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SIMPLIFIED, ANALYTICALLY SOLVABLE MODEL PROBLEM FOR NON-ANALOG MONTE CARLO METHODS

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Abstract- In Monte Carlo particle transport, it is important to change the variance of calculations of relatively rare events with a technique known as non-analog Monte Carlo. In order to reduce the variance and the computation time, biasing techniques are introduced to accelerate the calculation convergence without changing the outcome. However these variance reduction techniques are often complex and can only be solved by computer codes. In this study, a simplified, analytically solvable model problem is introduced for non-analog Monte Carlo methods. A sample problem for neutrons passing through a thick shield is simulated. The drawback of this simulation is the expensive computation time and large variance for analog Monte Carlo methods. So, biasing techniques like implicit capture and splitting are introduced and the problem is solved analytically.

Keywords- Non-analog Monte Carlo, variance reduction, neutron transport

1. INTRODUCTION

By the increase in the computational power of computers, Monte Carlo methods have become more popular and widely useable in several areas of science and technology. Today's applications of Monte Carlo techniques include diagnostic imaging, radiation therapy, traffic flow, stock-exchange forecasting, oil well exploration and reactor design [1]. In analog Monte Carlo methods, the desired confidence level is achieved by increasing the number of particle history and as a result computation time. Thus, the performance of the Monte Carlo method is measured by using the figure of merit and defined as measure of the efficiency and given by,

$$FOM = 1/(TE^2) \tag{1}$$

where T is total computation time and E is relative error and defined as,

$$E^2 = \sigma_{\bar{x}}^2 / (N\bar{x}^2) \tag{2}$$

where $\sigma_{\bar{x}}^2$ is sample variance, $\bar{x}$ is sample mean. N is the number of particle history. T could be defined as $t_p N$ and t_p is the average computation time per sample history. Finally, the figure of merit becomes,

$$FOM = \bar{x}^2 / t_p \sigma_{\bar{x}}^2 \tag{3}$$

For a given model problem, the numerical value for the figure of merit could be estimated by using true mean and true variance if the average computation time per history is known. To increase the efficiency of the Monte Carlo methods, either computation time or relative error should be reduced with a given number of particle histories. To reduce the relative error without increasing the number of histories, non-analog Monte Carlo techniques (variance reduction techniques) are introduced. The main goal of non-analog Monte Carlo technique is to reduce sample variance so that the relative error decreases. Variance reduction (biasing) techniques for Monte Carlo simulations can also reduce the amount of computer time required for obtaining results of sufficient precision [2]. On the contrary, different types of variance reduction techniques may increase the computation time per sample history [3].

Many of the variance reduction techniques produce and/or destroy particles during the simulation per history to produce outcomes closer to the solution. In this manuscript, implicit capture (survival biasing) and splitting techniques are chosen for variance reduction. To solve a non-analog Monte Carlo problem analytically, a simplified neutron transport model problem is introduced and analytical expressions for the variance are determined. These analytical expressions for variance may be used to discuss the improvement in efficiency by means of variance reduction techniques.

2. THE MODEL PROBLEM

In this study, the forward neutron transport through one region and two region homogenous slabs are introduced as the model problem. In the modeling, differential scattering kernel is chosen in such a way that scattered neutrons are allowed to travel in forward direction only, so that, the angular coordinate system will only have the component $\Omega_x = \cos\theta$.

2.1. Homogeneous Slab Problem

Let us assume that a neutron beam enter at x=0 into the system (fig. 1). The objective of the simulation is to determine the number of neutrons exiting at x=L. The slab is characterized by total cross section Σ_t and scattering ratio c.

