\ell} \Sigma(\bar{r} + \bar{\Omega}\ell', \bar{E})\, d\ell' \right] \tag{35}$$

Provided that a particle with the energy $\bar{E}'$ collides at the point $\bar{r}$, then

$$\int_V p_c(\bar{E} | \bar{E}', \bar{r})\, d\bar{E}, \tag{36}$$

is the probability that its new energy $\bar{E}$ lies in the volume V of the energy space. We assume that this probability is already normalized:

$$\int p_c(\bar{E} | \bar{E}', \bar{r})\, d\bar{E} = 1 \tag{37}$$

where the integral is taken over the whole energy space. This probability may be very complicated in analytical form.

The flux $\Phi(\overline{r},\overline{E})$ is defined through the relation

$$\Phi(\overline{r},\overline{E}) = \int \chi(\overline{r}',\overline{E})\, Q_T(\overline{r}|\overline{r}',\overline{E})\, d\overline{r}' \tag{38}$$

where

$$Q_T(\overline{r}|\overline{r}',\overline{E}) = 1 - P_T(\overline{r}|\overline{r}',\overline{E}) = \frac{p_T(\overline{r}|\overline{r}',\overline{E})}{\Sigma(\overline{r},\overline{E})} \tag{39}$$

is the probability that the next collision will occur "beyond the point $\overline{r}$". Using (30), (32), (33), (34), (38) and (39), one may show [2] that $\Phi(\overline{r},\overline{E})$ satisfies the following integro-differential equation.

$$\overline{\Omega} \cdot \text{grad}\, \Phi(\overline{r},\overline{E}) + \Sigma(\overline{r},\overline{E})\, \Phi(\overline{r},\overline{E}) =$$

$$= \iint \Sigma(\overline{r},\overline{E}')\, \Phi(\overline{r},\overline{E}')\, C(\overline{E}|\overline{E}',\overline{r})\, d\overline{E}' + p_o(\overline{r},\overline{E}) \tag{40}$$

where

$$C(\overline{E}|\overline{E}',\overline{r}) = c(\overline{E}')\, p_c(\overline{E}|\overline{E}',\overline{r}) \tag{41}$$

and where the gradient is taken with regard to $\overline{r}$.

3.2 A problem

Consider the following problem:
Calculate the integral

$$I = \int \Phi(\overline{r},\overline{E})\, f(\overline{r},\overline{E})\, d\overline{E} \tag{42}$$

where Φ is the flux, defined in (38), and f a given function.

Substituting (38) into the above integral, we get

3) $$I = \iint \chi(\overline{r}',\overline{E})\, g(\overline{r}',\overline{E};\overline{r})\, d\overline{r}'\, d\overline{E}$$

where

$$g(\overline{r}',\overline{E};\overline{r}) = Q_T(\overline{r}|\overline{r}',\overline{E})\, f(\overline{r},\overline{E})$$

---

3) The r -dependence is not indicated.

and where χ satisfies the integral equation (30).

The problem is now a special case of that considered in §2, and is solved in the same way provided that the decompositions (4) and (5) are possible.

Assuming (4), (5) and that

$$\int_0^\infty p_T(r + \overline{\Omega}\ell, \overline{E})\, d\ell = 1 \tag{43}$$

a straightforward Monte Carlo solution of our problem is as follows.

Generate a random walk

$$\gamma_N = (\overline{r}_o, \overline{E}_o; \overline{r}_1, \overline{E}_1; \ldots; \overline{r}_N, \overline{E}_N) \;,$$

where $\overline{E}_n = E_n \overline{\Omega}_n$, in the following way.

Sample first $\overline{r}_o, \overline{E}_o$ according to the frequency function

$$p_o(\overline{r}_o, \overline{E}_o)$$

Write

$$\overline{r}_\nu = \overline{r}_{\nu-1} + \overline{\Omega}_{\nu-1}\, \ell_\nu \tag{44}$$

and choose ℓ_ν from

$$p_T(\overline{r}_{\nu-1} + \overline{\Omega}_{\nu-1}\, \ell_\nu | \overline{r}_{\nu-1}, \overline{E}_{\nu-1})$$

Then choose $\overline{E}_\nu$ from

$$p_c(\overline{E}_\nu | \overline{E}_{\nu-1}, \overline{r}_\nu)$$

Repeat the above procedure for $\nu = 1, 2, \ldots, N$.

