Monte Carlo Neutron Transport Example

This short note provides a brief example of the Monte Carlo Simulation of Neutron Scattering. A description and relevant formulae for the various physical interaction and monte carlo sampling is provided.

Mathematical Preliminaries

Coordinate System

[4, p. 67]

The usual Cartesian coordinate system is used to locate a particle in space and its collision site, $\vec{r} = (x, y, z)$. The three direction cosines $(\hat{\mathbf{\Omega}}_x, \hat{\mathbf{\Omega}}_y, \hat{\mathbf{\Omega}}_z)$ with respect to the x, y, and z axes describe the particles direction of travel. The direction cosines are

$$\begin{aligned}
\hat{\mathbf{\Omega}}_x &= \sin\theta\cos\varphi \\
\hat{\mathbf{\Omega}}_y &= \sin\theta\sin\varphi \\
\hat{\mathbf{\Omega}}_z &= \cos\theta.
\end{aligned}$$

The linear displacement, S of a particle along the direction $\hat{\mathbf{\Omega}}$ from its position (x, y, z) is

$$\vec{r}\,' = \vec{r} + \hat{\mathbf{\Omega}} \cdot S \qquad \Longrightarrow \begin{cases} x' &= x + \hat{\mathbf{\Omega}}_x\, S \\ y' &= y + \hat{\mathbf{\Omega}}_y\, S \\ z' &= z + \hat{\mathbf{\Omega}}_z\, S. \end{cases}$$

Selection of the Initial Source Particle Position

[4, p. 67]

The first step in generating a particle history is to randomly assign an initial position $\vec{r}_o$, a trajectory $\hat{\mathbf{\Omega}}$, and energy E to the particle. Selection of the initial position is accomplished by sampling the normalized source distribution function $S(\vec{r}, \hat{\mathbf{\Omega}}, E)$. Let's examine a few simple cases:

1. A point source located at $\vec{r}_p$: $S(\vec{r}) = \delta(\vec{r}_p - \vec{r})$. No Sampling is necessary since $\vec{r}_o = \vec{r}_p$ always.

2. Uniformly distributed sources within cube with edge lengths A, B and C. The initial particle source position $\vec{r}_o$ is selected as follows (lower left-hand corner of cube is located at (x_p, y_p, z_p):

$$\begin{aligned}
x_o &= x_p + \xi_1 \cdot A \\
y_o &= y_p + \xi_2 \cdot B \\
z_o &= z_p + \xi_3 \cdot C
\end{aligned}$$

where ξ_1, ξ_2 and ξ_3 are three uniformly distributed random numbers on $(0, 1)$.

3. Uniformly distributed sources within a sphere with radius R. The origin of the sphere has the coordinates (x_p, y_p, z_p). The initial position $\vec{r}_o$ of a source particle is selected as follows (see the next section for the derivation of polar and azimuthal angle sampling):

$$\begin{aligned} x_o &= x_p + r \cdot \sin\theta\cos\varphi \\ y_o &= y_p + r \cdot \sin\theta\sin\varphi \\ z_o &= z_p + r \cdot \cos\theta \end{aligned}$$

where

$$\begin{aligned} r &= \xi_1^{1/3} \cdot R \\ \varphi &= 2\pi \cdot \xi_2 \\ \theta &= \arccos(2\,\xi_3 - 1) \end{aligned}$$

and ξ_1, ξ_2 and ξ_3 are three uniformly distributed random numbers on $(0, 1)$.

Selection of the Initial Particle Trajectory for Isotropically Emitting Sources

Spherically symmetric or isotropic distribution is given by:

$$P(\theta, \varphi) = \frac{d\mathbf{\Omega}}{4\pi} = \frac{\sin\theta\, d\theta}{2}\frac{d\varphi}{2\pi}$$

θ and φ are independent random variables. For this case the pdf can be separated into two single variable pdf's: $P(\theta, \varphi) = P_1(\theta)\, P_2(\varphi)$ meaning that θ and φ can be sampled separately.

