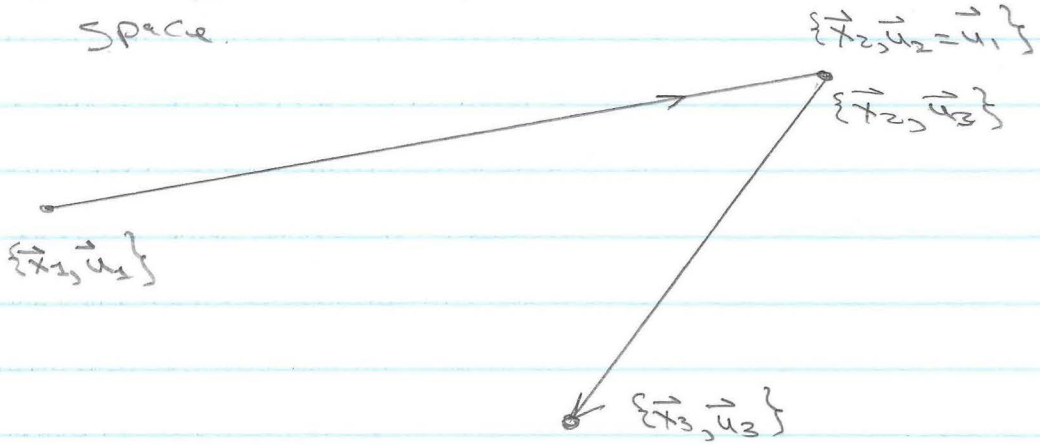
Ray Tracing & Rotations Chapter 7

"Ray Tracing" How a particle is moved around in space.



"Phase space"

$\{\vec{x}, \vec{u}, E, q, ir, t, wt\}$

- $\vec{x}$: 3D space
- $\vec{u}$: 3D direction
- E: energy
- q: particle type
- ir: region # (geometry)
- t: time

$\vec{x}$: 3D vector $\vec{x} : (x, y, z)$

$\vec{u}$: 3D normalized direction vector $\vec{u} \cdot \vec{u} = 1$ $\vec{u} : (u, v, w)$

$u = u_x$, $v = u_y$, $w = u_z$

(sinθcosφ, sinθsinφ, cosθ)

spider coord.

E : total or kinetic energy (usually kinetic)

q : particle type, q is usually an integer

e.g. electromagnetic code

$q = \pm 1 \Rightarrow$ positron (+1), electron (-1)

$= 0 \Rightarrow$ photon

wt = weight

For now, we shall focus on $\{\vec{x}, \vec{v}\}$

7.1 Displacements

Say we have a displacement of distances

(s comes from other physics) — distance to a surface, distance to an interaction

$$\{\vec{x}_0, \vec{v}_0\}$$

$$T\left(\{\vec{x}_0, \vec{v}_0\}, s\right) = \{\vec{x}_0 + \vec{v}_0 s, \vec{v}_0\}$$

$$= \{\vec{x}_1, \vec{v}_0\}$$

$\vec{x}_0$: $\{x_0, y_0, z_0\}$

or

$$x = x_0 + u s$$

$$y = y_0 + v s$$

$$z = z_0 + w s$$

7.2 Rotations of coordinate systems

Imagine 2 3D cartesian coordinate systems.

$\vec{x}$; lab system

$\vec{x}'$; particle system

where

$\vec{x}'$ has been rotated by angle ϕ in the positive (right hand rule) sense about the z axis, leaving the z, z' axes colinear

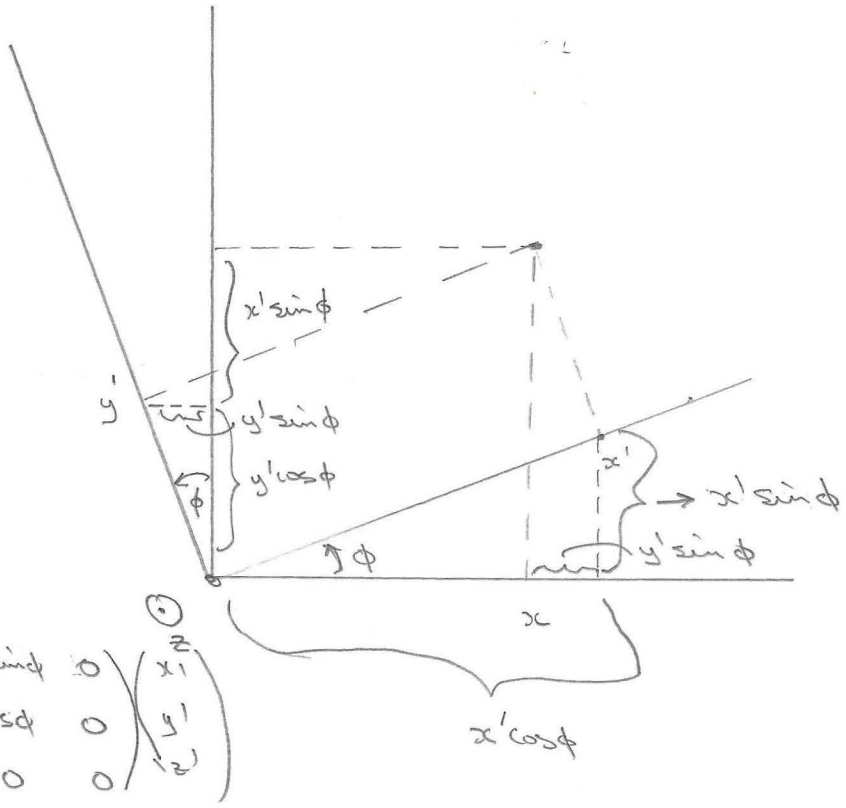
Consult the figure on the next page, and it can be shown that the coordinates of a point at (x,y,z) or (x',y',z') are related by the matrix equation