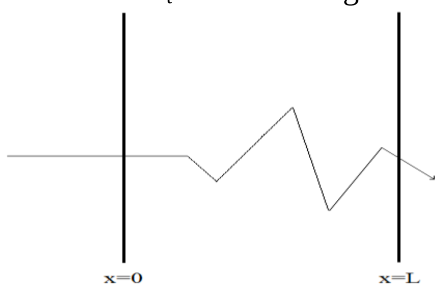

Figure 1. One region homogenous slab

The governing transport equation is written as,

$$\mu\frac{\partial\psi(x,\mu)}{\partial x}+\Sigma_T\psi(x,\mu)=c\Sigma_T\psi(x,\mu)\qquad 0<x<L \tag{4}$$

where $\mu = cos\ \theta$ (θ is the scattering angle at direction x) and ψ is the angular flux. The boundary conditions are,

$$\psi(0,\mu)=n_0\delta(\mu-1)\quad \text{and}\quad \psi(L,\mu)=0 \text{ for } \mu=-1 \tag{5}$$

2.2. Two Regions Homogeneous Slab Problem

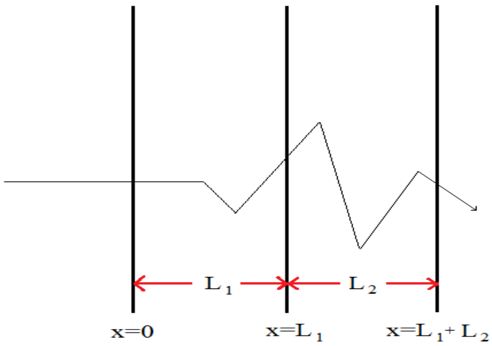

Figure 2. Two regions homogenous slab

For the two regions slab problem, it is again considered that a neutron beam enter the system at x=0. The slab is composed of two different regions of length L_1 and L_2. The objective of the simulation is to determine the number of neutrons exiting at x=L where $L=L_1+L_2$. In region-I and region-II, the total cross sections are defined as Σ_{T1} and Σ_{T2} and scattering ratios are defined as c_1 and c_2 respectively. The governing transport equation is written as,

$$\begin{aligned}\mu\frac{\partial\psi^{(1)}(x,\mu)}{\partial x}+\Sigma_{T1}\psi^{(1)}(x,\mu)&=\Sigma_{T1}c_1\psi^{(1)}(x,\mu)\qquad 0<x<L_1\\ \mu\frac{\partial\psi^{(2)}(x,\mu)}{\partial x}+\Sigma_{T2}\psi^{(2)}(x,\mu)&=\Sigma_{T2}c_2\psi^{(2)}(x,\mu)\qquad \mathrm{L}_1<x<L\end{aligned} \tag{6}$$

with boundary conditions,

$$\psi^{(1)}(0,\mu)=n_0\delta(\mu-1)\ \text{ and }\ \psi^{(2)}(L_2,\mu)=0 \text{ for } \mu=-1 \tag{7}$$

These equations are not coupled with each other and the solution of the transport equation for region-I become the boundary condition for region-II.

3. MULTI-COLLIDED FLUX METHOD

since the neutrons scatter in forward direction only, the neutrons which reach to $x = L_1$ surface are determined by using the multi-collided flux method in region-I. The solution of the m-times collided flux equation is as follows;

$$\mu \frac{\partial \psi^{(1),m}(x,\mu)}{\partial x} + \Sigma_{T1}\psi^{(1),m}(x,\mu) = \Sigma_{s1}\psi^{(1),m-1}(x,\mu) \qquad 0 < x < L_1$$
$$\psi^{(1),0}(0,\mu) = n_0\delta(\mu-1) \quad \text{and} \quad \psi^{(1),m}(0,\mu) = 0 \quad for \quad m \geq 1 \tag{8}$$

$$\psi^{(1),0}(x,\mu) = \psi^{(1)}(0,\mu)e^{-\Sigma_{T1}x/\mu}$$
$$\psi^{(1),1}(x,\mu) = \psi^{(1)}(0,\mu)\frac{\Sigma_{s1}x}{\mu}e^{-\Sigma_{T1}x/\mu}$$

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$$\psi^{(1),m}(x,\mu) = \psi^{(1)}(0,\mu)\frac{(\Sigma_{s1}x)^m}{m!\mu^m}e^{-\Sigma_{T1}x/\mu}$$