Sampling of θ proceeds as follows; the pdf for the θ distribution is

$$P(\theta)\, d\theta = \frac{\sin\theta}{2}\, d\theta = \frac{1}{2} d\mu,$$

applying the fundamental inversion theorem yields

$$\xi_1 = \frac{1}{2}\int_{-1}^{\mu} d\mu = \frac{1}{2}\,(\mu + 1) \qquad \Longrightarrow \qquad \mu = 2\,\xi_1 - 1$$

where $\mu = \cos\theta$. Using the fundamental inversion theorem for φ gives

$$\xi_2 = \frac{1}{2\pi}\int_0^{\varphi} d\varphi = \frac{\varphi}{2\pi}$$

thus

$$\varphi = 2\pi \cdot \xi_2$$

ξ_1 and ξ_2 are two uniformly distributed random numbers on (0,1).

Though the above procedure is quite simple, it requires the computation of the $\cos\varphi$ and $\sin\varphi$ functions to evaluate the direction cosines of the particle (see equation 1). On the other hand $\sin\theta$ can be easily evaluated; $\sin\theta = \sqrt{1 - \mu^2}$. A simple but elegant technique to compute the φ transcendental functions was derived by Van Neumann. It directly evaluates the $\sin\varphi$ and $\cos\varphi$ functions and involves the use of the rejection technique.

Suppose it is of interest to locate a point within a circle inscribed within the square shown in the figure above. Two uniformly distributed random numbers ξ_1 and ξ_2 are required to define the point's location:

$$x_1 = 2\xi_1 - 1 \qquad \text{and} \qquad x_2 = 2\xi_2 - 1$$

If $x_1^2 + x_2^2 < 1$ the sampled point is retained, otherwise it is rejected. Having defined the points location, the transcendental $\cos\varphi$ and $\sin\varphi$ functions can now be evaluated:

$$\cos\varphi = \frac{x_1}{\sqrt{x_1^2 + x_2^2}} \qquad \text{and} \qquad \sin\varphi = \frac{x_2}{\sqrt{x_1^2 + x_2^2}}.$$

To avoid having to take square roots, use is made of the double angle formulas from trigonometry. This leads to the following relations;

$$\cos\varphi = \frac{x_1^2 - x_2^2}{x_1^2 + x_2^2} \qquad \text{and} \qquad \sin\varphi = \frac{2\,x_1\,x_2}{x_1^2 + x_2^2}.$$

The efficiency of this process is the ratio of the area of the circle to that of the square; $\frac{\pi}{4}$.

The calculation of the direction cosines is as follows

a) Pick two random numbers, ξ_1 and ξ_2

b) Compute x_1 and x_2

c) Retain values of $x_1^2 + x_2^2 < 1$

d) Compute $\cos\varphi$ and $\sin\varphi$

e) Pick a third random number ξ_3 and retain the value if $\xi_3 < 0.5$

f) Then compute $\cos\theta = 2\xi_3 - 1$ and $\sin\theta = (1 - \cos^2\theta)^{1/2}$

and the direction cosines are

$$\begin{aligned} \hat{\mathbf{\Omega}}_x &= \sin\theta\cos\varphi \\ \hat{\mathbf{\Omega}}_y &= \sin\theta\sin\varphi \\ \hat{\mathbf{\Omega}}_z &= \cos\theta. \end{aligned}$$

Pathlength Travelled

A) Homogeneous Medium [1, p. 6], and [2, p. 303]

The probability of a first collision between ℓ and $\ell + d\,\ell$ along the particles line of sight is given by

$$p(\ell)\,d\ell = \Sigma_t\,e^{-\Sigma_t \ell}\,d\ell$$

Applying the fundamental inversion theorem gives

$$\xi = \int_0^x \sigma_t\,e^{-\Sigma_t \ell}\,d\ell = 1 - e^{-\Sigma_t x} \qquad \text{Solving for } x\text{:} \quad x = -\frac{1}{\Sigma_t}\,\ln(1-\xi)$$

$(1-\xi)$ is distributed in the same manner as ξ, hence the above can be written as

$$x = -\frac{1}{\Sigma_t}\,\ln(\xi)$$

where ξ is a uniformly distributed random number on (0,1).

