Why are you here?

- Use existing Monte Carlo codes to model data sets – set up source locations & luminosities, change density structure, get images and spectra to compare with observations
- Learn techniques so you can develop your own Monte Carlo codes
- General interest in computational radiation transfer techniques

Format

- Lectures & lots of “unscheduled time”
- Breakout sessions – tutorial exercises, using codes, informal discussions
- Coffee served at 10.30 & 15.30
- Lunch at 13.00 or 12.30
- Dinner at 7pm (different locations)

Lecturers

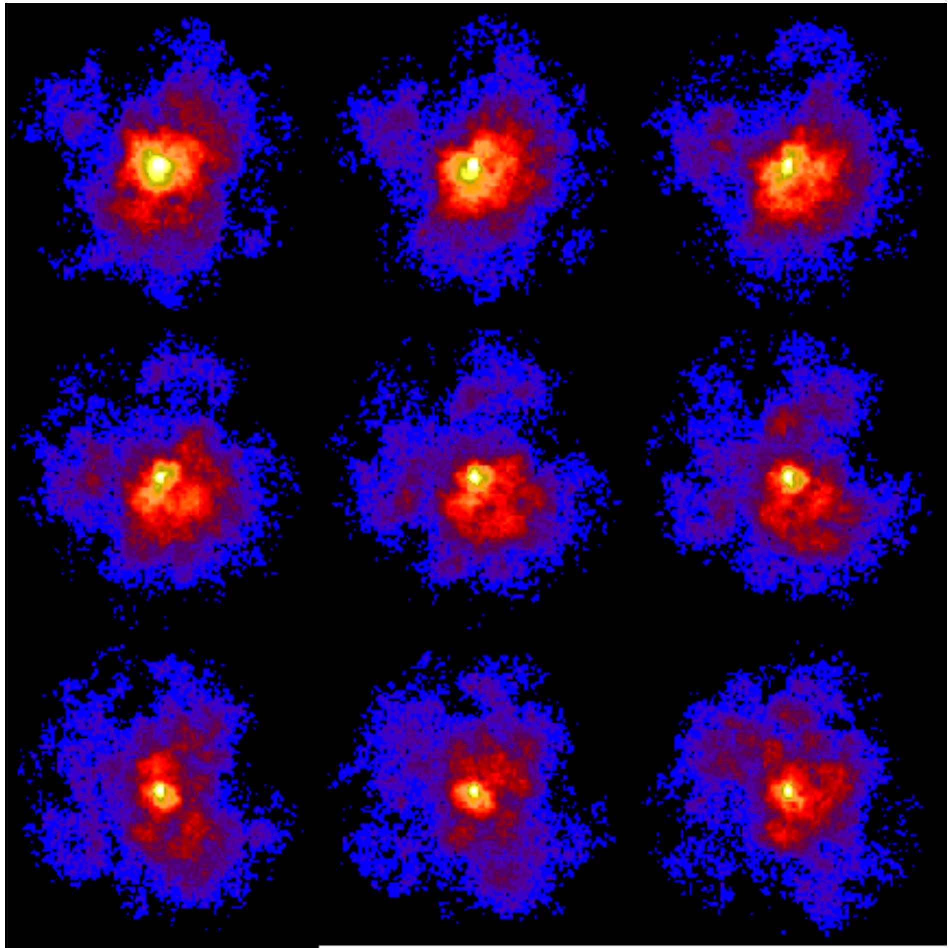
- Kenny Wood – general intro to MCRT, write a short scattered light code, photoionization code
- Tom Robitaille – radiative equilibrium, improving efficiency of MCRT codes, using HYPERION
- Tim Harries – 3D gridding techniques, radiation pressure, time dependent MCRT, using TORUS
- Michiel Hogerheijde – NLTE excitation, development of NLTE codes, using LIME
- Barbara Ercolano – photoionization, using MOCASSIN

Lecturers

- Stuart Sim – radiation hydrodynamics with MCRT
- Peter Camps – MCRT for modeling of dust in galaxies, SKIRT
- Steve Jacques – MCRT in medicine, laser-tissue interactions, planning cancer treatments, etc
- Jon Bjorkman (cancelled due to illness) – theory of MCRT, radiative equilibrium techniques, error estimates, normalizing output results

Reflection Nebulae: can reflections from grains diagnose albedo?