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}$$

or $\vec{x} = R_\phi \vec{x}'$

where R_ϕ is a 3×3 matrix

$$x = x'\cos\phi - y'\sin\phi$$
$$y = x'\sin\phi + y'\cos\phi$$



$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}$$

See demo code zrotphi

1.2.

$$\underbrace{\begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{R_\phi^T} \underbrace{\begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{R_\phi}$$

$$= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = I$$

$$R_\phi^{-1} R_\phi = I \Rightarrow R^T = R^{-1}$$

Similarly for a rotation in the positive sense by angle Θ about the y axis $\Rightarrow$

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \underbrace{\begin{pmatrix} \cos\Theta & 0 & \sin\Theta \\ 0 & 1 & 0 \\ -\sin\Theta & 0 & \cos\Theta \end{pmatrix}}_{R_\Theta} \begin{pmatrix} x'' \\ y'' \\ z'' \end{pmatrix} \quad (2)$$

has the same properties

$$R_\Theta^T = R_\Theta^{-1}$$

So,

Combining ① & ②

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix} \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x'' \\ y'' \\ z'' \end{pmatrix}$$

or

$$\vec{x} = R\vec{x}''$$

where

$$R = R_\theta R_\phi$$

$$= \begin{pmatrix} \cos\theta\cos\phi & -\sin\phi & \sin\theta\cos\phi \\ \cos\theta\sin\phi & \cos\phi & \sin\theta\sin\phi \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}$$

You may work out on your own that

$$R^T = R^{-1}$$

These are the basic rotation matrices of ray tracing.

How are they used?

For us, the lab system is $(\hat{x}, \hat{y}, \hat{z})$

Scattering angles, Θ, Φ are given

Θ = "theta", Φ = "phi" (we speak)

with respect to that.

So, say that a particle, with unit direction vector

$$\vec{u}_0 = (\sin\Theta_0\cos\phi_0, \sin\Theta_0\sin\phi_0, \cos\Theta_0)$$

undergoes a scattering by Θ, Φ

Then, the direction after scattering is

$$\vec{u} = R(\Theta_0,\phi_0)\, R(\Theta, \Phi)\, R^{-1}(\Theta_0,\phi_0)\, \vec{u}_0$$

$R^{-1}(\Theta_0,\phi_0)$: puts particle along z-axis

$R(\Theta, \Phi)$: redirects by Θ, Φ wrt the z-axis

$R(\Theta_0,\phi_0)$: Rotates back to the original direction

$$R \equiv R(\Theta_0,\phi_0)\,R(\Theta,\Phi)\,R^{-1}(\Theta_0,\phi_0)$$

is given explicitly by eq'n 7.13

$$\begin{aligned} u = \sin\theta\cos\phi &= u_0\cos\Theta + \sin\Theta(w_0\cos\Phi\cos\phi_0 - \sin\Phi\sin\phi_0) \\ v = \sin\theta\sin\phi &= v_0\cos\Theta + \sin\Theta(w_0\cos\Phi\sin\phi_0 + \sin\Phi\cos\phi_0) \\ w = \cos\theta &= w_0\cos\Theta - \sin\Theta\sin\theta_0\cos\Phi \end{aligned} \tag{7.13}$$

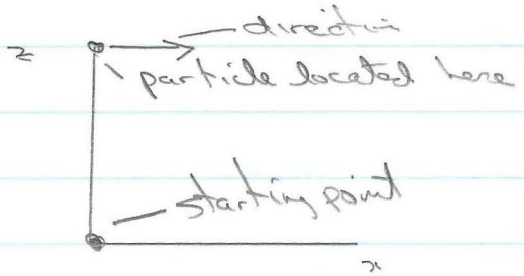
In our transport operator language

$$R(\{\vec{x}_0,\vec{u}_0\},\Theta,\Phi) = \{\vec{x}_0, R(\vec{u}_0,\Theta,\Phi)\} = \{\vec{x}_0,\vec{u}\}$$

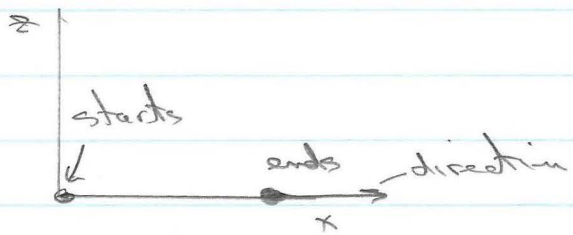
Note that T and R do not commute

e.g.