Thus, the angular neutron flux in region-I is given as,

$$\psi^{(1)}(x,\mu) = \psi^{(1)}(0,\mu)\sum_{m=0}^{\infty}\frac{(\Sigma_{s1}x)^m}{m!\mu^m}e^{-\Sigma_{T1}x/\mu} \tag{9}$$

The angular flux at the exit of region-I is used as a boundary condition to determine the m-times collided angular neutron flux in region-II by using the following transport equation;

$$\mu \frac{\partial \psi^{(2),m}(x,\mu)}{\partial x} + \Sigma_{T2}\psi^{(2),m}(x,\mu) = \Sigma_{s2}\psi^{(2),m-1}(x,\mu) \qquad L_1 < x < L \tag{10}$$

with boundary conditions,

$$\psi^{(2),0}(L_1,\mu) = \psi^{(1)}(0,\mu)\sum_{m=0}^{\infty}\frac{(\Sigma_{s1}L_1)^m}{m!\mu^m}e^{-\Sigma_{T1}L_1/\mu} \quad and \quad \psi^{(2),m}(L_1,\mu) = 0 \quad for \quad m \geq 1 \tag{11}$$

and the multi-collided angular fluxes in region-II are obtained as,

$$\begin{aligned}
&\psi^{(2),0}(x,\mu)=\psi^{(1)}(L_1,\mu)e^{-\Sigma_{T2}x/\mu}\\
&\psi^{(2),1}(x,\mu)=\psi^{(1)}(L_1,\mu)\frac{\Sigma_{s2}x}{\mu}e^{-\Sigma_{T2}x/\mu}\\
&.\\
&.\\
&\psi^{(2),m}(x,\mu)=\psi^{(1)}(L_1,\mu)\frac{\left(\Sigma_{s2}x\right)^m}{m!\mu^m}e^{-\Sigma_{T2}x/\mu}
\end{aligned} \tag{12}$$

Finally, the angular flux at region-II is written as,

$$\psi^{(2)}(x,\mu)=\psi^{(1)}(0,\mu)\sum_{k=0}^{\infty}\frac{\left(\Sigma_{s1}L_1\right)^k}{k!\mu^k}e^{-\Sigma_{T1}L_1/\mu}\sum_{m=0}^{\infty}\frac{\left(\Sigma_{s2}x\right)^m}{m!\mu^m}e^{-\Sigma_{T2}x/\mu} \tag{13}$$

Since the summation terms are equal to,

$$\sum_{k=0}^{\infty}\frac{\left(\Sigma_{s1}x\right)^k}{k!\mu^k}=e^{-\Sigma_{s1}x/\mu} \quad \text{and} \quad \sum_{m=0}^{\infty}\frac{\left(\Sigma_{s2}x\right)^m}{m!\mu^m}=e^{-\Sigma_{s2}x/\mu} \tag{14}$$

The angular neutron flux at $x=L$ is written as,

$$\psi^{(2)}(L,\mu)=\psi^{(1)}(0,\mu)e^{-\Sigma_{a1}L_1/\mu}e^{-\Sigma_{a2}L_2/\mu} \tag{15}$$

Thus, the number of neutrons leaked out from the system is determined by using the partial current definition as,

$$\int_0^1 \mu\psi^{(2)}(L,\mu)\,d\mu=n_0e^{-\Sigma_{a1}L_1}e^{-\Sigma_{a2}L_2} \tag{16}$$

The open form of angular flux could be written as,

$$\psi^{(2)}(L,\mu)=\psi^{(1)}(0,\mu)\sum_{k=0}^{\infty}\sum_{m=0}^{\infty}P_{1k}(L_1,\mu)P_{2m}(L_2,\mu) \tag{17}$$

where,

$$\begin{aligned}
P_{1k}(L_1,\mu)&=\frac{\left(\Sigma_{s1}L_1\right)^k}{k!\mu^k}e^{-\Sigma_{T1}L_1/\mu}\\
P_{2m}(L_2,\mu)&=\frac{\left(\Sigma_{s2}L_2\right)^m}{m!\mu^m}e^{-\Sigma_{T2}L_2/\mu}
\end{aligned} \tag{18}$$