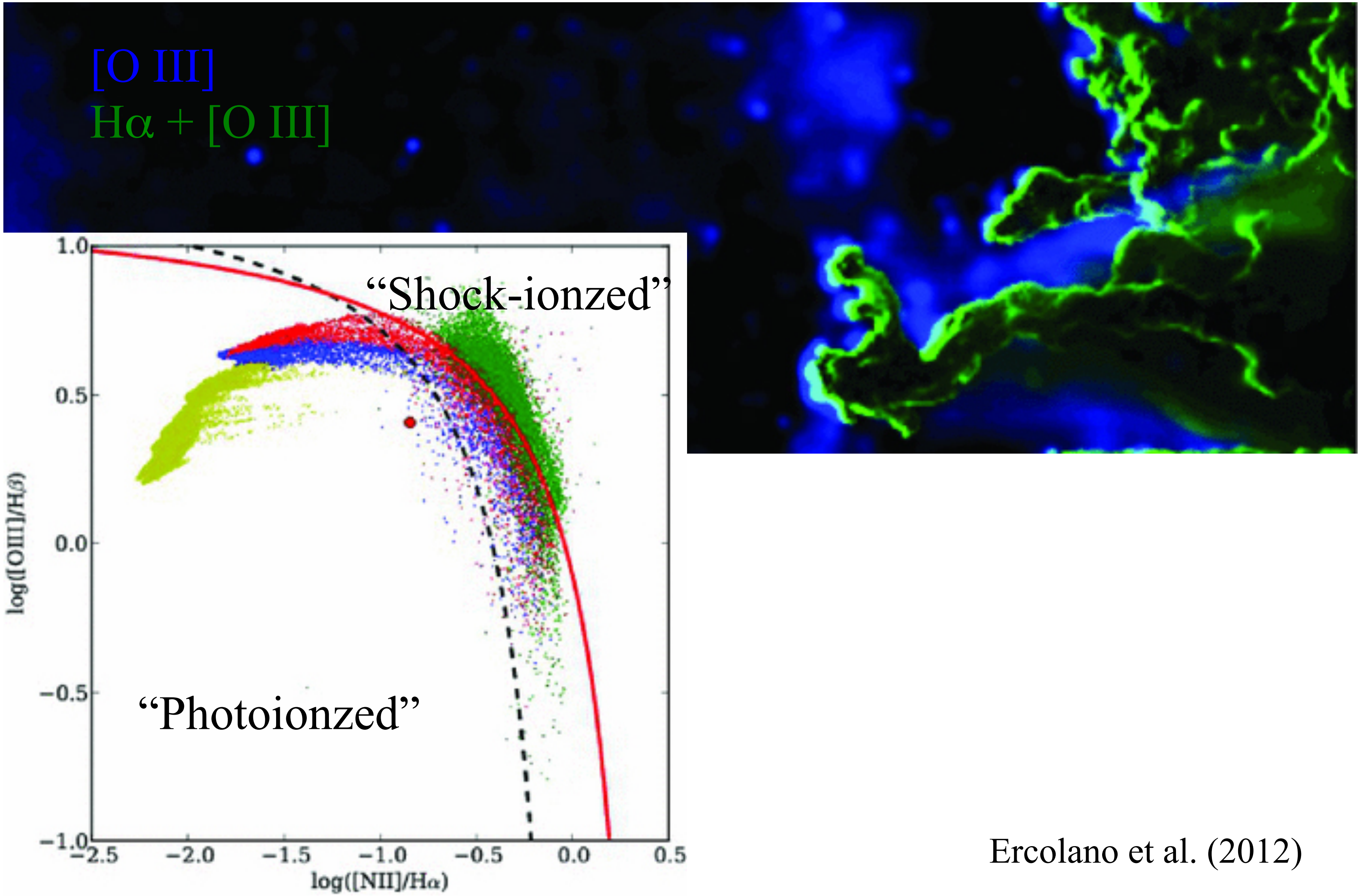
NGC 7023
Reflection Nebula



3D density: viewing angle effects

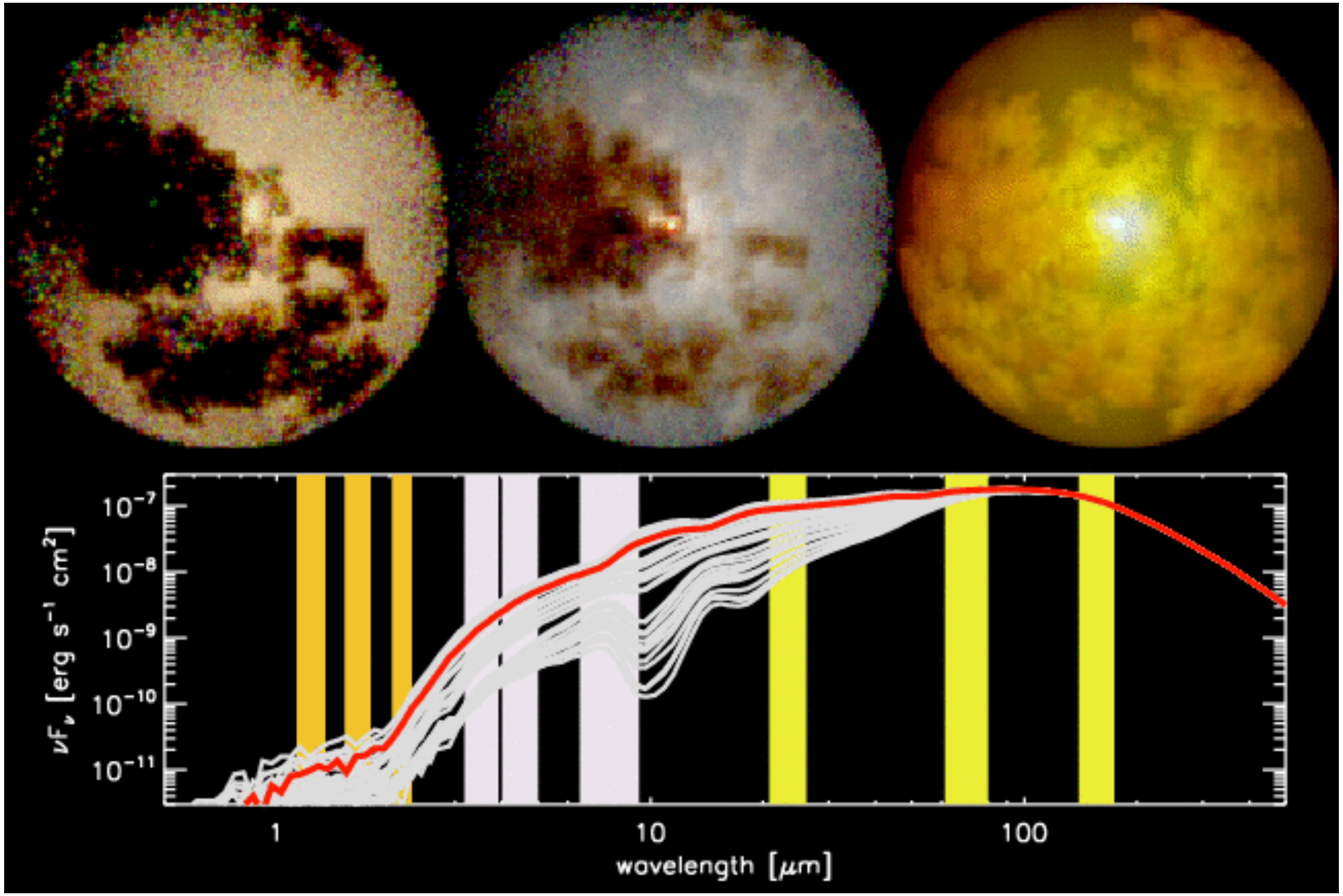
Mathis, Whitney, & Wood (2002)

Photo- or shock- ionization?



Ercolano et al. (2012)

Dusty Ultra Compact H II Regions



3D Models: Big variations with viewing angle

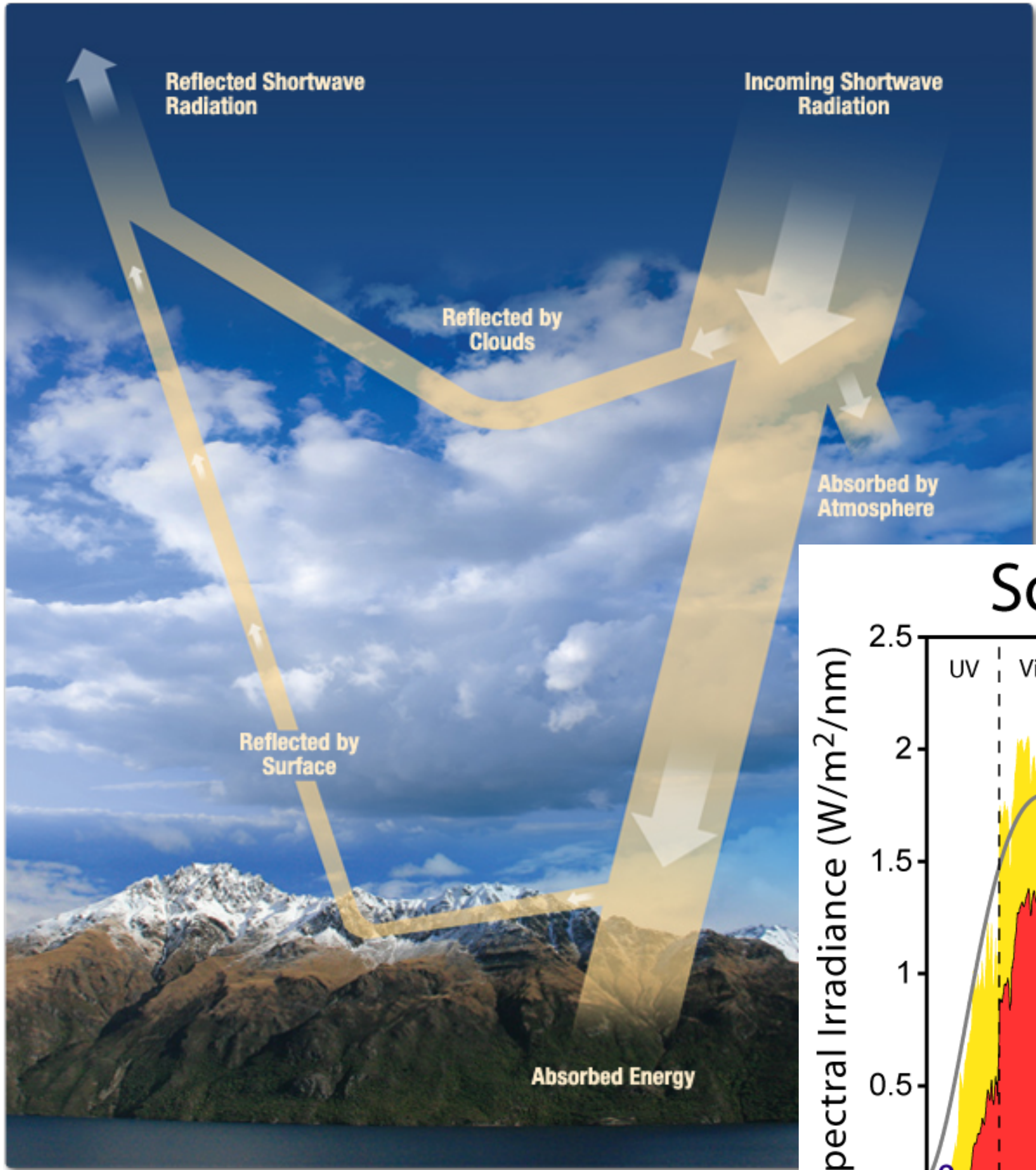
Indebetouw, Whitney, Johnson, & Wood (2006)

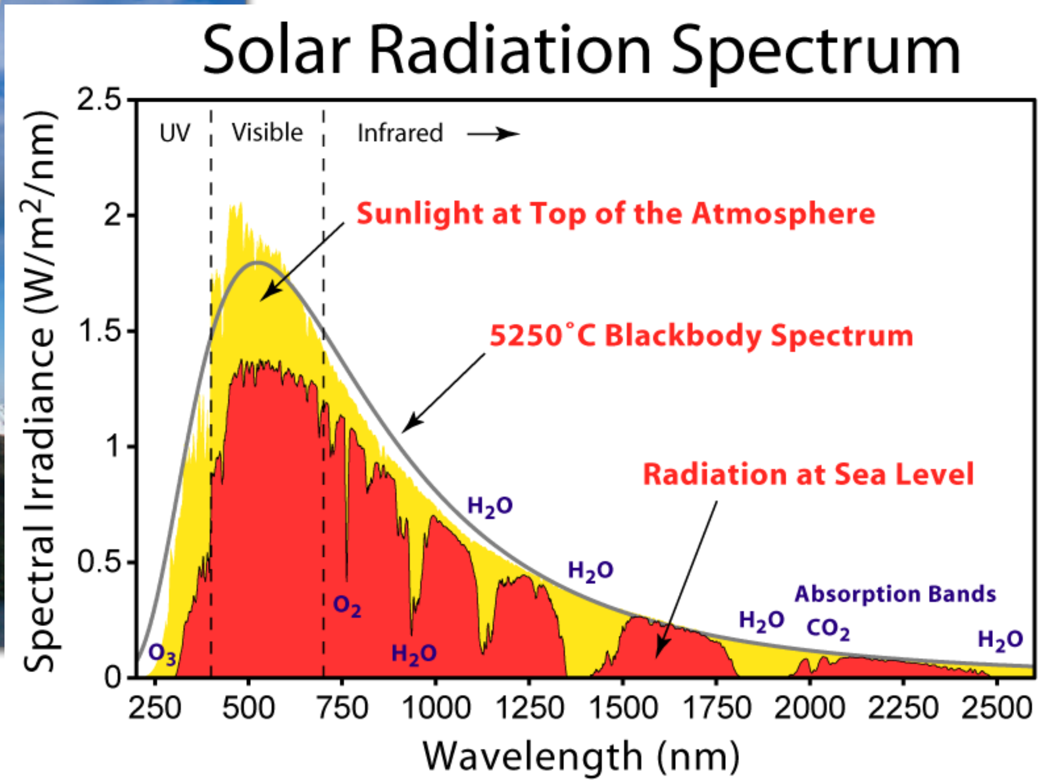
What happens physically?