$$R(\{T(\{0,\hat{z}\},1\},\tfrac{\pi}{2},\phi) = \{\hat{z},\hat{x}\}$$



$$T(\{R(\{0,\hat{z}\},\tfrac{\pi}{2},0\},1) = \{\hat{x},\hat{x}\}$$



An example illustrating these concepts is given in the demo

randomWalk.m

rotate.m (7.13)
azimuthal.m azimuthal random sampling

```
function [u,v] = azimuthal()
%azimuthal.m A function samples a random direction in 2D space
%
% FileName      : azimuthal.m
% Creation      : 09/29/2016
% Modifications : September 29, 2016 Initial creation
% Author(s)     : Alex Bielajew
%
% Inputs        : [] i.e. none
%
% Outputs
%  double
%     u :  x-axis direction cosine
%     v :  y-axis direction cosine
%
% Purpose       : NERS 544 Monte Carlo Methods
%               : Demonstration, production, part of the code library

phi = 2*pi*rand; % Random azimuthal direction in radians
u = cos(phi);    % x-axis direction cosine
v = sin(phi);    % y-axis direction cosine

return
```

```
function u = rotate(u0,ws)
%rotate.m Arbitrary direction vector deflection (random azimuth)
%
% FileName      : rotate.m
% Creation      : 09/29/2016
% Modifications : September 29, 2016 Initial creation
% Author(s)     : Alex Bielajew
%
% Inputs        : u0 (vector, double):
%                     = (u_0,v_0,w_0) initial (x,y,z)-axis direction cosines
%                     u = sin(theta_0)*cos(phi_0)
%                     v = sin(theta_0)*sin(phi_0)
%                     w = cos(theta_0)
%               : ws (scalar, double)
%                   = cos(Theta) cosine of the polar scattering angle, Theta
% Outputs
%               : u (vector, double)
%                     = (u,v,w) final (x,y,z)-axis direction cosines
%
% Purpose       : NERS 544 Monte Carlo Methods
%               : Deflects the particle direction into a random azimuthal angle
%                     about it's  direction u0, by cos(Theta) = ws
%               : From (7:13) of the Monte Carlo book
%               : Demonstration, production, part of the code library

if (ws == 1)
   u = u0; % There is no scattering, return the original vector
   return
end

% General scattering case

[us,vs] = azimuthal(); % Unit normalized 2-D transverse direction cosines
                       % i.e. cos(Phi), sin(Phi)

% Convert 2-D transverse to 3-D transverse direction cosines

sinThetas = sqrt((1 - ws)*(1 + ws)); % This handles the near 1 situation for
                                     % ws with more precision than
                                     % sqrt(1 - ws^2))
us = sinThetas*us;     % i.e. us = sin(Theta)*cos(Phi)
vs = sinThetas*vs;     % i.e. vs = sin(Theta)*sin(Phi)

u2v2 = u0(1)^2 + u0(2)^2;    % i.e. u2v2 = sin(theta_0)^2

if (u2v2 == 0) % Particle's original direction was along the z-axis,
               % a common source condition
   u(1) = us;
   u(2) = vs;
   u(3) = ws;
   return
end

sintheta  = sqrt(u2v2);       % i.e. sin(theta_0)
sinthetai = 1/sintheta;       % inverse used below
cosphi    = u0(1)*sinthetai;  % i.e. cos(phi)/sin(Theta)
sinphi    = u0(2)*sinthetai;  % i.e. sin(phi)

% Equation (7.13) from the book
u(1) = u0(1)*ws + us*u0(3)*cosphi - vs*sinphi;
u(2) = u0(2)*ws + us*u0(3)*sinphi + vs*cosphi;
u(3) = u0(3)*ws - us*sintheta;
return
```

This page is intentionally blank.

(Ask me about this in class!)

```
% randomWalks.m A Matlab script M-file demonstrating many type of random walks
%
% FileName      : randomWalks.m
% Creation      : 09/29/2016
% Modifications : September 29, 2016 Initial creation
% Author(s)     : Alex Bielajew
%

clear all
close all
format compact
clc

disp(sprintf('Several types of random walks are performed'))
disp(sprintf('=========================================='))
disp(sprintf('1: Equal steps, 2D, isotropic'))
disp(sprintf('2: Exponentionally distibuted steps, 2D, isotropic'))

Sim = input('Which simulation [1:4] would you like to see? ');

if ((floor(Sim) ~= Sim) || (Sim < 1) || (Sim > 4))
   disp('Input must be integer an between 0 and 4 incusive. Try again.')
   return
end

clc

if (Sim == 1)
   disp(sprintf('1: Equal steps, 2D, isotropic'))
   disp(sprintf('============================'))
   Nh   = input('Number of histories: ');
   smax = input('Number of step/history: ');

   % Size the trajectory arrays
   x = zeros(1,smax+1); % smax steps => smax+1 endpoints
   y = x;

   if (Nh <= smax)
      figure(1)
      hold on
   end

   %Loop over the number of histories
   maxmax = 0; % Used for axis scaling
   for n = 1:Nh
      x(1) = 0;
      y(1) = 0;

      % Loop over the individual steps/history
      for i = 1:smax
         [u,v] = azimuthal; % "azimuthal" is in the code library
         % Note that the first step is deflected before transport
         x(i+1) = x(i) + u;
         y(i+1) = y(i) + v;
      end

      % Display the histories cumulatively
      if (Nh <= smax)
         plot(x,y,'k-o')
         maxx = max(abs(x));
         maxy = max(abs(y));
         maxmax = max(maxmax,max(maxx, maxy));
         axis equal
         axis([-maxmax, maxmax, -maxmax, maxmax])
```

```
      if (n == 1)
         title(sprintf(' After %g history',n))
      else
         title(sprintf(' After %g histories',n))
      end
      if (n <= 10)
         pause
      else
         pause(0.01)
      end
      %close % Uncomment this to see individual histories
   end

   xend(n) = x(end); % Used for ploting the endpoints only
   yend(n) = y(end);

end % End of loop over histories

choice = input(' Plot all the endpoints? (0 => no) ');
if (choice)
   figure(2)
   plot(xend,yend,'ko')
end

% Calculate some stats
xbar = sum(xend)/Nh/smax
x2bar = sum(xend.^2)/Nh/smax
x3bar = sum(xend.^3)/Nh/smax
x4bar = sum(xend.^4)/Nh/smax/(smax - 1)


elseif (Sim == 2)

elseif (Sim == 3)

elseif (Sim == 4)


end
```

2D random walks, with a fixed step length

Consider a basic random walk in 2D, isotropic, steplength $s=1$. # of steps/history $= N_s$

$$\langle x \rangle = \left[\prod_{i=1}^{N_s} \left(\frac{1}{2\pi} \int_0^{2\pi} d\phi_i \right) \right] \sum_{i=1}^{N_s} \cos\phi_i$$