At this point it should be noted that the open form of the angular flux given by Eq.17 will be utilized in non-analog Monte Carlo games. The term $P_{1k}(L_1,\mu)P_{2m}(L_2,\mu)$ is the angular flux at $x=L$ due to a neutron undergoing k collisions in region-I and m collisions in region-II. Thus, the probability that a neutron will transmit through the system is given as,

$$P_{transm}(L) = \sum_{k=0}^{\infty}\sum_{m=0}^{\infty} P_{1k}(L_1, \mu = 1) P_{2m}(L_2, \mu = 1) = \sum_{k=0}^{\infty}\sum_{m=0}^{\infty} P_{1k}(L_1) P_{2m}(L_2) \tag{19}$$

The term $P_{1k}(L_1)P_{2m}(L_2)$ is the probability that a neutron entering into the system succeeds to escape after making k collisions in region-I and m collisions in region-II. If the summation is performed, the probability that a neutron transmits through the system is given as,

$$P_{transm}(L) = P_{transm}(L_1) P_{transm}(L_2) = e^{-\Sigma_{a1} L_1} e^{-\Sigma_{a2} L_2} \tag{20}$$

In analog Monte Carlo game, a neutron entering the system is followed until it is absorbed in the system or leaked out from the system. Leaked or absorbed neutron may undergo several scattering events and the history is terminated as a result of absorption or leakage. Thus, the particle will exit the system with weight unity or the particle will be absorbed in the system and will not contribute to the tally. Thus, the probability distribution function (PDF) for the weights of neutrons exiting from *x*= *L* is given as,

$$n_{\text{analog}}(L, \omega) = P_{transm} \delta(\omega - 1) + (1 - P_{transm}) \delta(\omega - 0) \tag{21}$$

and $n_{\text{analog}}(L, \omega) d\omega$ is the probability that a particle leaks out from the system having a weight ω within $d\omega$. The PDF is normalized to unity and given as,

$$\int_0^{\infty} n_{\text{analog}}(L, \omega) d\omega = 1 \tag{22}$$

Thus, mean of the weights is determined by using the PDF as,

$$m_{\bar{\omega}} = \int_0^{\infty} \omega n_{\text{analog}}(L, \omega) d\omega = \mathrm{P}_{transm}(L) = e^{-\Sigma_{a1} L_1} e^{-\Sigma_{a2} L_2} \tag{23}$$

The mean of the weight square is,

$$m_{\bar{\omega}^2} = \int_0^{\infty} \omega^2 n_{\text{analog}}(L, \omega) d\omega = \mathrm{P}_{transm}(L) = e^{-\Sigma_{a1} L_1} e^{-\Sigma_{a2} L_2} \tag{24}$$

Hence, the variance is determined by using the results given by Eq.23 and Eq.24 as,

$$\sigma^2_{\text{analog}} = m_{\bar{\omega}^2} - m_{\bar{\omega}}{}^2 = P_{transm}(L)(1 - P_{transm}(L)) = e^{-\Sigma_{a_1} L_1} \cdot e^{-\Sigma_{a_2} L_2} (1 - e^{-\Sigma_{a_1} L_1} \cdot e^{-\Sigma_{a_2} L_2}) \tag{25}$$

Since the process is binary, the variance could also be written as,

$$\sigma^2_{\text{analog}} = m_{\bar{\omega}}(1 - m_{\bar{\omega}}). \tag{26}$$

The derivation also allows determining mean of high order moments and could be used to determine variance of variance. Although these results are well known and explicitly given in literature, the method developed in this section will be adopted in non-analog Monte Carlo methods.