- Photons emitted, travel some distance, interact with material
- Scattered, absorbed, re-emitted
- Photon interactions heat material, change level populations, alter ionization balance and hence change opacity
- If medium in hydrostatic equilibrium: density structure related to temperature structure
- Density structure may depend on radiation field and vice versa

Atmospheric Physics

Clouds important for photon transport and temperature structure of atmosphere



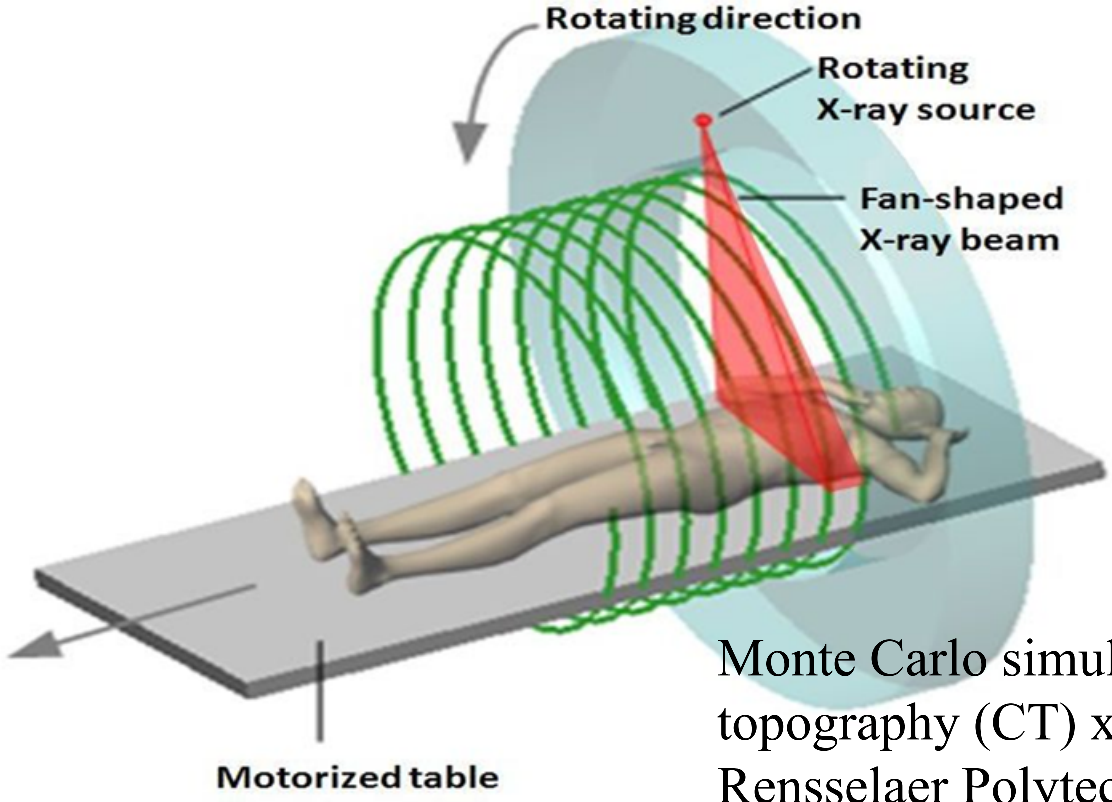


Medical Physics

Light activated treatments such as photodynamic therapy: how deep does the radiation penetrate into skin and tissue?

Imaging using x-ray, ultraviolet, optical, infrared, & polarised light

Optical tweezers, photo-acoustic imaging, nuclear medicine, etc, etc



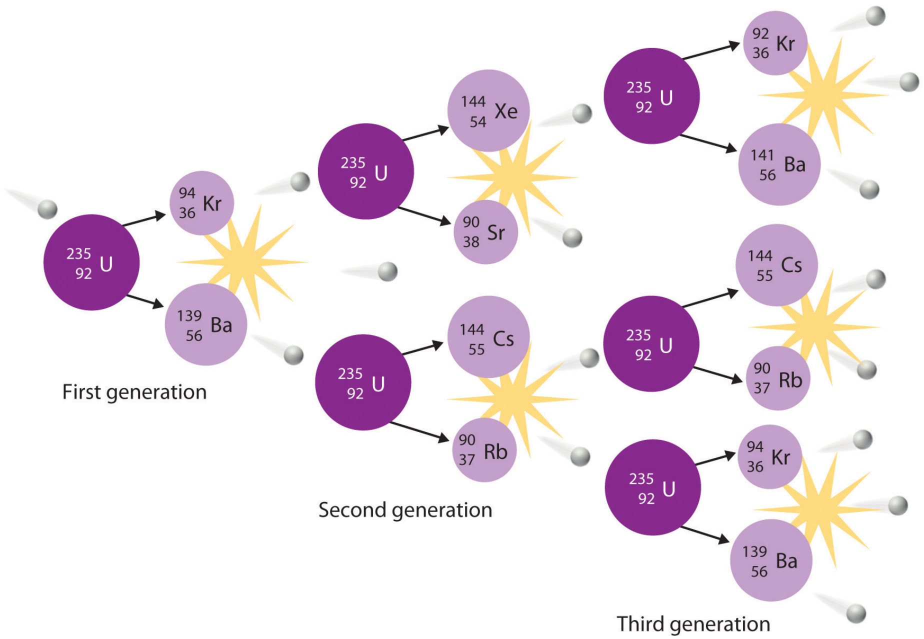
Monte Carlo simulations of computed topography (CT) x-ray imaging doses
Rensselaer Polytechnic Institute

Nuclear Physics & Neutron Transport

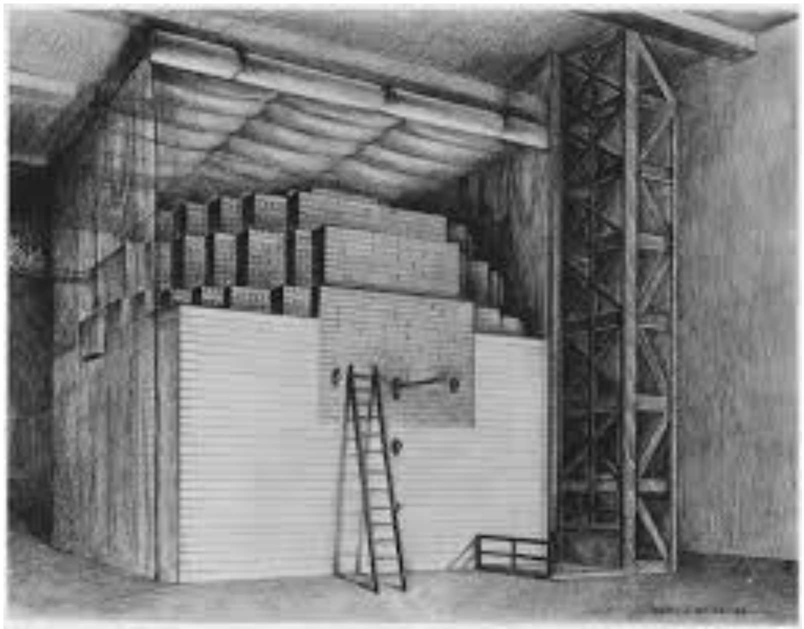
Compute controlled criticality assemblies & geometries for nuclear fission reactors