Similarly

$$\langle y \rangle = \left[\prod_{i=1}^{N_s} \left(\frac{1}{2\pi} \right) \int_0^{2\pi} d\phi_i \right] \sum_{i=1}^{N_s} \sin\phi_i$$

$\langle x \rangle = \langle y \rangle = 0$ since $\langle \sin \rangle \langle \cos \rangle = 0$ over a full cycle.

$$\langle x^2 \rangle = \left[\prod_{i=1}^{N_s} \frac{1}{2\pi} \int_0^{2\pi} d\phi_i \right] \left(\sum_{i=1}^{N_s} \cos\phi_i \right) \left(\sum_{j=1}^{N_s} \cos\phi_j \right)$$

$$= \left[\prod_{i=1}^{N_s} \frac{1}{2\pi} \int_0^{2\pi} d\phi_i \right] \sum_{i=1}^{N_s} \cos^2\phi_i$$

(all cross term vanish due to above argument)

$$= \frac{N_s}{2}$$

$$\langle y^2 \rangle = \frac{N_s}{2}$$

So,

$$\langle \rho^2 \rangle = \langle x^2 \rangle + \langle y^2 \rangle = N_s$$

So, the width of the random walk expands with time

$$\sqrt{\langle \rho^2 \rangle} = \sqrt{N_s}$$

You can see this in the plots

One expects

$$\langle x^3 \rangle = \langle y^3 \rangle = 0$$

What is $\langle x^4 \rangle$, $\langle y^4 \rangle$?

Would anyone like to work this out for extra credit?

hint: multi-nomials !

$$(x_1 + x_2 + x_3 \ldots x_m)^n =$$

$$\sum_{k_1 + k_2 \ldots = n} \underbrace{\left(\frac{n!}{k_1! k_2! \ldots k_m!} \right)}_{\text{multinomial coefficient}} \prod_{1 \le s \le m} x_s^{k_s}$$

I have a feeling that the variance of the variance also increases with N_s

Chapter 8

Transport in media, interaction models

In the previous chapter it was stated that a simulation provides us with a set of pathlengths, $(s_1, s_2, s_3 \cdots)$ and an associated set of deflections, $([\Theta_1, \Phi_1], [\Theta_2, \Phi_2], [\Theta_3, \Phi_3] \cdots)$ that enter into the transport and deflection machinery developed there. In this chapter we discuss how this data is produced and give some indication as to its origins. We also present some basic interaction models that are facsimiles of the real thing, just so that we can have something to model without a great deal of computational effort.

8.1 Interaction probability in an infinite medium

Imagine that a particle starts at position $\vec{x}_0$ in an arbitrary infinite scattering medium and that the particle is directed along an axis with unit direction vector $\vec{\mu}$. The medium can have a density or a composition that varies with position. We call the probability that a particle exists at position $\vec{x}$ relative to $\vec{x}_0$ *without having collided*, $p_{\rm s}(\vec{\mu}\cdot(\vec{x}-\vec{x}_0))$, the *survival probability.* The *change* in probability due to interaction is characterized by an interaction coefficient (in units L^{-1}) which we call $\mu(\vec{\mu}\cdot(\vec{x}-\vec{x}_0))$. This interaction coefficient can change along the particle flight path. The change in survival probability is expressed mathematically by the following equation:

$$\mathrm{d}p_{\rm s}(\vec{\mu}\cdot(\vec{x}-\vec{x}_0)) = -p_{\rm s}(\vec{\mu}\cdot(\vec{x}-\vec{x}_0))\mu(\vec{\mu}\cdot(\vec{x}-\vec{x}_0))\mathrm{d}(\vec{\mu}\cdot(\vec{x}-\vec{x}_0)) \ . \tag{8.1}$$

The minus sign on the right-hand-side indicates that the probability decreases with pathlength and the proportionality with $p_{\rm s}(\vec{\mu}\cdot(\vec{x}-\vec{x}_0))$ on the right-hand-side means the probability of loss is proportional to the probability of the particle *existing* at the location where the interaction takes place.

To simplify the notation we translate and rotate so that $\vec{x}_0 = (0,0,0)$ and $\vec{\mu} = (0,0,1)$. (We

can always rotate and translate back later if we want to.) However, the more complicated notation reinforces the notion that the starting position and direction can be arbitrary and that the interaction coefficient can change *along the path* of the particle's direction. In the simpler notation with a small rearrangement we have:

$$\frac{\mathrm{d}p_\mathrm{s}(z)}{p_\mathrm{s}(z)} = -\mu(z)\mathrm{d}z \ . \tag{8.2}$$

We can integrate this from $z = 0$ where we assume that $p(0) = 1$ to z and obtain:

$$p_\mathrm{s}(z) = \exp\left(-\int_0^z \mathrm{d}z'\mu(z')\right) \ . \tag{8.3}$$

The probability that a particle has interacted *within* a distance z is simply $1 - p_\mathrm{s}(z)$. This is also called the *cumulative probability:*

$$c(z) = 1 - p_\mathrm{s}(z) = 1 - \exp\left(-\int_0^z \mathrm{d}z'\mu(z')\right) \ . \tag{8.4}$$

Since the medium is infinite, $c(\infty) = 1$ and $p_\mathrm{s}(\infty) = 0$.