Estimate the Nth partial sum of the infinite series expansion (5) of the integral I by

$$\hat{J}_N(\gamma_N) = \hat{I}_o(\gamma_N) + \ldots + \hat{I}_N(\gamma_N)$$

where

1) $\hat{I}_n(\gamma_N) = c(E_o)\, c(E_1) \ldots c(E_{n-1})\, g(\bar{r}_n, \bar{E}_n; \bar{r})$, $n=0, 1, \ldots, N$ (45)

3.3 Derivation of an importance sampling technique

We shall now derive an importance sampling technique from a simple transformation of the flux. The transformation is

$$\Phi^*(\bar{r},\bar{E}) = \frac{\Phi(\bar{r},\bar{E})}{\psi(\bar{r},\bar{E})} \Bigg/ \iint \frac{p_o(\bar{r},\bar{E})}{\psi(\bar{r},\bar{E})}\, d\bar{r}\, d\bar{E} \qquad (46)$$

where the function ψ is

a) positive

b) continuous with continuous derivatives (not a necessary condition)

c) such that

$$\Sigma(\bar{r},\bar{E}) + \bar{\Omega} \cdot \frac{\text{grad}\, \psi(\bar{r},\bar{E})}{\psi(\bar{r},\bar{E})} \geq 0 \qquad (47)$$

Write the transport equation (40) for the flux Φ into the form

$$L(\Sigma, C)\ \Phi = p_o \qquad (48)$$

where L symbolizes the integro-differential operator defined in the equation (40). The transformation (46) introduced into the equation (48) gives birth to a new transport equation (see Appendix)

$$L(\Sigma^*, C^*)\ \Phi^* = p_o^* \qquad (49)$$

---

1) (Put $c(E-1) = 1$)

where

$$\begin{cases} \Sigma^*(\bar{r},\bar{E}) = \Sigma(\bar{r},\bar{E}) + \bar{\Omega} \cdot \dfrac{\text{grad } \psi(\bar{r},\bar{E})}{\psi(\bar{r},\bar{E})} & (50) \\ \\ C^*(\bar{E}|\bar{E}',\bar{r}) = \dfrac{\Sigma(\bar{r},\bar{E})}{\Sigma^*(\bar{r},\bar{E})} \cdot \dfrac{\psi(\bar{r},\bar{E}')}{\psi(\bar{r},\bar{E})} \cdot C(\bar{E}|\bar{E}',\bar{r}) & (51) \\ \\ p_o^*(\bar{r},\bar{E}) = \dfrac{p_o(\bar{r},\bar{E})}{\psi(\bar{r},\bar{E})} \Bigg/ \displaystyle\iint \dfrac{p_o(\bar{r},\bar{E})}{\psi(\bar{r},\bar{E})}\, d\bar{r}\, d\bar{E} & (52) \end{cases}$$

The frequency function which gives birth to the new cross section Σ^* is

$$p_T^*(\bar{r}+\bar{\Omega}\ell|\bar{r},\bar{E}) = \Sigma^*(\bar{r}+\bar{\Omega}\ell,\bar{r}) \cdot \text{EXP}\left[-\int_0^\ell \Sigma^*(\bar{r}+\bar{\Omega}\ell',\bar{E})\, d\ell'\right], \quad (53)$$

or, if we introduce (50) and take account of the assumption b) and of (33),

$$p_T^*(\bar{r}+\bar{\Omega}\ell|\bar{r},\bar{E}) = \Sigma^*(\bar{r}+\bar{\Omega}\ell,\bar{E})\, \text{EXP}\left\{-\int_0^\ell \left[\Sigma(\bar{r}+\bar{\Omega}\ell',\bar{E}) + \frac{\frac{d}{d\ell'}\psi(\bar{r}+\bar{\Omega}\ell',\bar{E})}{\psi(\bar{r}+\bar{\Omega}\ell',\bar{E}}\right] d\ell'\right\}$$