Nuclear safety – radioactive shielding calculations

Uncontrolled reactions – critical masses for bombs



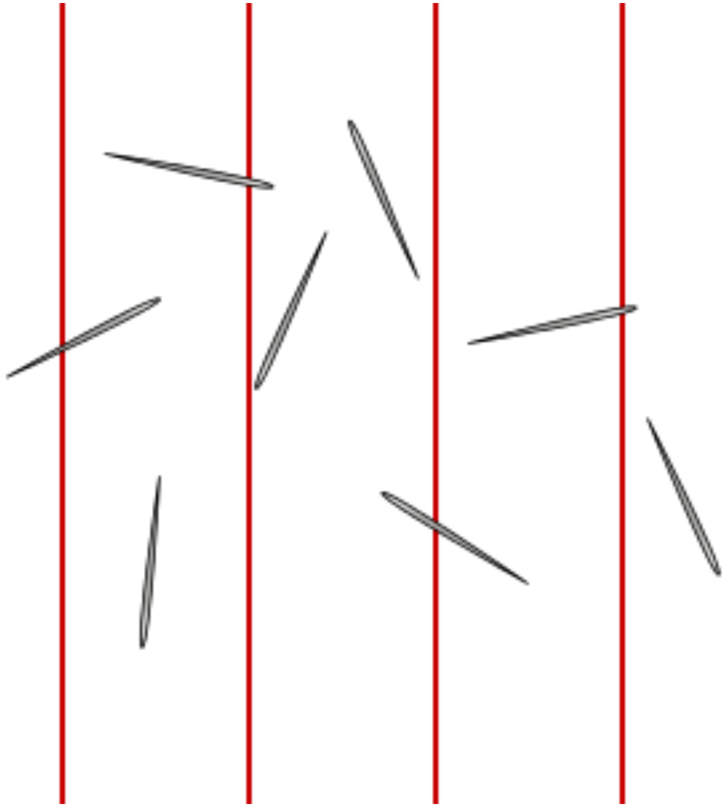
Chain reaction in ^{235}U



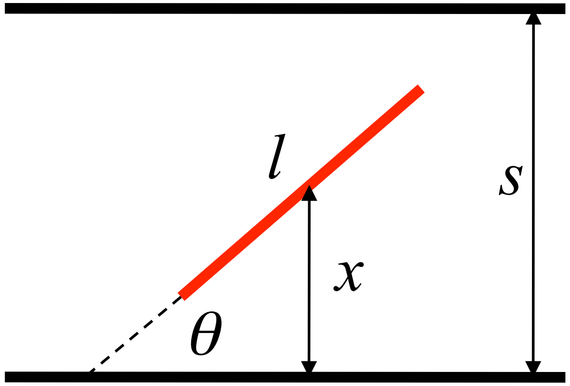
Chicago Pile 1, December 1942
World's first artificial nuclear reactor

Buffon’s needles

Georges-Louis Leclerc
Comte de Buffon
1707-1788



What is the probability that a needle will cross a line?



Needles of length l
Line separation s
x = distance from needle centre to closest line
Needle touches/crosses line if

$$x \le \frac{l}{2}\sin\theta$$

Probability density function: function of a variable that gives probability for variable to take a given value

Exponential distribution: $p(x) = e^{-x}$, for x in range 0 to infinity

Uniform distribution: $p(x) = 1/L$, for x in range 0 to L

Normalised over all x: $\int_0^\infty p(x)\,dx = 1$

Probability x lies in range $a < x < b$ is ratio of "areas under the curve"

$$P = \frac{\int_a^b p(x)\,dx}{\int_0^\infty p(x)\,dx}$$

x is distributed uniformly between $(0, s/2)$, θ in range $(0, \pi/2)$

$$p(x) = 2/s, \qquad p(\theta) = 2/\pi$$

Variables x and θ independent, so joint probability is

$$p(x, \theta) = 4/(s\,\pi)$$

Probability of a needle touching a line ($l < s$) is

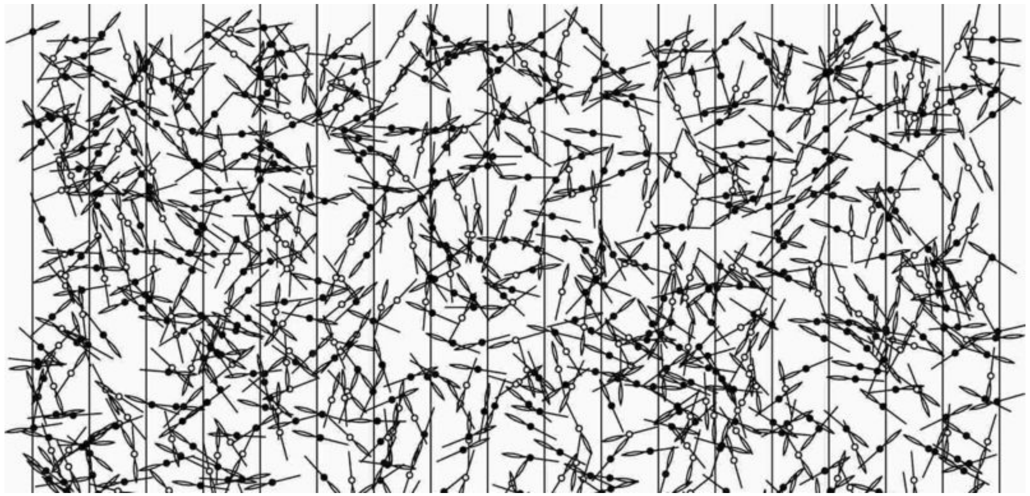
$$P = \int_0^{\pi/2} \int_0^{l/2 \sin\theta} \frac{4}{s\pi} \, dx \, d\theta = \frac{2l}{s\pi}$$

Drop lots of needles. Probability of needle crossing line is

$$P = \frac{\text{Number of needles crossing lines}}{\text{Total number of needles dropped}}$$

Can estimate π :

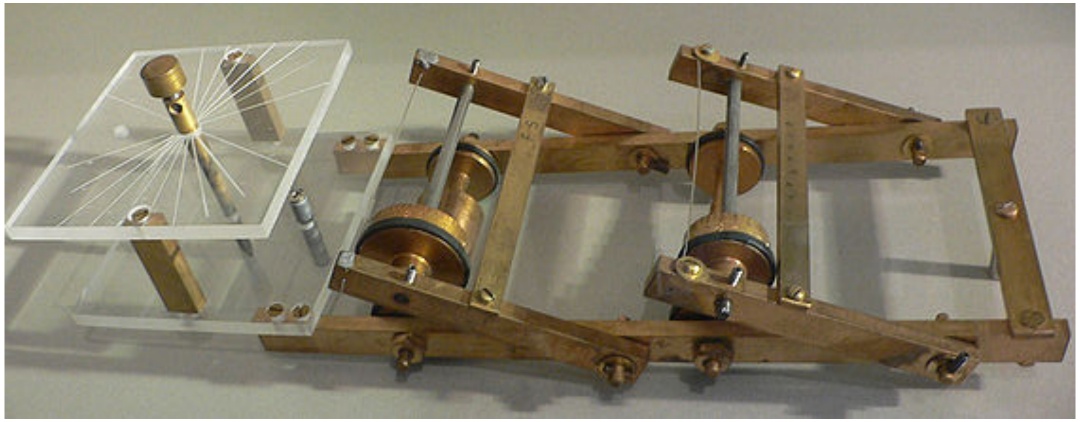
$$\pi = \frac{2l}{sP}$$

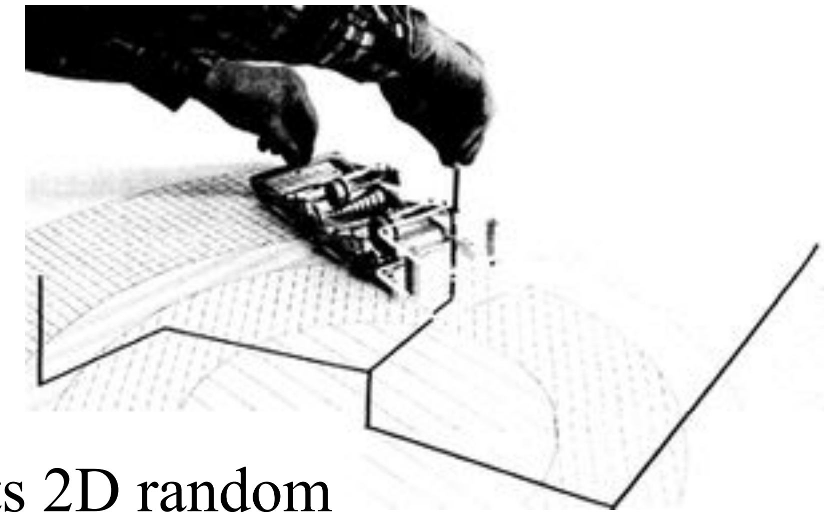


Brief History

- Buffon's needles – first Monte Carlo simulation
- Statistical sampling – draw conclusions on an entire population by conducting a study on a small subset of the population.
- Used in maths since 1800s, but slow before computers.
- Lord Kelvin studied kinetic theory using random sampling to evaluate integrals. Generated random numbers by pulling pieces of paper from a jar.
- Fission of ^{235}U by neutrons discovered in 1938, possibility of chain reactions for power and explosives
- Enrico Fermi developed mechanical machine, the FERMIAC, to simulate neutron random walks