The differential (per unit length) probability for interaction *at* z can be obtained from the derivative of the cumulative probability $c(z)$:

$$p(z) = \frac{\mathrm{d}}{\mathrm{d}z}\left[1 - \exp\left(-\int_0^z \mathrm{d}z'\mu(z')\right)\right] = \mu(z)\exp\left(-\int_0^z \mathrm{d}z'\mu(z')\right) = \mu(z)p_\mathrm{s}(z) \ . \tag{8.5}$$

There is a critical assumption in the above expression! It is assumed that the existence of a particle at z means that it has not interacted in any way. $p_\mathrm{s}(z)$ is after all, the survival probability. Why is this important? The interaction coefficient $\mu(z)$ may represent a number of possibilities. Choosing which interaction channel the particle takes is *independent* of whatever happened along the way so long as it has survived and what happens is only dependent on the local $\mu(z)$. There will be more discussion of this subtle point later.

8.1.1 Uniform, infinite, homogeneous media

This is the usual case where it is assumed that μ is a constant, independent of position within the medium. That is, the scattering characteristic of the medium is uniform. (The interaction can depend on the energy ofthe incoming particle, however.) In this case we have the simplification:

$$p_\mathrm{s}(z) = e^{-\mu z} \ , \tag{8.6}$$

which is the well-known exponential attenuation law for the survival probability of particles as a function of depth. The cumulative probability is:

$$c(z) = 1 - p_\mathrm{s}(z) = 1 - e^{-\mu z} \ , \tag{8.7}$$

and the differential probability for interaction z is:

$$p(z) = \frac{\mathrm{d}}{\mathrm{d}z}[1 - e^{-\mu z}] = \mu e^{-\mu z} = \mu p_{\mathrm{s}}(z) \ . \tag{8.8}$$

The use of random numbers to sample this probability distribution was given in Chapter 4.

8.2 Finite media

In the case where the medium is finite, our notion of probability distribution seems to break down since:

$$c(\infty) = 1 - p_{\mathrm{s}}(\infty) = 1 - \exp\left(-\int_0^\infty \mathrm{d}z'\mu(z')\right) < 1 \ . \tag{8.9}$$

That is, the cumulative probability at infinity is less than one because either the particle escapes a finite geometry or $\mu(z)$ is zero beyond some limit. (These are two ways of saying the same thing!)

We can recover our notion of probability theory by drawing a boundary at $z = z_{\mathrm{b}}$ at the end of the geometry and rewrite the cumulative probability as:

$$c(z) = 1 - p_{\mathrm{s}}(z) = 1 - \exp\left(-\int_0^z \mathrm{d}z'\mu(z')\right) + \exp\left(-\int_0^{z_{\mathrm{b}}} \mathrm{d}z'\mu(z')\right)\theta(z - z_{\mathrm{b}}) \ , \tag{8.10}$$

where we assume that $\mu(z) = 0$ for $z \geq z_{\mathrm{b}}$. The probability distribution becomes:

$$p(z) = \mu(z)\exp\left(-\int_0^z \mathrm{d}z'\mu(z')\right) + p_{\mathrm{s}}(z_{\mathrm{b}})\delta(z - z_{\mathrm{b}}) \ . \tag{8.11}$$

The interpretation is that once the particle reaches the boundary, it reaches it with a cumulative probability equal to one minus its survival probability. Probability **is** conserved. In fact, this is *exactly* what is done in a Monte Carlo simulation. If a particle reaches the bounding box of the simulation it is absorbed at that boundary and transport discontinues. If this were not the case, an attempt at particle transport simulation would put the logic into an infinite loop with the particle being transported elsewhere looking for more medium to interact in. In a sense, this is exactly what happens in nature! Particles escaping the earth go off into outer space until they interact with another medium or else they transport to the end of the universe. It is simply a question of conservation of probability!

8.3 Regions of different scattering characteristics

Let us imagine that our "universe" contains regions of different scattering characteristics such that it is convenient to write:

$$\mu(z) \quad = \quad \mu_1(z)\theta(z)\theta(b_1 - z)$$

$$\begin{aligned}\mu(z) &= \mu_2(z)\theta(z-b_1)\theta(b_2-z)\\ \mu(z) &= \mu_3(z)\theta(z-b_2)\theta(b_3-z)\\ &\vdots\end{aligned} \tag{8.12}$$

Typically, the μ's may be constant in their own domains. However, the analysis about to be presented is much more general. Note also that there is no fundamental restriction to layered media. Since we have already introduced arbitrary translations and rotations, the notation just means that along the flight path the interaction changes in some way at certain distances that we wish to assign a particular status to.

The interaction probability for this arrangement is:

$$\begin{aligned}p(z) &= \theta(z)\theta(b_1-z)\mu_1(z)e^{-\int_0^z \mathrm{d}z'\mu_1(z')}\\ &+ \theta(z-b_1)\theta(b_2-z)\mu_2(z)e^{-\int_0^{b_1}\mathrm{d}z'\mu_1(z')}e^{-\int_{b_1}^{z}\mathrm{d}z'\mu_2(z')}\\ &+ \theta(z-b_2)\theta(b_3-z)\mu_3(z)e^{-\int_0^{b_1}\mathrm{d}z'\mu_1(z')}e^{-\int_{b_1}^{b_2}\mathrm{d}z'\mu_2(z')}e^{-\int_{b_2}^{z}\mathrm{d}z'\mu_3(z')}\\ &\vdots\end{aligned} \tag{8.13}$$

Another way of writing this is:

$$\begin{aligned}p(z) &= \theta(z)\theta(b_1-z)\mu_1(z)e^{-\int_0^z \mathrm{d}z'\mu_1(z')}\\ &+ p_{\mathrm{s}}(b_1)\theta(z-b_1)\theta(b_2-z)\mu_2(z)e^{-\int_{b_1}^{z}\mathrm{d}z'\mu_2(z')}\\ &+ p_{\mathrm{s}}(b_2)\theta(z-b_2)\theta(b_3-z)\mu_3(z)e^{-\int_{b_2}^{z}\mathrm{d}z'\mu_3(z')}\\ &\vdots\end{aligned} \tag{8.14}$$