4. IMPLICIT CAPTURE

One of the techniques used in non-analog Monte Carlo methods is the implicit capture (survival biasing). Implicit capture is introduced at the interaction point and a neutron undergoing collision is survived with the new weight $\omega_{new} = c \cdot \omega_{old}$. In neutron transport, c is defined as the scattering ratio. Since the neutrons at the interaction points are survived, the multi-collided fluxes are determined by using the biased transport equation given as,

$$\mu \frac{\partial \psi_{IC}^{(1),m}(x,\mu)}{\partial x} + \Sigma_{T1}\psi_{IC}^{(1),m}(x,\mu) = \Sigma_{T1}\psi_{IC}^{(1),m-1}(x,\mu) \qquad 0 < x < L_1 \tag{27}$$

with boundary conditions,

$$\psi_{IC}^{(1),0}(0,\mu) = n_0\delta(\mu-1) \quad for \quad m=0 \quad and \quad \psi_{IC}^{(1),m}(0,\mu) = 0 \quad for \quad m \geq 1 \tag{28}$$

Solving biased transport equation in region-I with implicit capture for angular flux,

$$\psi_{IC}^{(1)}(x,\mu) = \psi_{IC}^{(1)}(0,\mu)\sum_{m=0}^{\infty}\frac{(\Sigma_{T1}x)^m}{m!\mu^m}e^{-\Sigma_{T1}x/\mu} \tag{29}$$

The angular flux at the exit of region-I is used as a boundary condition to determine the m-times collided angular neutron flux in region-II by using the following biased transport equation;

$$\mu \frac{\partial \psi_{IC}^{(2),m}(x,\mu)}{\partial x} + \Sigma_{T2}\psi_{IC}^{(2),m}(x,\mu) = \Sigma_{s2}\psi^{(2),m-1}(x,\mu) \qquad L_1 < x < L_2 \tag{30}$$

with boundary conditions,

$$\psi_{IC}^{(2),0}(L_1,\mu) = \psi_{IC}^{(1)}(0,\mu)\sum_{m=0}^{\infty}\frac{(\Sigma_{T1}L_1)^m}{m!\mu^m}e^{-\Sigma_{T1}L_1/\mu} \text{ and } \psi_{IC}^{(2),m}(L_1,\mu) = 0 \quad for \quad m \geq 1 \tag{31}$$

and m-times collided angular fluxes in region-II are obtained as,

$$\psi_{IC}^{(2),m}(x,\mu) = \psi_{IC}^{(1)}(L_1,\mu)\frac{(\Sigma_{T2}x)^m}{m!\mu^m}e^{-\Sigma_{T2}x/\mu} \tag{32}$$

Hence, for the non-analog Monte Carlo game, the PDF for neutrons exiting at $x=L$ is given by,

$$n_{IC}(L,\omega)=\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}P_{1i,IC}(L_1)P_{2j,IC}(L_2)\delta(\omega-c_1^i c_2^j) \tag{33}$$

where $n_{IC}(L,\omega)\, d\omega$ is the probability that a particle having weight between ω and $\omega+d\omega$ will leak out from the system. $P_{1i,IC}P_{2j,IC}$ is the probability that a particle entering into the system will leak out after undergoing i collisions in region-I and j collisions in region-II due to biasing and given as,

$$P_{1i,IC}(L_1)P_{2j,IC}(L_2)=\frac{(\Sigma_{t1}L_1)^i}{i!}e^{-\Sigma_{t1}L_1}\cdot\frac{(\Sigma_{t2}L_2)^j}{j!}e^{-\Sigma_{t2}L_2} \tag{34}$$

Since $n_{IC}(L,\omega)$ is defined as the PDF, $\int_0^{\infty} n_{\mathrm{IC}}(\mathrm{L},\omega)d\omega$ is normalized to unity and the number of particles exiting from the system will be equal to the number of particles entering into the system. The mean of the weights and mean of the square weights are determined by using the PDF as,

$$m_{\varpi,IC}=\int\omega n_{IC}(\omega)d\omega=\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}P_{1i,IC}(L_1)P_{2j,IC}(L_2)\omega_{ij}\quad=e^{-\Sigma_{a_1}L_1}e^{-\Sigma_{a_2}L_2} \tag{35}$$

where $\omega_{ij}=c_1^i c_2^j$

$$m_{\varpi^2,IC}=\int\omega^2 n_{IC}(L,\omega)d\omega=(P_{tranm}(L_1))^{(1+c_1)}\cdot(P_{tranm}(L_2))^{(1+c_2)} \tag{36}$$