Enrico Fermi and the FERMIAC



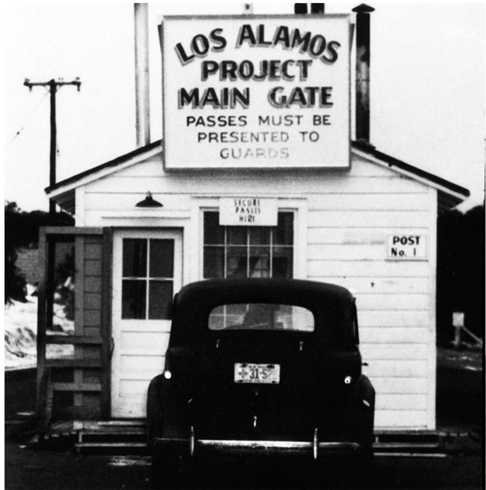


Mechanical device that plots 2D random
walks of slow and fast neutrons in fissile material

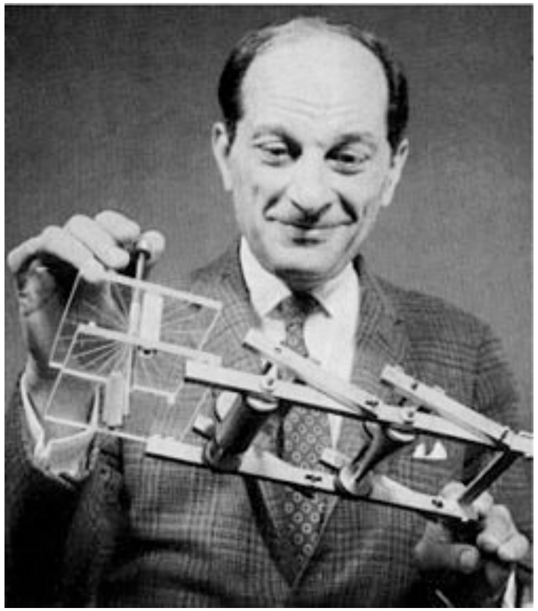
Los Alamos

- Development of computers from the 1940s made Monte Carlo practical – the ENIAC, MANIAC, etc
- Ideas from Metropolis, Ulam, von Neumann, Teller developed for neutron propagation



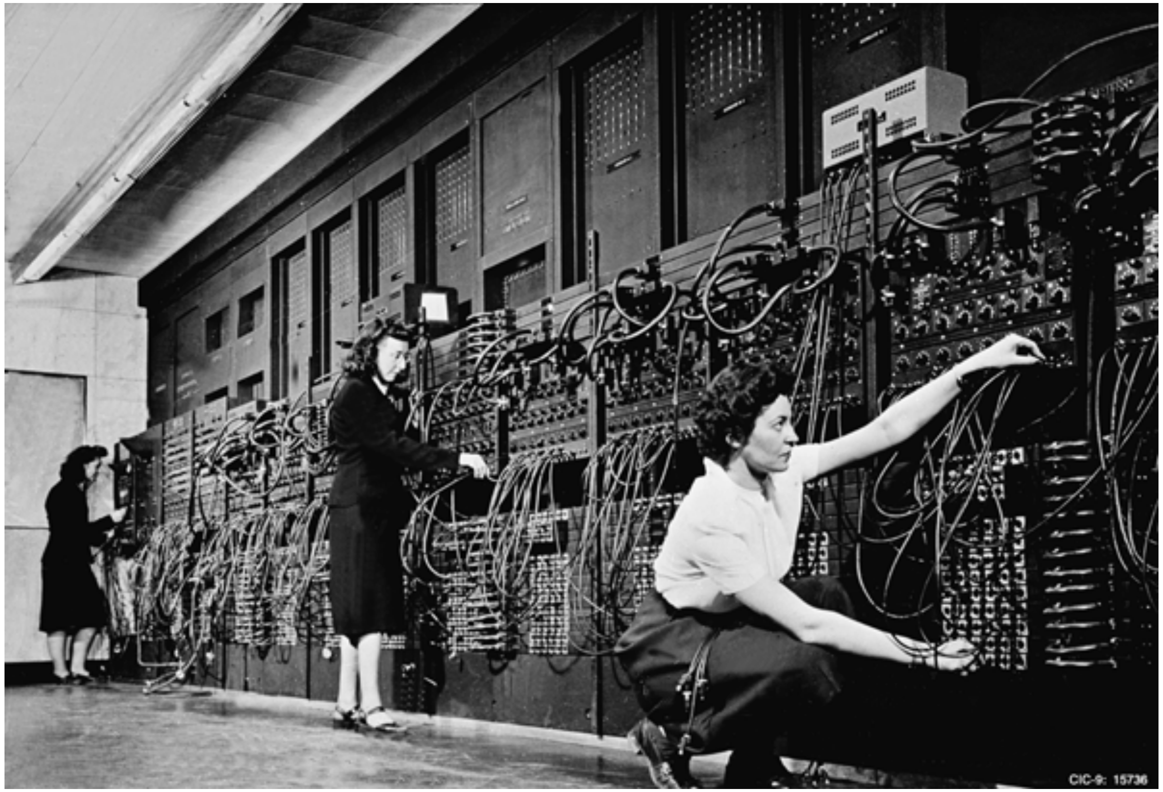



No whining about fortran…!!!!



Stan Ulam with the FERMIAC

The ENIAC
Electronic Numerical Integrator and Computer



MANIAC: Mathematical Analyzer Numerical Integrator and Computer

- Stan Ulam had ideas on numerical simulations when he was ill and playing solitaire (patience)
- Technique given name by Nick Metropolis
- First declassified paper published in 1949 by Metropolis & Ulam: “The Monte Carlo Method”

Just in case you think you're doing something new…

THE INSTITUTE FOR ADVANCED STUDY
Founded by Mr. Louis Bamberger and Mrs. Felix Fuld
PRINCETON, NEW JERSEY
School of Mathematics

March 11, 1947

IA AIRMAIL: REGISTERED

Mr. R. Richtmyer
Post Office Box 1663
Santa Fe, New Mexico

Dear Bob:

This is the letter I promised you in the course of our telephone conversation on Friday, March 7th.

I have been thinking a good deal about the possibility of using statistical methods to solve neutron diffusion and multiplication problems, in accordance with the principle suggested by Stan Ulam. The more I think about this, the more I become convinced that the idea has great merit. My present conclusions and expectations can be summarized as follows:

(1) The statistical approach is very well suited to a digital treatment. I worked out the details of a criticality discussion under the following ...itions: ...metry ...position along the

Just in case you think you’re doing something new…

Dear Bob,

I have been thinking a good deal about the possibility of using statistical methods to solve the neutron diffusion and multiplication problem, in accordance with the principle suggested by Stan Ulam…

If and when the problem of neutron diffusion has been satisfactorily handled… it will be time to investigate the more general case, where hydrodynamics also come into play… I think I know how to set up this problem, too…

John von Neumann had Monte Carlo radiation transport coupled with hydrodynamics all figured out… in 1947!!

Recap of radiation transfer basics

- Intensities
- Opacities
- Mean free path
- Equation of radiation transfer

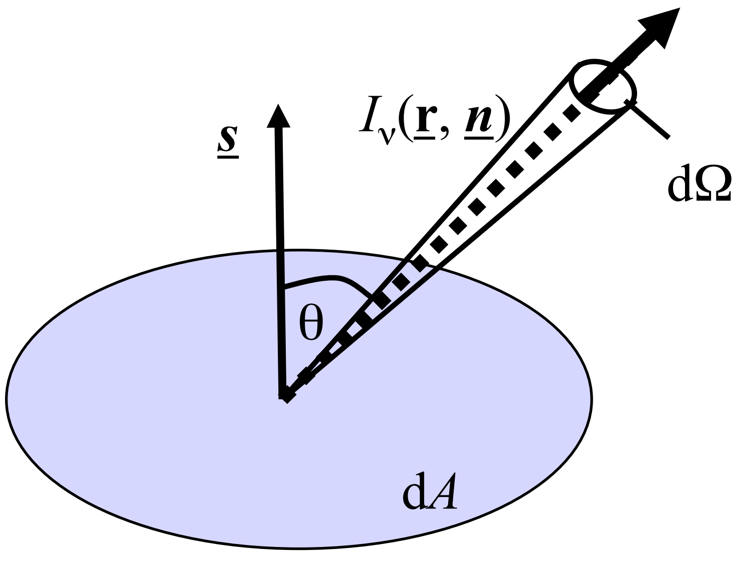
Specific Intensity

$$\mathrm{d}E_\nu = I_\nu \cos\theta \, \mathrm{d}A \, \mathrm{d}t \, \mathrm{d}\nu \, \mathrm{d}\Omega$$

Units of I_ν: J/m^2/s/Hz/sr (ergs/cm^2/s/Hz/sr)