$$= \Sigma^*(\bar{r}+\bar{\Omega}\ell,\bar{E})\, \frac{\psi(\bar{r},\bar{E})}{\psi(\bar{r}+\bar{\Omega}\ell,\bar{E})}\, \text{EXP}\left[-\int_0^\ell \Sigma(\bar{r}+\bar{\Omega}\ell',\bar{E})\, d\ell'\right]$$

$$= \frac{\Sigma^*(\bar{r}+\bar{\Omega}\ell,\bar{E})}{\Sigma(\bar{r}+\bar{\Omega}\ell,\bar{E})} \cdot \frac{\psi(\bar{r},\bar{E})}{\psi(\bar{r}+\bar{\Omega}\ell,\bar{E})} \cdot p_T(\bar{r}+\bar{\Omega}\ell|\bar{r},\bar{E}) \quad (54)$$

The corresponding distribution function is

$$p_T^*(\bar{r}+\bar{\Omega}\ell|\bar{r},\bar{E}) = 1 - \frac{\psi(\bar{r},\bar{E})}{\psi(\bar{r}+\bar{\Omega}\ell,\bar{E})}\, \text{EXP}\left[-\int_0^\ell \Sigma(\bar{r}+\bar{\Omega}\ell',\bar{E})\, d\ell'\right] \quad (55)$$

Consider now the frequency function for the initial state

$$p_o^*(\bar{r},\bar{E})$$

and the frequency function for transition from state $(\bar{r}_{\nu-1},\bar{E}_{\nu-1})$ to $(\bar{r}_\nu,\bar{E}_\nu)$:

$$p^*(\bar{r}_\nu,\bar{E}_\nu \,|\bar{r}_{\nu-1},\bar{E}_{\nu-1}) = p_T^*(\bar{r}_\nu|\bar{r}_{\nu-1},\bar{E}_{\nu-1})p_c(\bar{E}_\nu|\bar{E}_{\nu-1},\bar{r}_\nu) \quad (56)$$

According to the above frequency functions, we generate a random walk

$$\gamma_N = (\bar{r}_o,\bar{E}_o;\bar{r}_1,\bar{E}_1; \ldots;\bar{r}_N,\bar{E}_N)$$

and estimate the Nth partial sum for the series (5) for I by

$$\hat{J}_N^*(\gamma_N) = \hat{I}_o^*(\gamma_N) + \hat{I}_1(\gamma_N) + \ldots + I_N^*(\gamma_N) \qquad (57)$$

where

$$\hat{I}_N^*(\gamma_N) = \frac{p_o(\bar{r}_o,\bar{E}_o)\prod_{\nu=1}^{n} K(\bar{r}_\nu,\bar{E}_\nu|\bar{r}_{\nu-1},\bar{E}_{\nu-1})}{p_o^*(\bar{r}_o,\bar{E}_o)\prod_{\nu=1}^{n} p^*(\bar{r}_\nu,\bar{E}_\nu|\bar{r}_{\nu-1},\bar{E}_{\nu-1})} \cdot g(\bar{r}_n,\bar{E}_n;\bar{r}) \qquad (57a)$$

Into the above estimator we put the expression for K, p_o^* and p^*, as they are defined in (32), (33), (52) and (56). We then get

$$\hat{I}_N^{*}(\gamma_N) = S \cdot \psi(\bar{r}_o,\bar{E}_o)\prod_{\nu=1}^{n}\frac{p_T(\bar{r}_\nu|\bar{r}_{\nu-1},\bar{E}_{\nu-1})\,c(\bar{E}_{\nu-1})}{p_T^*(\bar{r}_\nu|\bar{r}_{\nu-1},\bar{E}_{\nu-1})} \cdot g(\bar{r}_n,\bar{E}_n;\bar{r})$$

where

$$S = \int \frac{p_o(\bar{r},\bar{E})}{\psi(\bar{r},\bar{E})}\,d\bar{r}\,d\bar{E} \qquad (57b)$$

