

MCRT: L4

A Monte Carlo Scattering Code

- Plane parallel scattering slab
- Optical depths & physical distances
- Emergent flux & intensity
- Internal intensity moments



Constant density slab, vertical optical depth $\tau_{\max} = n \sigma z_{\max}$
 Normalized length units $z = z / z_{\max}$, so $0 < z < 1$

Emit packets

Packets scatters in slab until:

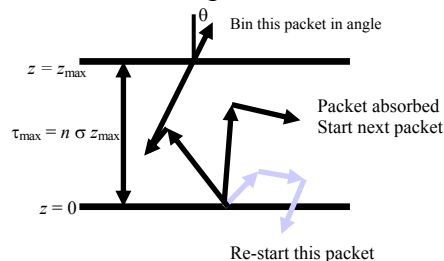
absorbed: terminate, start new packet

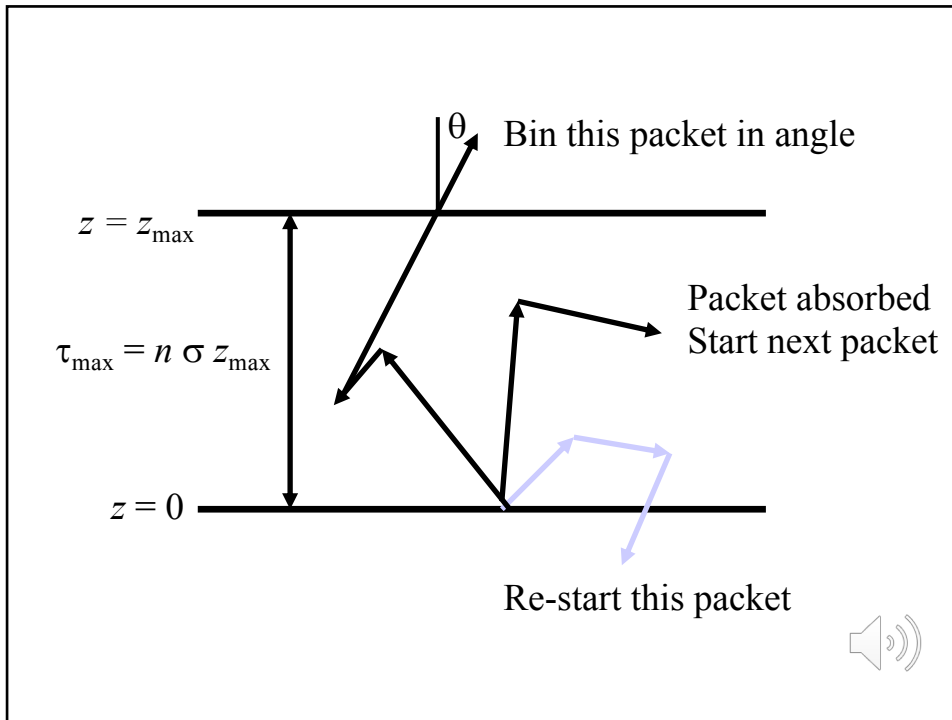
$z < 0$: re-emit packet

$z > z_{\max}$: escapes, "bin" packet

Loop over packets

Pick optical depths, test for absorption, test if still in slab





Emitting Packets: Packets need an initial starting location and direction. Uniform specific intensity from a surface.

Start packet at $(x, y, z) = (0, 0, 0)$

$$I_v(\mu) = \frac{dE}{\mu dA dt dv d\Omega} \Rightarrow \frac{dE}{dA dt dv d\Omega} \propto \frac{dN}{d\Omega} \propto \mu I_v(\mu)$$

Emission direction: sample $\phi = 2\pi\xi$

Sample μ from $P(\mu) = \mu I(\mu)$ using cumulative distribution.

Normalization: emitting outward from lower boundary,

so $0 < \mu < 1$

$$\xi = \frac{\int_0^\mu P(\mu) d\mu}{\int_0^1 P(\mu) d\mu} = \mu^2 \Rightarrow \mu = \sqrt{\xi}$$

$$n_x = \sin\theta \cos\phi$$

$$n_y = \sin\theta \sin\phi$$

$$n_z = \cos\theta$$

Distance Traveled: Random optical depth $\tau = -\log \xi$,
and $\tau = n \sigma L$, so distance traveled is:

$$L = \frac{\tau}{\tau_{\max}} z_{\max}$$

$$x = x + L n_x$$

$$y = y + L n_y$$

$$z = z + L n_z$$

Scattering: Assume isotropic scattering, so new packet
direction is:

$$\theta = \cos^{-1}(2\xi - 1)$$

$$\phi = 2\pi \xi$$

$$n_x = \sin\theta \cos\phi$$

$$n_y = \sin\theta \sin\phi$$

$$n_z = \cos\theta$$

Two different ξ values!!