Function of position and direction

Independent of distance when no sources or sinks



s is normal to dA

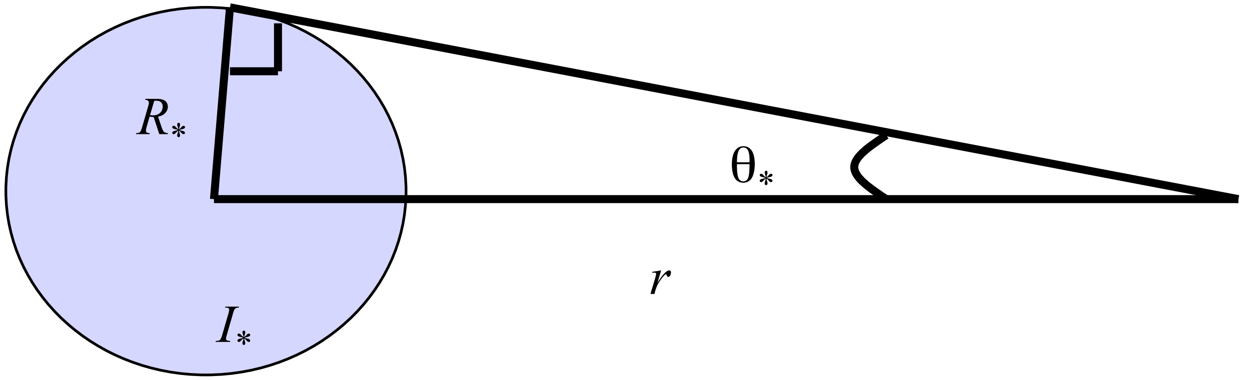
Mean Intensity

$$J_\nu = \frac{1}{4\pi}\int I_\nu \, \mathrm{d}\Omega = \frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi} I_\nu \sin\theta \, \mathrm{d}\theta \, \mathrm{d}\phi$$

Same units as I_ν

Function of position

Determines heating, ionization, level populations, etc



What is J_ν at r from a star with uniform specific intensity I_* across its surface?

$I = I_*$ for $0 < \theta < \theta_*$ $(\mu_* < \mu < 1)$; $\mu = \cos\theta$

$I = 0$ for $\theta > \theta_*$ $(\mu < \mu_*)$

$$J = \frac{1}{2}\int_{\mu_*}^{1} I \, \mathrm{d}\mu = \tfrac{1}{2} I_* (1 - \mu_*)$$

$$J = I_* \tfrac{1}{2}\left(1 - \sqrt{1 - R_*^2 / r^2}\right) = w I_*$$

w = *dilution factor*

Large r, $w = R^2/4r^2$

Monochromatic Flux

$$\mathcal{F}_\nu = \int I_\nu \cos\theta \, \mathrm{d}\Omega = \int_0^{2\pi} \int_0^{\pi} I_\nu \cos\theta \sin\theta \, \mathrm{d}\theta \, \mathrm{d}\phi$$

Energy passing through a surface. Units: J/s/m^2/Hz

Stellar Luminosity

Flux = energy/second per area/Hz
Luminosity = energy/second/Hz

$$L_\nu = \mathcal{F}_\nu A_* = 4\pi R_*^2 \pi I_\nu$$

Assume $I_\nu = B_\nu$ and integrate to get total luminosity:

$$L = \int L_\nu \, d\nu = 4\pi R_*^2 \pi \int B_\nu \, d\nu = 4\pi R_*^2 \sigma T^4$$

Energy Density & Radiation Pressure

$$u_\nu = \frac{1}{c}\int I_\nu \, \mathrm{d}\Omega = \frac{4\pi}{c} J_\nu$$

$$p_\nu = \frac{1}{c}\int I_\nu \cos^2\theta \, \mathrm{d}\Omega$$

u_ν : J/m^3/Hz

p_ν : N/m^2/Hz

Isotropic radiation: $p_\nu = u_\nu/3$

Radiation pressure analogous to gas pressure: pressure of the photon gas

Moments of the Radiation Field

First three moments of specific intensity are named *J* (zeroth moment), *H* (first), and *K* (second):

$$J_\nu = \frac{1}{4\pi}\int I_\nu \, \mathrm{d}\Omega$$

$$H_\nu = \frac{1}{4\pi}\int I_\nu \cos\theta \, \mathrm{d}\Omega$$

$$K_\nu = \frac{1}{4\pi}\int I_\nu \cos^2\theta \, \mathrm{d}\Omega$$

Physically: J = mean intensity; $H = \mathcal{F} / 4\pi$

K related to radiation pressure:

$$p_\nu = \frac{4\pi}{c} K_\nu$$

Photon Interactions

- Scattering: change direction (and energy)
- Absorption: energy added to K.E. of particles: photon thermalized
- Emission: energy taken from thermal energy of particles

Emission Coefficient

$$\mathrm{d}E_\nu \equiv j_\nu \, \mathrm{d}V \, \mathrm{d}t \, \mathrm{d}\nu \, \mathrm{d}\Omega$$

Energy, $\mathrm{d}E_\nu$, added:

- stimulated emission
- spontaneous emission
- thermal emission
- energy scattered into the beam

Intensity contribution from emission along ds:

$$\mathrm{d}I_\nu(s) = j_\nu(s)\,\mathrm{d}s$$

Extinction Coefficient

Energy removed from beam

Defined per particle, per mass, or per volume

$$\mathrm{d}I_\nu(s) = -I_\nu\,\sigma_\nu\,n\,\mathrm{ds}$$

σ_ν = cross section per particle (m^2)

n = particle density (m^{-3})

$$\mathrm{d}I_\nu(s) = -I_\nu\,\alpha_\nu\,\mathrm{ds}$$

α_ν: units of m^{-1}

$$\mathrm{d}I_\nu(s) = -I_\nu\,\kappa_\nu\,\rho\,\mathrm{ds}$$

κ_ν: units $m^2\ kg^{-1}$

ρ = density ($kg\ m^{-3}$)

Source Function

Same units as intensity:

$$S_\nu \equiv \frac{j_\nu}{\alpha_\nu}$$

Multiple processes contribute to emission and extinction:

$$S_\nu^{\mathrm{tot}} = \frac{\sum j_\nu}{\sum \alpha_\nu}$$

e.g., a spectral line:

$$S_\nu^{\mathrm{tot}} = \frac{j_\nu^c + j_\nu^l}{\alpha_\nu^c + \alpha_\nu^l} = \frac{S_\nu^c + \eta_\nu S_\nu^l}{1 + \eta_\nu}$$

$\eta_\nu = \alpha_\nu^l / \alpha_\nu^c$ = line-to-continuum extinction ratio;
S_ν^c, S_ν^l are continuum and line source functions

Optical Depth

$$\mathrm{d}\tau_\nu = \alpha_\nu(s)\,\mathrm{d}s = \rho(s)\kappa_\nu\,\mathrm{d}s$$

$$\tau_\nu = \int_0^s \alpha_\nu\,\mathrm{d}s = \int_0^s \rho\kappa_\nu\,\mathrm{d}s$$

Function of frequency via the opacity, and direction

Physically τ_ν is number of photon mean free paths

Mean free path = $1 / \alpha = 1 / (n\,\sigma) = 1 / (\rho\,\kappa)$

Equation of Radiation Transfer

ERT along a ray: $$\frac{\mathrm{d}I_\nu}{\mathrm{d}\tau_\nu} = S_\nu - I_\nu$$

Solution: $$I_\nu(\tau_\nu) = I_\nu(0)\,\mathrm{e}^{-\tau_\nu} + \int_0^{\tau_\nu} S_\nu(t_\nu)\,\mathrm{e}^{-(\tau_\nu - t_\nu)}\,\mathrm{d}t_\nu$$

Goal: Determine source function!

Interconnectedness

Moments (J_ν, H_ν, K_ν) depend on I_ν

Need to solve ERT to get I_ν

I_ν (and hence J_ν) depends on position and direction

I_ν depends on S_ν, hence on emissivity and opacity

Opacity depends on temperature and ionization

Temperature and ionization depends on J_ν

$$J_\nu = \frac{1}{4\pi}\int I_\nu \,\mathrm{d}\Omega$$

$$H_\nu = \frac{1}{4\pi}\int I_\nu \cos\theta \,\mathrm{d}\Omega$$

$$K_\nu = \frac{1}{4\pi}\int I_\nu \cos^2\theta \,\mathrm{d}\Omega$$

$$\frac{\mathrm{d}I_\nu}{\mathrm{d}\tau_\nu} = S_\nu - I_\nu$$

$$S_\nu \equiv \frac{j_\nu}{\alpha_\nu}$$

$$\mathrm{d}\tau_\nu = \alpha_\nu(s)\,\mathrm{d}s = \rho(s)\kappa_\nu\,\mathrm{d}s$$