If we take account of (54), we get

$$\hat{I}_n^*(\gamma_N) = S \cdot \psi(\bar{r}_o, \bar{E}_o) \left[\prod_{\nu=1}^{n} \frac{\Sigma(\bar{r}_\nu, \bar{E}_{\nu-1})\ \psi(\bar{r}_\nu, \bar{E}_{\nu-1})\ c(\bar{E}_{\nu-1})}{\Sigma^*(\bar{r}_\nu, \bar{E}_{\nu-1})\ \psi(\bar{r}_{\nu-1}, \bar{E}_{\nu-1})} \right] \cdot$$

$$\cdot\ g(\bar{r}_n, \bar{E}_n; \bar{r}) \tag{57c}$$

According to (51) and (41) we may also write

$$\hat{I}_n^*(\gamma_N) = S \left[\prod_{\nu=1}^{n} \frac{C^*(\bar{E}_\nu | \bar{E}_{\nu-1}, \bar{r}_\nu)}{p_c(\bar{E}_\nu | \bar{E}_{\nu-1}, \bar{r}_\nu)} \right] \cdot \psi(\bar{r}_n, \bar{E}_n)\ g(\bar{r}_n, \bar{E}_n; \bar{r}) \tag{57d}$$

3.3.1 Example 1

The problem is now to calculate the particle flux Φ in the neighbourhood of the point $\bar{r} = \bar{r}_Q$ in the spatial space.

For simplicity, assume that the total cross section does not depend on the spatial vector $\bar{r}$:

$$\Sigma = \Sigma(\bar{E})$$

Denote

$$\bar{r} = ix + jy + kz$$

$$\bar{\Omega} = i\alpha + j\beta + k\gamma$$

where α, β, γ are the ordinary direction cosines.

We should like to construct a new flux Φ^* which emphasizes the particle motion against the point $\bar{r}_Q$. Consider the transformation

$$\Phi^*(\bar{r}, \bar{E}) = \text{const.} \cdot \Phi(\bar{r}, \bar{E}) / \psi(\bar{r}, \bar{E})$$

where

$$\psi(\bar{r}, \bar{E}) = \text{EXP}\left[c(E)\Sigma(E) \left| \bar{r} - \bar{r}_Q \right| \right], \tag{58}$$

$$0 < c(E) < 1 ,$$

$|\bar{r}-\bar{r}_Q|$ = distance between $\bar{r}$ and $\bar{r}_Q$

This transformation gives birth to a new transport frequency function

$$p_T^*(\bar{r}+\bar{\Omega}\ell\,|\,\bar{r},\bar{E}) = \Sigma^*(\bar{r}+\bar{\Omega}\ell,\bar{E})\ \mathrm{EXP}\left[-\int_0^{\ell}\Sigma^*(\bar{r}+\bar{\Omega}\ell',\bar{E})\ d\ell'\right]$$

with

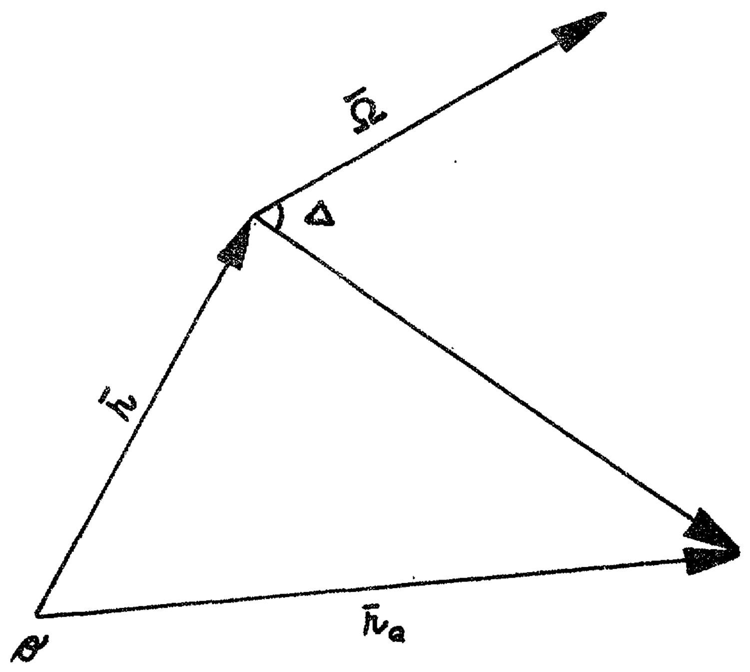
$$\Sigma^* = \Sigma + \bar{\Omega}\cdot\frac{\mathrm{grad}\,\psi}{\psi}$$