Absorb or Scatter: Scatter if $\xi < a$, otherwise packet
absorbed, exit “do while in slab” loop and start a new
packet



Structure of FORTRAN program:

```

do i = 1, npackets
1   call emit_packet
      do while ( (z .ge. 0.) .and. (z .le. zmax) ) ! packet is in slab
          L = -log(ran) * zmax / taumax
          z = z + L * nz      ! update packet position, x,y,z
          if ((z.lt.0.).or.(z.gt.zmax)) goto 2 ! packet exits
          if (ran .lt. albedo) then
              call scatter
          else
              goto 3      ! terminate packet
          end if
      end do
2   if (z .le. 0.) goto 1 ! re-start packet
      bin packet according to direction
3   continue ! exit for absorbed packets, start a new packet
end do

```



Fortran functions and subroutines: Pass variables and a FUNCTION performs maths, algebra, geometry, to return a single result, e.g., random number generators. SUBROUTINES are similar, but can return many different results. The order that variables are passed must be the same in the call statement and the subroutine. In main program have the call statement:

```
call emit_packet(iseed,x,y,z,nx,ny,nz)
```

```
subroutine emit_packet(iseed,x,y,z,nx,ny,nz)
implicit none
```

```
integer iseed
real x,y,z,nx,ny,nz,ran2
```

Set packet position and direction using equations

```
return
end
```



Binning Packets

Bin escaping packets according to direction of travel in ϕ (azimuth) and θ (polar). Bins of equal ϕ and equal $[\cos(\theta)]$, gives bins of equal solid angle.

Can also have internal spatial bins to sum quantities for computing number of interactions, fluxes, pressures, etc. See lectures on 3D grid codes.

Can also bin in time when doing time-dependent simulations. In general the time for a particle to traverse a distance is simply $t = d / v$, where v is photon or particle speed in the medium.



Error Estimation

Recall expected value (mean), variance, standard deviation:

$$E(x) = \bar{x} = \frac{1}{n} \sum_{i=1}^n x_i \quad \text{var}(x) = \sigma^2 = \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2$$

Where x can be number of photons in a bin (spatial or angular); number of scatterings per photon; counters for mean intensity, fluence, number of absorptions, radiation pressure; etc, etc
 Compute sum of x and x^2 in each bin (angular or spatial) and estimate σ using:

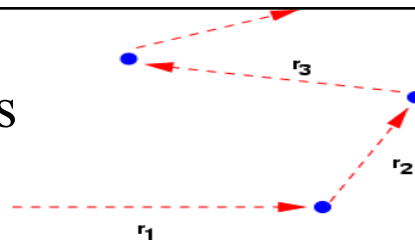
$$\sigma^2 = \text{var}(x) = E(x^2) - [E(x)]^2$$

Variance of the mean is σ^2 / n

Standard deviation of the estimate of the mean is $\sigma / n^{1/2}$



Random walks



Net displacement of a single photon from starting position after N mean free paths between scatterings is:

$$\mathbf{R} = \mathbf{r}_1 + \mathbf{r}_2 + \dots + \mathbf{r}_N$$

Square and average to get distance $|R|$ travelled :

$$l_*^2 \equiv \langle \mathbf{R}^2 \rangle = \langle \mathbf{r}_1^2 \rangle + \langle \mathbf{r}_2^2 \rangle + \dots + \langle \mathbf{r}_N^2 \rangle + 2\langle \mathbf{r}_1 \cdot \mathbf{r}_2 \rangle + \dots$$

The cross terms are all of the form:

$$2\langle \mathbf{r}_1 \cdot \mathbf{r}_2 \rangle = 2\langle |\mathbf{r}_1| |\mathbf{r}_2| \cos \delta \rangle$$

where δ is the angle of deflection during the scattering.

For isotropic scattering, $\langle \cos \delta \rangle = 0$, cross-terms vanish.

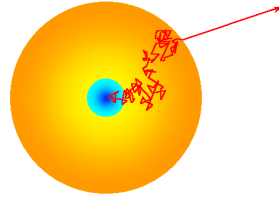


Thus, for a random walk from centre to edge of sphere of radius l_* , we can determine average number of scatterings, N , from

$$l_*^2 \equiv \langle \mathbf{R}^2 \rangle = \langle \mathbf{r}_1^2 \rangle + \langle \mathbf{r}_2^2 \rangle + \dots + \langle \mathbf{r}_N^2 \rangle$$

$$\alpha^2 l_*^2 = \tau_{\max}^2 = N \alpha^2 \langle \mathbf{r}^2 \rangle = N \langle \tau^2 \rangle$$

$$N = \tau_{\max}^2 / \langle \tau^2 \rangle = \tau_{\max}^2 / 2$$



Using: $\langle \tau^2 \rangle = \int_0^{\infty} p(\tau) \tau^2 d\tau = \int_0^{\infty} e^{-\tau} \tau^2 d\tau = 2$

If the medium is optically thin, then the probability of scattering is $1 - e^{-\tau}$

Using $1 - e^{-\tau} \cong \tau$ then $N \approx \tau$, $\tau \ll 1$

Therefore $N \approx \tau + \tau^2 / 2$ is a more accurate approximation