Now consider a change of variables $b_{i-1} \le z_i \le b_i$ and introduce the conditional survival probability $p_{\mathrm{s}}(b_i|b_{i-1})$ which is the probability that a particle does not interact in the region $b_{i-1} \le z_i \le b_i$ given that it has not interacted in a previous region either. By conservation of probability:

$$p_{\mathrm{s}}(b_i) = p_{\mathrm{s}}(b_{i-1})p_{\mathrm{s}}(b_i|b_{i-1})\ . \tag{8.15}$$

Then Equation 8.14 can be rewritten:

$$p(z) = p(z_1, z_2, z_3\cdots) = p(z_1) + p_{\mathrm{s}}(b_1)[p(z_2) + p_{\mathrm{s}}(b_2|b_1)[p(z_3) + p_{\mathrm{s}}(b_3|b_2)[\cdots \tag{8.16}$$

What this means is that the variables $z_1, z_2, z_3\cdots$ can be treated as independent. If we consider the interactions over z_1 as independent, then from Equation 8.11 we have:

$$p(z_1) = \mu_1(z_1)\exp\left(-\int_0^{z_1}\mathrm{d}z'\mu_1(z')\right) + p_{\mathrm{s}}(b_1)\delta(z-b_1)\ . \tag{8.17}$$

If the particle makes it to $z = b_1$ we consider z_2 as an independent variable and sample from:

$$p(z_2) = \mu_2(z_2) \exp\left(-\int_0^{z_2} \mathrm{d}z' \mu_2(z')\right) + p_\mathrm{s}(b_2|b_1)\delta(z - b_2) \ . \tag{8.18}$$

If the particle makes it to $z = b_2$ we consider z_3 as an independent variable and sample from:

$$p(z_3) = \mu_3(z_3) \exp\left(-\int_0^{z_3} \mathrm{d}z' \mu_3(z')\right) + p_\mathrm{s}(b_3|b_2)\delta(z - b_3) \ , \tag{8.19}$$

and so on.

A simple example serves to illustrate the process. Consider only two regions of space on either side of $z = b$ with different interaction coefficients. That is:

$$\mu(z) = \mu_1\theta(b - z) + \mu_2\theta(z - b) \ . \tag{8.20}$$

The interaction probability for this example is:

$$p(z) = \theta(b - z)\mu_1 e^{-\mu_1 z} + \theta(z - b)\mu_2 e^{-\mu_1 b} e^{\mu_2(z-b)} \tag{8.21}$$

Now, treat z_1 as independent, that is

$$p(z_1) = \mu_1 e^{-\mu_1 z} + e^{-\mu_1 b}\delta(z - b) \tag{8.22}$$

If the particle makes it to $z = b$ we consider z_2 as an independent variable and sample from:

$$p(z_2) = \mu_2 e^{-\mu_2 z_2} \tag{8.23}$$

which is the identical probability distribution implied by Equation 8.21.

The importance of this proof is summarized as follows. The interaction of a particle is dependent only on the local scattering conditions. If space is divided up into regions of locally constant interaction coefficients, then we may sample the distance to an interaction by considering the space to be uniform in the local interaction coefficient. We sample the distance to an interaction and transport the particle. If a boundary demarcating a region of space with different scattering characteristics interrupts the particle transport, *we may stop at that boundary and resample using the new interaction coefficient of the region beyond the boundary.* The alternative approach would be to invert the cumulative probability distribution implied by Equation 8.4,

$$\int_0^z \mathrm{d}z' \mu(z') = -\log(1 - r) \ , \tag{8.24}$$

where r is a uniform random number between 0 and 1. The interaction distance z would be determined by summing the interaction coefficient until the equality in Equation 8.24 is satisfied. In some applications it may be efficient to do the sampling directly according to the above. In other applications it may be more efficient to resample every time the interaction coefficient changes. It is simply a trade-off between the between the time taken to index the look-up table for $\mu(z)$ and recalculating the logarithm in a resampling procedure.

8.4 Obtaining μ from microscopic cross sections

A microscopic cross section is the probability per unit pathlength that a particle interacts with one scattering center per unit volume. Thus,

$$\sigma = \frac{\mathrm{d}p}{n\,\mathrm{d}z} \ , \tag{8.25}$$

where $\mathrm{d}p$ is the differential probability of "some event" happening over pathlength $\mathrm{d}z$ and n is the number density of scattering centers that "make the event happen". The units of cross section are L^2. A special quantity has been defined to measure cross sections, the *barn*. It is equal to 10^{-24} cm^2. This definition in terms of areas is essentially a generalization of the classical concept of "billiard ball" collisions.

Consider a uniform beam of particles with cross sectional area A_b impinging on a target of thickness $\mathrm{d}z$ as depicted in Figure 8.1. The scattering centers all have cross sectional area σ. The density of scattering centers is n so that there are $nA_\mathrm{b}\mathrm{d}z$ scattering centers in the beam. Thus, the probability per unit area that there will be an interaction is:

$$\mathrm{d}p = \frac{nA_\mathrm{b}\mathrm{d}z\sigma}{A_\mathrm{b}} \ , \tag{8.26}$$

which is just the fractional area occupied by the scattering centers. Hence,

$$\frac{\mathrm{d}p}{\mathrm{d}z} = n\sigma \ , \tag{8.27}$$

which is the same expression given in Equation 8.25. While the classical picture is useful for visualizing the scattering process it is a little problematic in dealing with cross sections that can be dependent on the incoming particle energy or that can include the notion that the scattering center may be much larger or smaller than its physical size. The electromagnetic scattering of charged particles (*e.g.* electrons) from unshielded charged centers (*e.g.* bare nuclei) is an example where the cross section is much larger than the physical size. Much smaller cross sections occur when the scattering centers are transparent to the incoming particles. An extreme example of this would be neutrino-nucleon scattering. On the other hand, neutron-nucleus scattering can be very "billiard ball " in nature. Under some circumstances contact has to be made before a scatter takes place.