$$= \Sigma(E) + c(E)\ \Sigma(E)\ (i\alpha + j\beta + k\gamma)\ \mathrm{grad}\sqrt{(x-x_Q)^2+(y-y_Q)^2+(z-z_Q)^2}$$

$$= \Sigma(E)\left[1 + c(E)\ (i\alpha + j\beta + k\gamma)\ \left(i\,\frac{x-x_Q}{|r-r_Q|} + j\,\frac{y-y_Q}{|r-r_Q|} + k\,\frac{z-z_Q}{|r-r_Q|}\right)\right]$$

$$= \Sigma(E)\ (1 - c(E)\cos\Delta) \qquad (59)$$

where Δ is the angle between the direction $\bar{\Omega}$ and the direction from $\bar{r}$ to $\bar{r}_Q$.



If L^* is the distance to the next collision, we may write

$$P(\ell < L^* \leq \ell + d\ell \,|\, L^* > \ell) = \Sigma^* = \Sigma(1 - c \cdot \cos \Delta) \tag{60}$$

and hence the cross section Σ^* may be considered as a "mortal intensity". This conditional probability has a minimum equal to $\Sigma(1 - c)$ for $\Delta = 0$, increases with increasing Δ and takes its maximum value $\Sigma(1 + c)$ for $\Delta = \Pi$. This means that the considered transformation (58) emphasizes the particle flux against the point $\overline{r}_Q$. The distribution function for the distance L^* to the next collision is, according to (55),

$$p_T^*(\overline{r}+\Omega\ell \,|\, \overline{r}, E\overline{\Omega}) = Pr(L^* \leq \ell \,|\, \overline{r}, \overline{E})$$

$$= 1 - EXP\left[-\Sigma(E)[\ell + c(E)(r_\ell - r_o)]\right] \tag{61}$$

where

$$r_\ell = |\overline{r} + \overline{\Omega}\ell - \overline{r}_Q|$$

Similar examples are found in [1], [2] and [6a].

3.4 Forced next collisions

If the point $\overline{r}_Q$ where the flux is to be calculated in the former example is near the outer boundary of the spatial space, important particles have a great probability of passing through this boundary and hence a great deal of information is missed. (Important particles are particles which have been observed in the neighbourhood of $\overline{r}_Q$).

Such disadvantages may be overcome by transformations of the old flux Φ to a new Φ^* , which vanishes at the outer boundary, which is the same as using transformation functions ψ which approach infinity at this boundary. We shall now construct such a transformation.

Consider first a transformation function which does not depend on the direction $\overline{\Omega}$

$$\psi = \psi(\overline{r}, E) \tag{62}$$

which has given birth to the cross section

$$\Sigma^*(\bar{r},\bar{E}) = \Sigma(\bar{r},E) + \bar{\Omega}\cdot\frac{\text{grad }\psi(\bar{r},E)}{\psi(\bar{r},E)} \tag{63}$$

with corresponding transport frequency function

$$p_T^*(\bar{r}+\bar{\Omega}\ell\,|\,\bar{r},\bar{E}) = \Sigma^*(\bar{r}+\bar{\Omega}\ell,\bar{r},\bar{E})\ \text{EXP}\left[-\int_0^{\ell}\Sigma^*(\bar{r}+\bar{\Omega}\ell',\bar{r},E)\,d\ell'\right] \tag{64}$$

and distribution function

$$P_T^*(\bar{r}+\bar{\Omega}\ell\,|\,\bar{r},\bar{E}) = 1 - \text{EXP}\left[-\int_0^{\ell}\Sigma^*(r+\bar{\Omega}\ell',\bar{r},\bar{E})\,d\ell'\right] \tag{65}$$