Example: Model H II Region

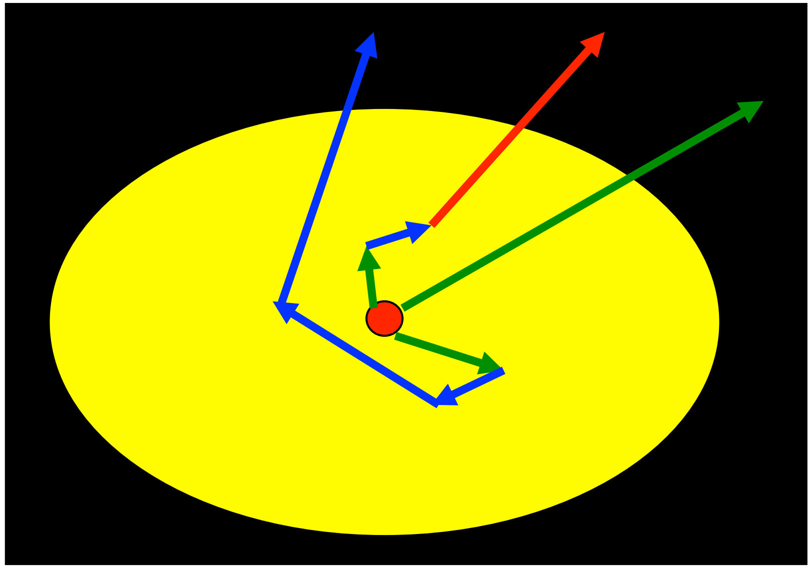
- Sources of ionizing photons
- Opacity from neutral H: bound-free
- 1st iteration:
  - Medium fully ionized (no neutral H) so opacity is zero
  - Solve ERT throughout medium to get J_ν
  - Solve for ionization structure, some regions neutral
- 2nd iteration:
  - new opacity structure,
  - different solution for ERT, different J_ν values
  - new ionization and opacity structure
- Iterate until get convergence: solution of ERT, J_ν, ionization structure do not change with further iterations

Monte Carlo Radiation Transfer I

- Monte Carlo "Photons" and interactions
- Sampling from probability distributions
- Optical depths, isotropic emission, scattering

Monte Carlo Basics

- Emit luminosity packet, hereafter a “photon”
- Photon travels some distance
- Something happens…



- Scattering, absorption, re-emission

Luminosity Packets

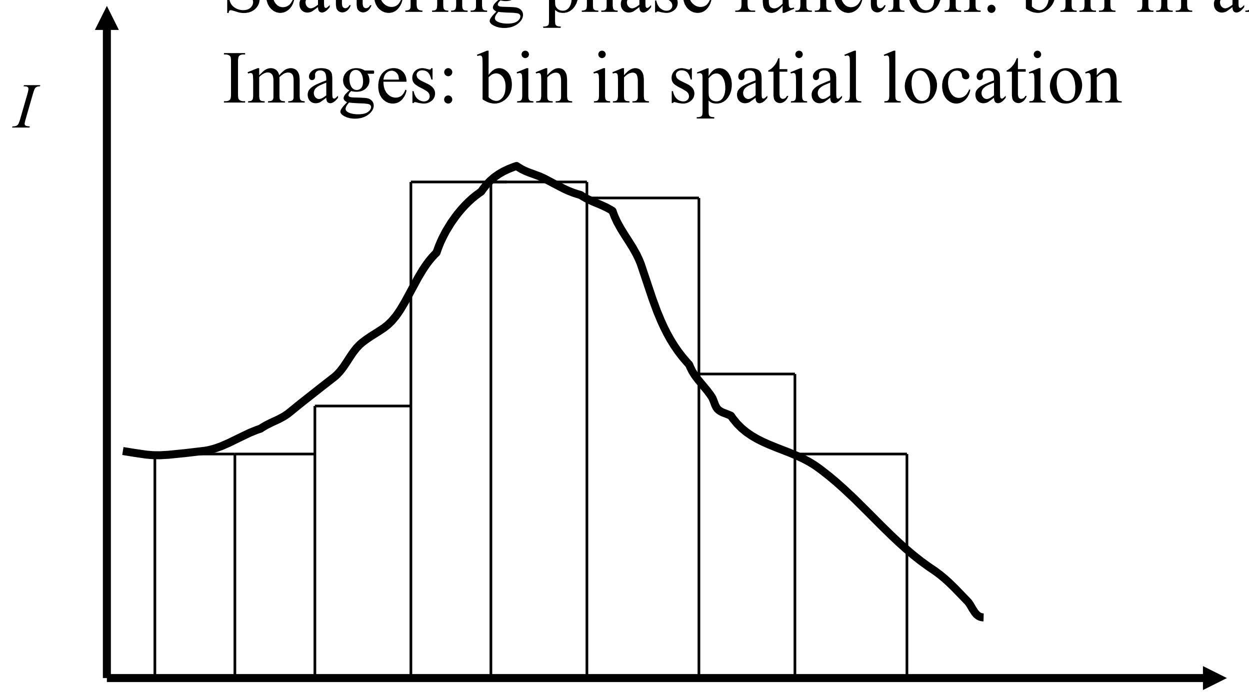
Total luminosity = L (J/s, erg/s)
Each packet carries energy $E_i = L\,\Delta t\,/\,N$,
N = number of Monte Carlo photons.
MC photon represents N_γ real photons, where $N_\gamma = E_i\,/\,h\nu_i$
MC photon packet moving in direction θ contributes to the specific intensity:

$$I_\nu = \frac{\mathrm{d}E_\nu}{\cos\theta\,\mathrm{d}A\,\mathrm{d}t\,\mathrm{d}\nu\,\mathrm{d}\Omega}$$

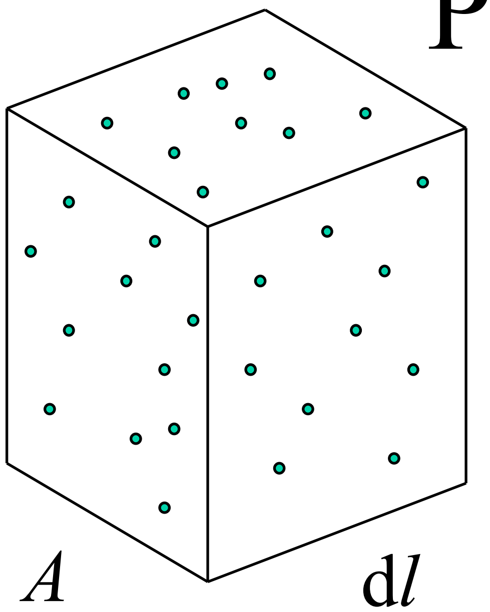
$$\Delta I_\nu = \frac{E_i}{\cos\theta\,\Delta A\,\Delta t\,\Delta\nu\,\Delta\Omega}$$

I_ν is a ***distribution function***. MC works with ***discrete*** energies. Binning the photon packets into directions, frequencies, etc, enables us to simulate a distribution function:

- Spectrum: bin in frequency
- Scattering phase function: bin in angle
- Images: bin in spatial location



Photon Interactions



Volume = A dl

Number density n

Cross section σ

Energy removed from beam per particle /t / ν / dΩ= I_ν σ

Intensity differential over dl is $dI_\nu = - I_\nu\, n\, \sigma\, dl$. Therefore

$$I_\nu (l) = I_\nu (0) \exp(-n\, \sigma\, l)$$

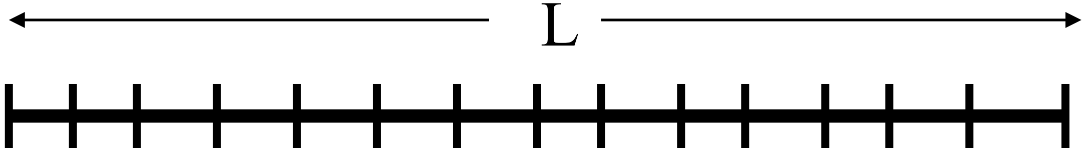
Fraction scattered or absorbed / length = $n\, \sigma$

$n\, \sigma$ = volume absorption coefficient = $\rho\, \kappa$

Mean free path = $1 / n\, \sigma$ = average dist between interactions

Probability of interaction over dl is $n\, \sigma\, dl$

Probability of traveling dl without interaction is $1 - n\, \sigma\, dl$



N segments of length L / N

Probability of traveling L before interacting is

$$P(L) = (1 - n\, \sigma\, L / N)\, (1 - n\, \sigma\, L / N) \ldots$$

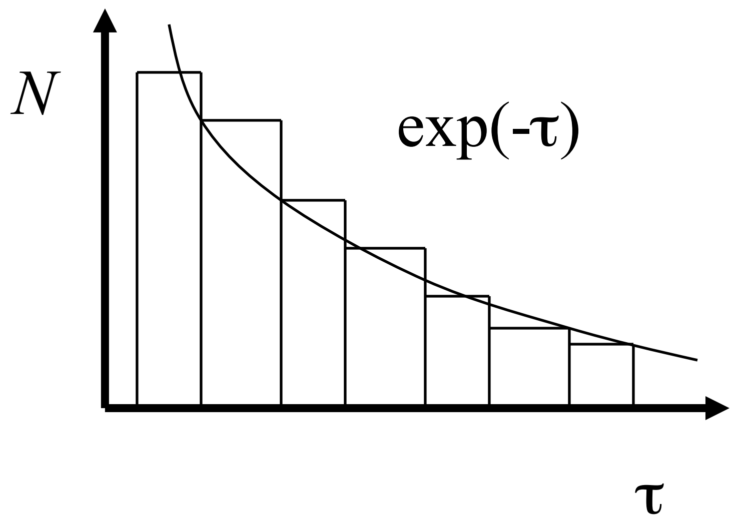
$$= (1 - n\, \sigma\, L / N)^N = \exp(-n\, \sigma\, L) \text{ (as N -> infty)}$$

$$P(L) = \exp(-\tau)$$

τ = number of mean free paths over distance L.