Another problem arises when one can no longer treat the scattering centers as independent. Classically this would happen if the targets were squeezed so tightly together that their cross sectional areas overlapped. Another example would be where groups of targets would act together collectively to influence the scattering. These phenomena are treated with special techniques that will not be dealt with directly in this book.

The probability per unit length, $\mathrm{d}p\,\mathrm{d}z$ is given a special symbol μ. That is,

$$\mu = \frac{\mathrm{d}p}{\mathrm{d}z} \ , \tag{8.28}$$

which we have been discussing in the previous sections.

The cross section, σ can also depend on the energy, E, of the incoming particle. In this case we may write the cross section differential in energy as $\sigma(E)$. The symbol σ is reserved for total cross section. If there is a functional dependence it is assumed to be differential in that quantity.

Once the particle interacts, the scattered particle can have a different energy, E' and direction, Θ, Φ relative to the initial z directions. The cross section can be differential in these parameters as well. Thus,

$$\sigma(E) = \int \mathrm{d}E'\, \sigma(E, E') = \int \mathrm{d}\Omega\, \sigma(E, \Theta, \Phi) = \int \mathrm{d}E' \int \mathrm{d}\Omega\, \sigma(E, E', \Theta, \Phi) \ , \tag{8.29}$$

relates the cross section to its differential counterparts. The interaction coefficient μ can have similar differential counterparts.

Now, consider a cross section differential both in scattered energy and angle. We may write this as:

$$\mu(E, E', \Theta, \Phi) = \mu(E) p(E, E', \Theta, \Phi) \ , \tag{8.30}$$

where $p(E, E', \Theta, \Phi)$ is a normalized probability distribution function, which describes the scattering of particle with energy E into energy E' and angles Θ, Φ. We are now ready to specify the final ingredients in particle transport.

Given a particle with energy E and cross section $\sigma(E, E', \Theta, \Phi)$:

- Form its interaction coefficient,

$$\mu(E) = n \int \mathrm{d}E' \int \mathrm{d}\Omega\, \sigma(E, E', \Theta, \Phi) \ . \tag{8.31}$$

- Usually the number density n is not tabulated but it can be determined from:

$$n = \frac{\rho}{A} N_{\mathrm{A}} \ . \tag{8.32}$$

  where ρ is the mass density, A is the atomic weight (g/mol) and N_{A} is Avogadro's number, the number of atoms per mole ($6.0221367(36) \times 10^{23}$ mol^{-1}) [C. 98][1].

- Assuming $\mu(E)$ does not depend on position, provide the distance to the interaction point employing (now familiar) sampling techniques:

$$s = -\frac{1}{\mu(E)} \log(1 - r) \ , \tag{8.33}$$

  where r is a uniformly distributed random number between 0 and 1. Provide this s and execute the transport step $\vec{x} = \vec{x_o} + \vec{\mu} s$. (Do not confuse the direction cosine vector $\vec{\mu}$ with the interaction coefficient μ!)

[1] The latest listing of physical constants and many more good things are available from the Particle Data Group's web page: `http://pdg.lbl.gov/pdg.html`

- Form the marginal probability distribution function in E':

$$m(E, E') = \int \mathrm{d}\Omega \, p(E, E', \Theta, \Phi) \ , \tag{8.34}$$

  and sample E'.

- Form the conditional probability distribution function in Θ, Φ:

$$p(E, \Theta, \Phi | E') = \frac{p(E, E', \Theta, \Phi)}{m(E, E')} \ , \tag{8.35}$$

  sample from it and provide $[\Theta, \Phi]$ to the rotation mechanism that will obtain the new direction after the scattering.

8.5 Compounds and mixtures

Often our scattering media are made up of compounds (*e.g.* water, H_2O) or homogeneous mixtures (*e.g.* air, made up of nitrogen, oxygen, water vapor and a little bit of Argon). How do we form interaction coefficients for these?

We can employ Equations 8.27 and 8.28 and extend them to include partial fractions, n_i of atoms each with its own cross section σ_i:

$$\mu(E) = \sum_i n_i \sigma_i \ . \tag{8.36}$$

Often, however, compounds are specified by fractional weights, w_i, the fraction of mass due to one atomic species compared to the total. From Equation 8.36 and 8.32:

$$\mu(E) = \sum_i \frac{\tilde{\rho}_i}{A_i} N_\mathrm{A} \sigma_i \ . = \sum_i \tilde{\rho}_i \left(\frac{\mu_i}{\rho_i} \right) = \rho \sum_i w_i \left(\frac{\mu_i}{\rho_i} \right) \ , \tag{8.37}$$

or

$$\frac{\mu(E)}{\rho} = \sum_i w_i \left(\frac{\mu_i}{\rho_i} \right) \ . \tag{8.38}$$

where ρ_i is the "normal" density of atomic component i (very often it is μ_i/ρ_i, called the mass attenuation coefficient, that is provided in numerical tabulations), $\tilde{\rho}_i$ is the "actual" mass density of the atomic species in the compound, ρ is the mass density of the compound and the fractional weight of atomic component i in the compound is $w_i = \tilde{\rho}_i / \rho$.