Consider then the transformation

$$\Phi_1^* = \Phi/\psi_1 \tag{66}$$

where the function ψ_1 is

$$\psi_1(\bar{r}+\bar{\Omega}\ell,\bar{E}) = \frac{\text{EXP}\left[\int_{\ell}^{G}\Sigma(\bar{r}+\bar{\Omega}\ell',E)\,d\ell'\right]}{\text{EXP}\left[\int_{\ell}^{G}\Sigma^*(\bar{r}+\bar{\Omega}\ell',\bar{E})\,d\ell'\right]-1} \tag{67}$$

where Σ is a given total cross section and Σ^* is defined in (63) and where

$$G = G(\bar{r}+\bar{\Omega}\ell,\bar{\Omega}) \tag{68}$$

is the distance from the point $\bar{r}+\bar{\Omega}\ell$ to the outer boundary in the direction $\bar{\Omega}$.

The above transformation gives birth to the following cross section

$$\Sigma_1^*(\bar{r}+\bar{\Omega}\ell,\bar{E}) = \Sigma(\bar{r}+\bar{\Omega}\ell) + \frac{d}{d\ell}\,\psi_1(\bar{r}+\bar{\Omega}\ell,\bar{E})/\psi_1(\bar{r}+\bar{\Omega}\ell,\bar{E})$$

where

$$\frac{\frac{d}{d\ell}\psi_1}{\psi_1} = \frac{-\dfrac{\mathrm{EXP}\left[\int_\ell^G \Sigma\, d\ell'\right]}{\mathrm{EXP}\left[\int_\ell^G \Sigma^* d\ell'\right]-1}\Sigma + \dfrac{\mathrm{EXP}\left[\int_\ell^G \Sigma\, d\ell'\right]}{\left[\mathrm{EXP}\left[\int_\ell^G \Sigma^* d\ell'\right]-1\right]^2}\cdot \mathrm{EXP}\left[\int_\ell^G \Sigma^* d\ell'\right]\Sigma^*}{\dfrac{\mathrm{EXP}\left[\int_\ell^G \Sigma\, d\ell'\right]}{\mathrm{EXP}\left[\int_\ell^G \Sigma^* d\ell'\right]-1}} =$$

$$= -\Sigma + \frac{\Sigma^* \mathrm{EXP}\left[\int_\ell^G \Sigma^* d\ell'\right]}{\mathrm{EXP}\left[\int_\ell^G \Sigma^* d\ell'\right] - 1}$$

and hence

$$\Sigma_1^*(\overline{r}+\overline{\Omega}\ell, \overline{E}) = \frac{\Sigma^*(\overline{r}+\overline{\Omega}\ell, \overline{E})}{1 - \mathrm{EXP}\left[-\int_\ell^G \Sigma^*(\overline{r}+\overline{\Omega}\ell', \overline{E})\, d\ell'\right]} \tag{69}$$

For the corresponding distribution function we have

$$p^*_{T_1}(\overline{r}+\overline{\Omega}\ell\,|\,\overline{r},\overline{E}) = 1 - \mathrm{EXP}\left[-\int_0^\ell \Sigma_1^*(\overline{r}+\overline{\Omega}\ell', \overline{r}, \overline{E})\, d\ell'\right]$$

$$= 1 - \frac{\psi_1(\overline{r},\overline{E})}{\psi_1(\overline{r}+\overline{\Omega}\ell, \overline{E})}\, \mathrm{EXP}\left[-\int_0^\ell \Sigma(\overline{r}+\overline{\Omega}\ell', E)\right]$$

$$= 1 - \frac{\mathrm{EXP}\left[\int_0^G \Sigma\, d\ell'\right]}{\mathrm{EXP}\left[\int_0^G \Sigma^* d\ell'\right] - 1} \cdot \frac{\mathrm{EXP}\left[\int_\ell^G \Sigma^* d\ell'\right] - 1}{\mathrm{EXP}\left[\int_\ell^G \Sigma\, d\ell'\right]} \cdot \mathrm{EXP}\left[-\int_0^\ell \Sigma\, d\ell'\right]$$