B) Distance Between Particle Collisions in a Bounded Absorber (Also known as forced collisions) [4, p. 63], [2,p. 336]
Let t be the distance along the particle path between its point of origin and the absorber boundary. The probability that the photon experiences a collision over the distance t is $1 - e^{-\Sigma_t t}$. The probability that the particle interacts within ℓ and $\ell + d\ell$ is $\Sigma_t\, e^{-\Sigma_t \ell}\, d\ell$. The conditional probability $P(\ell|\ell \leq t)$ that the particle collides after traveling a distance ℓ, given that it interacts within the absorber, is

$$P\left(\ell|\ell \leq t\right) = \frac{\Sigma_t\, e^{-\Sigma_t \ell}\, d\ell}{1 - e^{-\Sigma_t t}}$$

Thus,

$$\xi = \int_0^x \frac{\Sigma_t\, e^{-\Sigma_t \ell}\, d\ell}{1 - e^{-\Sigma_t t}} \quad = \quad \frac{1 - e^{-\Sigma_t x}\, d\ell}{1 - e^{-\Sigma_t t}}$$

Solving for x:

$$x = -\frac{1}{\Sigma_t} \ln\left(1 - \xi\left(1 - e^{-\Sigma_t t}\right)\right)$$

where ξ is a uniformly distributed random number on (0,1). For heterogeneous media see [3, p 39]. If there is more than one nuclear species in the medium, then the total cross section for all nuclear species.

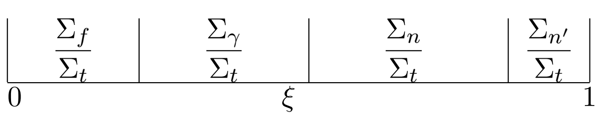
Interactions: Absorptions, Scattering

[2, p. 305].

Does a collision result in fission, capture, elastic scattering or inelastic scattering? To obtain our answer with a random number generator we note that

$$\Sigma_t = \Sigma_f + \Sigma_\gamma + \Sigma_n + \Sigma_{n'}$$

and the unit interval is divided into lengths: $\frac{\Sigma_f}{\Sigma_t}$, $\frac{\Sigma_\gamma}{\Sigma_t}$, $\frac{\Sigma_n}{\Sigma_t}$, and $\frac{\Sigma_{n'}}{\Sigma_t}$.



A random number is chosen uniformly distributed between 0 and 1 and the reaction chosen depends into which interval the random number falls:

interval 1: $0 \leq \xi < \frac{\Sigma_f}{\Sigma_t}$; interval 2: $\frac{\Sigma_f}{\Sigma_t} \leq \xi < \frac{\Sigma_f + \Sigma_\gamma}{\Sigma_t}$; interval 3: $\frac{\Sigma_f + \Sigma_\gamma}{\Sigma_t} \leq \xi < \frac{\Sigma_f + \Sigma_\gamma + \Sigma_n}{\Sigma_t}$;

and interval 4: $\frac{\Sigma_f + \Sigma_\gamma + \Sigma_n}{\Sigma_t} \leq \xi \leq \frac{\Sigma_f + \Sigma_\gamma + \Sigma_n + \Sigma_{n'}}{\Sigma_t}$.

If there is more than one nuclear species, then each reaction is the total over each species. Once a reaction is chosen by a random number, then another random number is chosen to determine the species. For radiative capture in a medium with N nuclear species we have:

$$\Sigma_\gamma = \sum_{i=1}^{N} \Sigma_\gamma^i = \Sigma_\gamma^1 + \Sigma_\gamma^2 + \Sigma_\gamma^3 + \cdots + \Sigma_\gamma^N$$

and the interval (0,1) is divided into lengths: $\frac{\Sigma_\gamma^1}{\Sigma_\gamma}, \frac{\Sigma_\gamma^2}{\Sigma_\gamma}, \frac{\Sigma_\gamma^3}{\Sigma_\gamma}, \ldots, \frac{\Sigma_\gamma^N}{\Sigma_\gamma}$.