8.6 Branching ratios

Sometimes the interaction coefficient represents the compound process:

$$\mu(E) = \sum_i \mu_i(E) \ . \tag{8.39}$$

For example, a photon may interact through the photoelectric, coherent (Rayleigh), incoherent (Compton) or pair production processes. Thus, from Equation 8.5 we have:

$$p(z) = \sum_i p_i(z) = \sum_i \mu_i(E) e^{-z\mu(E)} = \sum_i \mu_i(E) p_{\rm s}(z) \ , \tag{8.40}$$

where we assume (a non-essential approximation) that the $\mu_i(E)$'s do not depend on position. Thus the fractional probability for interaction channel i is:

$$P_i = \frac{p_i(z)}{p(z)} = \frac{\mu_i(E)}{\mu(E)} \ . \tag{8.41}$$

In other words, the interaction channel is decided upon the relative attenuation coefficients at the location of the interaction, not on how the particle arrived at that point.

This is one of the few examples of discrete probability distributions and we emphasize this by writing an uppercase P for this probability. The sampling of the branching ratio takes the form of the following recipe:

1. Choose a random number r. If $r \leq \ \mu_1(E)/\mu(E)$, interact via interaction channel 1. Otherwise,
2. if $r \leq \ [\mu_1(E) + \mu_2(E)]/\mu(E)$, interact via interaction channel 2. Otherwise,
3. if $r \ \leq \ \ [\mu_1(E) + \mu_2(E) + \mu_3(E)]/\mu(E)$, interact via interaction channel 3. Otherwise...and so on.

The sampling must stop because $\sum_i \mu_i(E)/\mu(E)$ and a random number must always satisfy one of the conditions along the way.

Note that this technique can be applied directly to sampling from the individual atomic species in compounds and mixtures. The fractional probabilities can be calculated according to the discussion of the last section and the sampling procedure above adopted.

8.7 Other pathlength schemes

For complete generality it should be mentioned that there are other schemes for selecting pathlengths. We shall see this in the later chapter on electron transport. In many applications, electron transport steps are provided in a pre-prescribed, non-stochastic way, such as

the pathlength for which a certain average energy loss would be obtained, or a pathlength that produces a given amount of angular deflection. Deeper discussion would invoke a long discussion that we will defer until later, after we have built up all the basic of the Monte Carlo technique that we will need to solve a broad class of problems.

8.8 Model interactions

In this section we will introduce several model interactions and employ them to study some basic characteristics of Monte Carlo results.

8.8.1 Isotropic scattering

The scattering of low to medium-energy neutrons (before resonances begin to appear) is nearly isotropic in the center-of-mass. Therefore the scattering of low to medium-energy neutrons from heavy nuclei is very nearly isotropic. Isotropic scattering is sampled from the distribution function:

$$p(\Theta,\Phi)\,\mathrm{d}\Theta\,\mathrm{d}\Phi = \frac{1}{4\pi}\sin\Theta\,\mathrm{d}\Theta\,\mathrm{d}\Phi\ . \tag{8.42}$$

The sampling procedure is:

$$\begin{aligned}\cos\Theta &= 1-2r_1\\ \Phi &= 2\pi r_2\end{aligned} \tag{8.43}$$

where the r_i are uniform random numbers between 0 and 1.

8.8.2 Semi-isotropic or P_1 scattering

The first order correction to isotropic scattering of low to medium-energy neutrons, a correction that becomes increasingly important for scattering from lighter nuclei is the semi-isotropic cross angular distribution:

$$p(\Theta,\Phi)\,\mathrm{d}\Theta\,\mathrm{d}\Phi = \frac{1}{4\pi}(1+a\cos\Theta)\sin\Theta\,\mathrm{d}\Theta\,\mathrm{d}\Phi \qquad |a|\le 1\ . \tag{8.44}$$

The sampling procedure is:

$$\begin{aligned}\cos\Theta &= \frac{2-a-4r_1}{1+\sqrt{1-a(2-a-4r_1)}}\\ \Phi &= 2\pi r_2\end{aligned} \tag{8.45}$$

where the r_i are uniform random numbers between 0 and 1.

8.8.3 Rutherfordian scattering

A reasonable approximation to the elastic scattering of charged particles is the Rutherfordian distribution:

$$p(\Theta,\Phi)\,\mathrm{d}\Theta\,\mathrm{d}\Phi = \frac{a(2+a)}{4\pi}\frac{\sin\Theta\,\mathrm{d}\Theta\,\mathrm{d}\Phi}{(1-\cos\Theta+a)^2} \qquad 0 \le a < \infty\ . \tag{8.46}$$

The sampling procedure is:

$$\begin{aligned}\cos\Theta &= 1 - 2a\frac{1-r_1}{a+2r_1}\\ \Phi &= 2\pi r_2\end{aligned} \tag{8.47}$$

where the r_i are uniform random numbers between 0 and 1. An interesting feature f the Rutherfordian distribution is that it becomes the isotropic distribution in the limit $a \longrightarrow \infty$ and the "no-scattering" distribution $\delta(1-\cos\Theta)$ in the limit $a \longrightarrow 0$.

8.8.4 Rutherfordian scattering—small angle form

One approximation that is made to the Rutherfordian distribution in the limit of small a is to make the small-angle approximation to Θ as well. The distribution then takes the form:

$$p(\Theta,\Phi)\,\mathrm{d}\Theta\,\mathrm{d}\Phi = \frac{2a}{\pi}\frac{\Theta\,\mathrm{d}\Theta\,\mathrm{d}\Phi}{(\Theta^2+2a)^2} \qquad 0 \le a < \infty\ , 0 \le \Theta < \infty\ . \tag{8.48}$$

The sampling procedure is:

$$\begin{aligned}\Theta &= \sqrt{\frac{2ar}{1-r}}\\ \Phi &= 2\pi r_2\end{aligned} \tag{8.49}$$

If $\Theta > \pi$ is sampled in the first step, it is rejected and the distribution in Θ is resampled. One also has to take care that the denominator in the $\sqrt{\ }$ does not become numerically zero through some quirk of the random number generator.