$$= \frac{\mathrm{EXP}\left[\int_0^G \Sigma^* d\ell'\right] - 1 - \mathrm{EXP}\left[\int_\ell^G \Sigma^* d\ell'\right] + 1}{\mathrm{EXP}\left[\int_0^G \Sigma^* d\ell'\right] - 1}$$

$$= \frac{\mathrm{EXP}\left[\int_0^G \Sigma^* d\ell'\right] \left\{1 - \mathrm{EXP}\left[-\int_0^\ell \Sigma^* d\ell'\right]\right\}}{\mathrm{EXP}\left[\int_0^G \Sigma^* d\ell'\right] \left\{1 - \mathrm{EXP}\left[-\int_0^G \Sigma^* d\ell'\right]\right\}}$$

$$= \frac{p_T^*(\overline{r}+\overline{\Omega}\ell \,|\, \overline{r}, \overline{E})}{p_T^*(\overline{r}+\overline{\Omega}G \,|\, \overline{r}, \overline{E})} \qquad 0 \leq \ell \leq G \qquad (70)$$

We observe that the above distribution function is normalized on the interval $(0, G)$, and hence the next collision is forced to occur inside the outer boundary.

3.4.1 Example 2

The problem is to calculate the flux Φ in the neighbourhood of the point $\overline{r} = \overline{r}_Q$ in a bounded medium. For simplicity, assume that $\Sigma = \Sigma(E)$ is a function of E only.

Consider the transformation in the former example:

$$\psi(\overline{r}, \overline{E}) = \text{const.} \cdot \mathrm{EXP}\left[c(E)\,\Sigma(E)|\overline{r} - r_Q|\right] \qquad (71)$$

with the corresponding cross section

$$\Sigma^*(\overline{r}, \overline{E}) = \Sigma(E)\,(1 - c(E)\cos\Delta) \qquad (72)$$

Consider then the transformation ψ_1 in (67) with the above expression for Σ^* . This transformation

a) emphasizes particles against the point $\overline{r}_Q$

b) does not allow any particle to escape at the boundary.

The distribution function for the distance to the next collision is, according to (70) and (61),

$$p^{*}_{T_1}(\bar{r}+\bar{\Omega}\ell\,|\,\bar{r},\bar{E}) = \frac{1 - \mathrm{EXP}\,\{-\Sigma(E)\,[\ell + c(E)\,(r_\ell - r_o)]\}}{1 - \mathrm{EXP}\,\{-\Sigma(E)\,[G + c(E)\,(r_G - r_o)]\}} \qquad (73)$$

where

$$r_t = |\bar{r} + \bar{\Omega}t - r_Q|$$

for

$$t = 0,\ \ell \text{ and } G\ ,\quad \text{where}\quad 0 \le \ell \le G$$

Numerical calculation indicate that the best choice of the function $c(E)$ is near unity.

Examples of similar importance sampling techniques are found in [4] and [6].

An extention of the above importance sampling technique has been used by the author to the problem of calculating the neutron-flux and the neutron dose in a bulkshield of a rather complicated configuration. This shield consists of a laminated cylinder through which a duct, divided into plugs, runs. Different materials and vacuum are allowed in each region of the shield. Numerical results will be published elsewhere.

4. Appendix

4.1 A transformation of the transport equation for the neutron flux

Introduce the transformation

$$\Phi^*(\bar{r},\bar{E}) = \frac{\Phi(\bar{r},\bar{E})}{\psi(\bar{r},\bar{E})} \Bigg/ S$$

where

$$S = \iint \frac{p_o(\bar{r},\bar{E})}{\psi(\bar{r},\bar{E})}\, d\bar{r}\; d\bar{E}$$

into the transport equation

$$\Omega \cdot \text{grad}\Phi(\bar{r},\bar{E}) + \Sigma(\bar{r}',\bar{E})\;\Phi(\bar{r},\bar{E})$$
$$= \iint \Sigma(\bar{r},\bar{E}')\;\Phi(\bar{r},\bar{E}')\;C(\bar{E},\bar{E}',\bar{r})\;dE' + p_o(\bar{r},\bar{E})$$