$\frac{\Sigma_\gamma^1}{\Sigma_\gamma}$	$\frac{\Sigma_\gamma^2}{\Sigma_\gamma}$	$\frac{\Sigma_\gamma^3}{\Sigma_\gamma}$	$\ldots$	$\frac{\Sigma_\gamma^N}{\Sigma_\gamma}$
0	ξ			1

A random number is chosen uniformly distributed between 0 and 1 and the nuclear species chosen depends into which interval the random number falls:

interval 1: $0 \le \xi < \frac{\Sigma_\gamma^1}{\Sigma_\gamma}$; interval 2: $\frac{\Sigma_\gamma^1}{\Sigma_\gamma} \le \xi < \frac{\Sigma_\gamma^1 + \Sigma_\gamma^2}{\Sigma_\gamma}$; interval 3: $\frac{\Sigma_\gamma^1 + \Sigma_\gamma^2}{\Sigma_\gamma} \le \xi < \frac{\Sigma_\gamma^1 + \Sigma_\gamma^2 + \Sigma_\gamma^3}{\Sigma_\gamma}$;

and the Nth interval: $\frac{\sum_{i=1}^{N-1} \Sigma_\gamma^i}{\Sigma_\gamma} \le \xi \le \frac{\sum_{i=1}^{N} \Sigma_\gamma^i}{\Sigma_\gamma}$.

Elastic Scattering

[2, p. 340], [3, p. 48].
The discussion here will restrict itself to isotropic scattering in the center-of-mass (CMS) system. In an elastic scattering event the momentum and the kinetic energy of the neutrons is conserved. The first order of business is to determine the cosine of the scattering angle in the CMS. For this case the cosine of the scattering angle is determined by sampling an uniform probability density function over the interval $-1 \le \mu_{cm} \le 1$:

$$\mu_{cm} = \cos(\theta)_{cm} = 2\,\xi_1 - 1.$$

Once μ_{cm} has been determined, we can determine the final energy after a scattering event. For isotropic scattering in the CMS, the energy of the neutron after the scattering event is

$$E' = \frac{E}{2}((1+\alpha) + (1-\alpha)\,\cos(\theta)_{cm}) = \frac{E}{2}((1+\alpha) + (1-\alpha)\,\mu_{cm}) \quad \text{where} \quad \alpha = \left(\frac{A-1}{A+1}\right)^2.$$

The cosine of the scattering angle in the laboratory reference frame is determined from the expression:

$$\cos(\theta) = \frac{1 + A\,\cos(\theta)_{cm}}{\sqrt{A^2 + 1 + 2\,A\,\cos(\theta)_{cm}}} = \frac{1 + A\,\mu_{cm}}{\sqrt{A^2 + 1 + 2\,A\,\mu_{cm}}}$$

or

$$\cos(\theta) = \frac{(A+1)}{2}\sqrt{\frac{E}{E'}} - \frac{(A-1)}{2}\sqrt{\frac{E'}{E}}.$$

We now turn our attention to determining the new direction cosines of the scattered neutron. The cosine of the scattering angle, $\cos(\theta)$, was computed above. Hence, $\sin(\theta) = \sqrt{1-\cos^2(\theta)}$. The azimuthal scattering angle, φ, must still be determined before the final direction $\hat{\mathbf{\Omega}}'$ is determined. We can use the Van Neumann's method presented earlier or $\varphi = 2\,\pi\,\xi$, where ξ is a uniformly distributed random number (also presented earlier). The new direction cosines for $\hat{\mathbf{\Omega}}'$ in terms of the old direction cosines $\hat{\mathbf{\Omega}}$ are [2, p. 341] (note the expression $\hat{\mathbf{\Omega}}'_x$ in ref. 2 is incorrect and has been corrected below)