Hence, the variance is determined by using the results given by Eq.35 and Eq.36 as,

$$\sigma_{\mathrm{IC}}^2=P_{tranm}(L_1)\cdot P_{tranm}(L_2).((P_{tranm}(L_1))^{c_1}\cdot(P_{tranm}(L_2))^{c_2}-P_{tranm}(L_1)\cdot P_{tranm}(L_2)) \tag{37}$$

At this point, it should be noted that in the limiting case where scattering ratios converge to zero, implicit capture solution produces analog Monte Carlo results.

5. SPLITTING

In the splitting game, a neutron passing through $x=L_1$ splits into n_s neutrons with new weights $\omega_{new}=\frac{1}{n_s}\omega_{old}$. For n_s equal to two, the PDF for neutrons that pass through $x=L$ is given as,

$$\begin{aligned}&n_{split,2}(L,\omega)=(1-P_{tranm}(L_1))\delta(\omega-0)+\\&P_{tranm}(L_1)[P_{tranm}(L_2)^2\delta(\omega-1)+2P_{tranm}(L_2)(1-P_{tranm}(L_2))\delta(\omega-\tfrac{1}{2})+(1-P_{tranm}(L_2))^2\delta(\omega-0)]\end{aligned} \tag{38}$$

$n_{split,2}(L,\omega)$ is the probability that a particle having a weight of ω about dω reaches the surface at $x=L$.

$$\int n_{split,2}(L,\omega)d\omega = 1 \tag{39}$$

If a neutron splits into n_s neutrons, with each neutron having a weight of $\omega_{new} = 1/n_s \, . \, \omega_{old}$, the PDF is given as,

$$n_{split,n_s}(L,\omega) = (1 - P_{tranm}(L_1))\delta(\omega - 0) + P_{tranm}(L_1)\sum_{i=0}^{n_s} C(n_s,i) P_{tranm}^{n_s - i}(L_2)(1 - P_{tranm}(L_2))^i \delta(\omega - \frac{n_s - i}{n_s}) \tag{40}$$

where $C(n_s, i)$ is the binomial expansion coefficient. For splitting into n_s neutrons the mean of the weights is determined as,

$$m_{\bar{\omega}} = \int \omega n_{split,n_s}(L,\omega)d\omega = n_{split,n_s}(L,\omega) = P_{tranm}(L_1)\sum_{i=0}^{n_s} C(n_s,i) P_{tranm}^{n_s - i}(L_2)(1 - P_{tranm}(L_2))^i \frac{n_s - i}{n_s} \tag{41}$$

$$m_{\bar{\omega}} = P_{tranm}(L_1) P_{tranm}(L_2)$$

The mean of the square weights is determined as,

$$m_{\bar{\omega}^2} = \int \omega^2 n_{split,n_s}(L,\omega)d\omega = P_{tranm}(L_1) P_{tranm}(L_2) \left\{ \frac{\left[1 + (n_s - 1) P_{tranm}(L_2)\right]}{n_s} \right\} \tag{42}$$

Hence, by using the definition of variance with Eq.41 and Eq.42

$$\sigma^2_{split-n_s} = P_{tranm}(L_1) P_{tranm}(L_2) \left\{ \frac{\left[1 + (n_s - 1) P_{tranm}(L_2)\right]}{n_s} - P_{tranm}(L_1) P_{tranm}(L_2) \right\} \tag{43}$$

6. CONCLUSIONS

Non-analog Monte Carlo methods are widely used in particle transport; such as, transport of radionuclides in a porous medium [4], cross-section biasing [5] and convergence acceleration of neutronic calculations [6]. However, these variance reduction techniques often require additional computational work. In this study, the analytical solutions of implicit capture and splitting games have been introduced for non-analog Monte Carlo methods. These methods can be used for educational purposes and may provide a better understanding of non-analog Monte Carlo methods.

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