We then get, when we take account of

$$\Phi(\bar{r},\bar{E}) = S\;\Phi^*(\bar{r},\bar{E})\;\psi(\bar{r},\bar{E})$$

and

$$\text{grad}\Phi = S\;\text{grad}(\Phi^*\psi) = S\;\psi\;\text{grad}\Phi^* + S\;\Phi^*\;\text{grad}\;\psi\;,$$

the following

$$\Omega \cdot (S\;\psi(\bar{r},\bar{E})\;\text{grad}\Phi^*(\bar{r},\bar{E}) + S\;\Phi^*(\bar{r},\bar{E})\;\text{grad}\psi(\bar{r},\bar{E})\,)$$
$$+\;\Sigma(\bar{r},\bar{E})\;S\;\psi(\bar{r},\bar{E})\;\Phi^*(\bar{r},\bar{E})$$
$$= \iint \Sigma(\bar{r},\bar{E})\;\Phi^*(\bar{r},\bar{E}')\;\psi(\bar{r},\bar{E}')\;S\;C(\bar{E},\bar{E}',\bar{r})\;d\bar{E}' + p_o(\bar{r},\bar{E})$$

Divide by $S \cdot \psi(\bar{r},\bar{E})$ and group together terms containing Φ^*

$$\Omega \cdot \operatorname{grad}\Phi^{*}(\overline{r},\overline{E}) + \left(\Sigma(\overline{r},\overline{E}) + \Omega \frac{\operatorname{grad}\psi(\overline{r},E)}{\psi} \right) \Phi^{*}(\overline{r},\overline{E})$$

$$= \iint \Sigma(\overline{r},E)\ \Phi^{*}(\overline{r},\overline{E})\ \frac{\psi(\overline{r},\overline{E}')}{\psi(\overline{r},\overline{E})}\ C(\overline{E}|\overline{E}',\overline{r})\ d\overline{E}' + \frac{p_o(\overline{r},\overline{E})}{\psi(\overline{r},\overline{E})} \Big/ S$$

Denote

$$\begin{cases} \Sigma^{*}(\overline{r},\overline{E}) = \Sigma(\overline{r},\overline{E}) + \overline{\Omega}\ \dfrac{\operatorname{grad}\ \psi(\overline{r},\overline{E})}{\psi(\overline{r},\overline{E})} \\[2ex] C^{*}(\overline{E}|\overline{E}',\overline{r}) = \dfrac{\Sigma(\overline{r},\overline{E})\ \psi(\overline{r},\overline{E}')}{\Sigma^{*}(\overline{r},\overline{E})\ \psi(\overline{r},\overline{E})}\ C(\overline{E}|\overline{E}',\overline{r}) \\[2ex] p_o^{*}(\overline{r},\overline{E}) = \dfrac{p_o(\overline{r},\overline{E})}{\psi_o(\overline{r},\overline{E})} \Big/ S \end{cases}$$

We may then write

$$\overline{\Omega}\ \operatorname{grad}\Phi^{*}(\overline{r},\overline{E}) + \Sigma^{*}(\overline{r},\overline{E})\ \Phi^{*}(\overline{r},\overline{E})$$

$$= \iint \Sigma^{*}(\overline{r},\overline{E})\ \Phi^{*}(\overline{r},\overline{E})\ C^{*}(\overline{E}|\overline{E}',\overline{r})\ dE' + p_o^{*}(\overline{r},\overline{E})$$

The original equation has thus been transformed to a similar equation.

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Notations

$P_r(A)$	: the probability of the event A
X , Y	: stochastic variables
$p(x)$	: frequency function of X
$P(x) = \int_{-\infty}^{x} p(x)\,dx$	: distribution function of X
$p(x\|y)$	: Conditional frequency function of X given Y
$P(x\|y) = \int_{-\infty}^{x} p(x\|y)\,dx$	: conditional distribution function of X given Y
$E\,X = \int_{-\infty}^{+\infty} x\,f(x)\,dx$	: mean value of X

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