$$
\begin{aligned}
\hat{\mathbf{\Omega}}'_x &= \frac{\sin(\theta)}{\sqrt{1-\hat{\mathbf{\Omega}}_z^2}} \left[\hat{\mathbf{\Omega}}_y \sin(\varphi) - \hat{\mathbf{\Omega}}_z\, \hat{\mathbf{\Omega}}_x \cos(\varphi)\right] + \hat{\mathbf{\Omega}}_x \cos(\theta) \\
\hat{\mathbf{\Omega}}'_y &= \frac{\sin(\theta)}{\sqrt{1-\hat{\mathbf{\Omega}}_z^2}} \left[-\hat{\mathbf{\Omega}}_x \sin(\varphi) - \hat{\mathbf{\Omega}}_z\, \hat{\mathbf{\Omega}}_y \cos(\varphi)\right] + \hat{\mathbf{\Omega}}_y \cos(\theta) \\
\hat{\mathbf{\Omega}}'_z &= \sin(\theta)\sqrt{1-\hat{\mathbf{\Omega}}_z^2}\,\cos\varphi + \hat{\mathbf{\Omega}}_z \cos(\theta).
\end{aligned}
$$

If the medium in which the scattering takes place is hydrogen, the energy loss and cosine of the scattering angel in the laboratory frame equation can be simplified. This is because for all practical purposes, the neutron and proton masses are considered equal. For neuron energies below 10 MeV, the elastic scattering of a neutron with a proton is isotropic in the CMS. For neutrons in this energy range, the scattering event can be modeled using one random number ξ_1.

$$E' = \xi_1\, E \qquad \text{and} \qquad (\cos(\theta))_{\text{lab}} = \sqrt{\xi_1}$$

Multiple Species

If there is more than one nuclear species in the medium, then the species off of which the neutron will scatter must be determined prior to computing the energy loss, the laboratory scattering angle and the new direction cosines.

Once the collision site has been determined, a random number is generated to determine the nuclide with which the neutron will scatter. To obtain the answer with a random number generator, we note that the total scattering cross section is given by

$$\Sigma_s = \sum_{i=1}^{N} \Sigma_s^i = \Sigma_s^1 + \Sigma_s^2 + \Sigma_s^3 + \cdots + \Sigma_s^N$$

and the interval (0,1) is divided into lengths: $\frac{\Sigma_s^1}{\Sigma_s}, \frac{\Sigma_s^2}{\Sigma_s}, \frac{\Sigma_s^3}{\Sigma_s}, \ldots, \frac{\Sigma_s^N}{\Sigma_s}$.

$\frac{\Sigma_s^1}{\Sigma_s}$	$\frac{\Sigma_s^2}{\Sigma_s}$	$\frac{\Sigma_s^3}{\Sigma_s}$	$\ldots$	$\frac{\Sigma_s^N}{\Sigma_s}$

0 $\qquad\qquad\qquad\qquad$ ξ $\qquad\qquad\qquad\qquad$ 1

A random number is chosen uniformly distributed between 0 and 1 and the nuclear species chosen depends into which interval the random number falls:

interval 1: $0 \leq \xi < \dfrac{\Sigma_s^1}{\Sigma_s}$; interval 2: $\dfrac{\Sigma_s^1}{\Sigma_s} \leq \xi < \dfrac{\Sigma_s^1 + \Sigma_s^2}{\Sigma_s}$; interval 3: $\dfrac{\Sigma_s^1 + \Sigma_s^2}{\Sigma_s} \leq \xi < \dfrac{\Sigma_s^1 + \Sigma_s^2 + \Sigma_s^3}{\Sigma_s}$;

and the Nth interval: $\dfrac{\sum_{i=1}^{N-1} \Sigma_s^i}{\Sigma_s} \leq \xi \leq \dfrac{\sum_{i=1}^{N} \Sigma_s^i}{\Sigma_s}$.

References

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4. Richard L. Morin, Editor, Monte Carlo Simulation in the Radiological Sciences, Chapter 4, CRC Press, Inc., Boca Raton, Florida (1988).