Probability Distribution Function

PDF for photons to travel τ before an interaction is exp(-τ). If we pick τ uniformly over the range 0 to infinity we will not reproduce exp(-τ). Want to pick lots of small τ and fewer large τ. Same with a scattering phase function: want to get the correct number of photons scattered into different directions, forward and back scattering, etc.



Cumulative Distribution Function

$$\text{CDF} = \text{Area under PDF} = \int P(x)\,\mathrm{d}x$$

Randomly choose τ, θ, λ, … so that PDF is reproduced

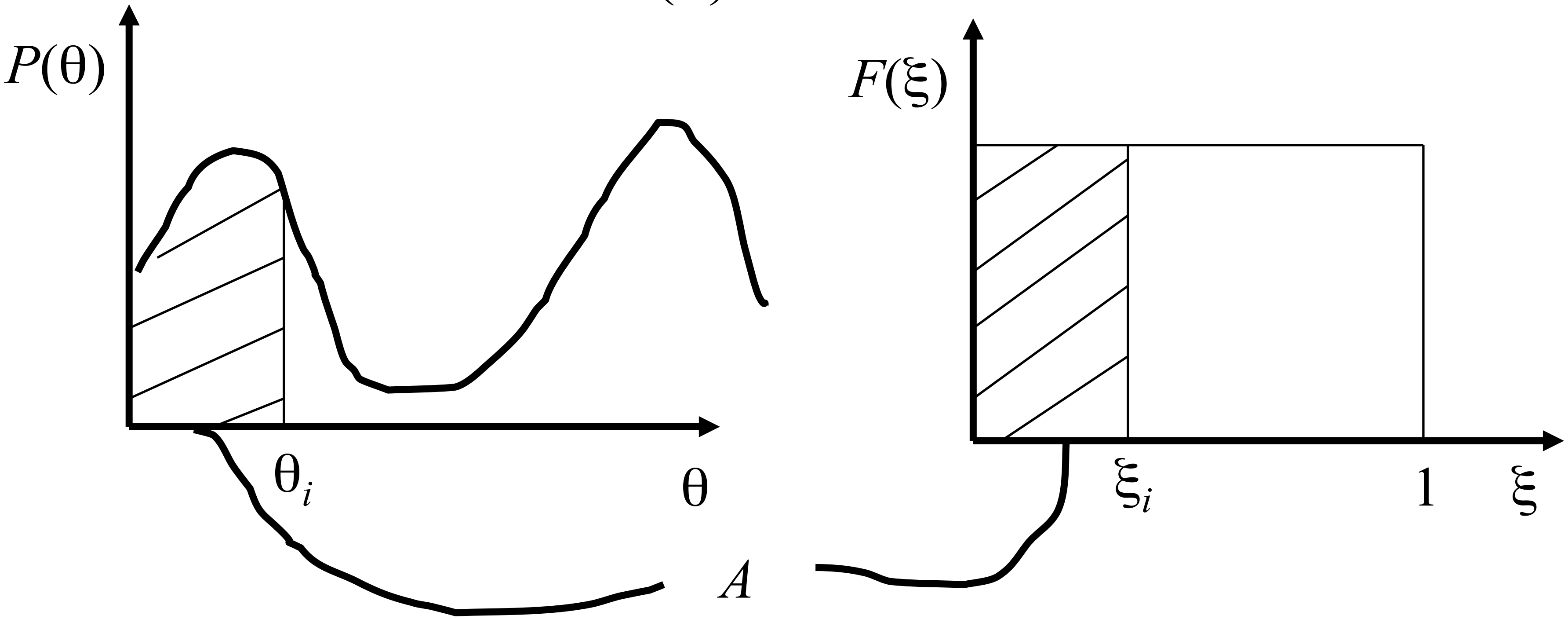
ξ is a random number uniformly chosen in range [0,1]

$$\xi = \int_a^X P(x)\,\mathrm{d}x \Rightarrow X$$

$$\int_a^b P(x)\,\mathrm{d}x = 1$$

This is the ***fundamental principle*** behind Monte Carlo techniques and is used to sample randomly from PDFs.

e.g., $P(\theta) = \cos\theta$ and we want to map ξ to θ. Choose random θs to "fill in" $P(\theta)$



$$\xi_i = \int_0^{\theta_i} P(\theta)\,\mathrm{d}\theta = \sin\theta_i \Rightarrow \theta_i = \sin^{-1}\xi_i$$

Sample many random θ_i in this way and "bin" them, we will reproduce the curve $P(\theta) = \cos\theta$.

Choosing a Random Optical Depth

$P(\tau) =$ exp(-τ), i.e., photon travels τ before interaction

$$\xi = \int_0^{\tau} e^{-\tau}\, d\tau = 1 - e^{-\tau} \Rightarrow \tau = -\log(1 - \xi)$$

Since ξ is in range [0,1], then (1-ξ) is also in range [0,1], so we may write:

$$\tau = -\log \xi$$

Physical distance, L, that the photon has traveled from:

$$\tau = \int_0^{L} n \sigma \, ds$$

Random Isotropic Direction

Solid angle is $d\Omega = \sin\theta \, d\theta \, d\phi$, choose (θ, ϕ) so they fill in PDFs for θ and ϕ. $P(\theta)$ normalized over $[0, \pi]$, $P(\phi)$ normalized over $[0, 2\pi]$:

$$P(\theta) = \tfrac{1}{2} \sin\theta \qquad\qquad P(\phi) = 1 / 2\pi$$

Using fundamental principle from above:

$$\xi = \int_0^\theta P(\theta)\mathrm{d}\theta = \frac{1}{2}\int_0^\theta \sin\theta \mathrm{d}\theta = \frac{1}{2}(1-\cos\theta)$$

$$\xi = \int_0^\phi P(\phi)\mathrm{d}\phi = \frac{1}{2\pi}\int_0^\phi \mathrm{d}\phi = \frac{\phi}{2\pi}$$

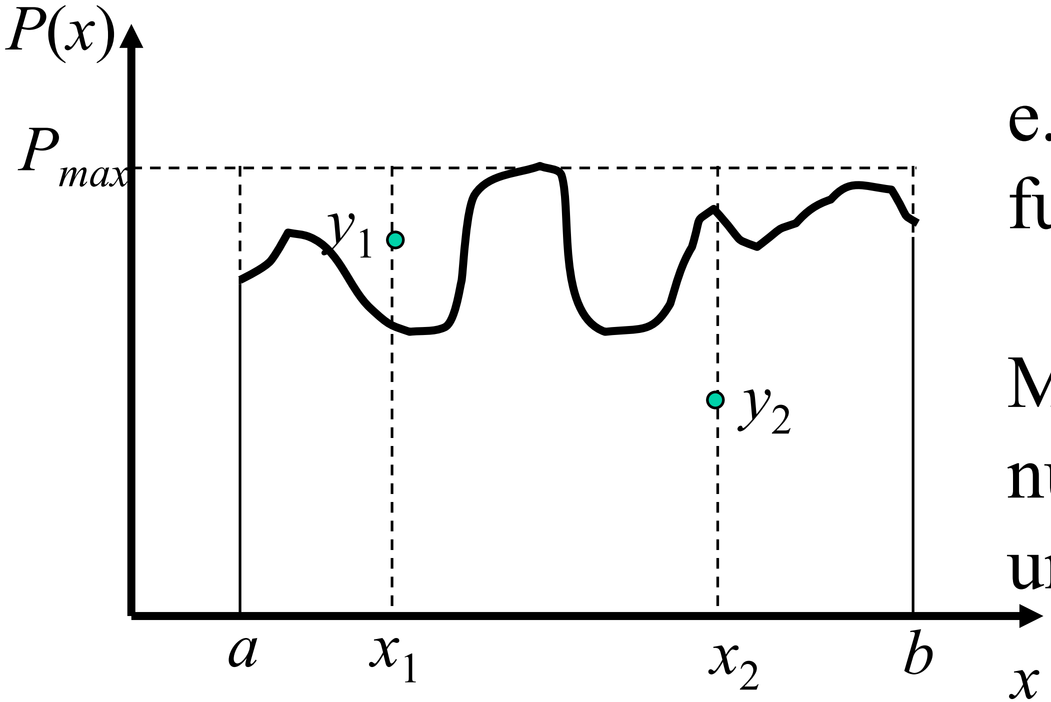
$$\theta = \cos^{-1}(2\xi - 1)$$

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

Use this for emitting photons isotropically from a point source, or choosing isotropic scattering direction.

Rejection Method

Used when we cannot invert the PDF as in the above examples to obtain analytic formulae for random θ, λ, etc.

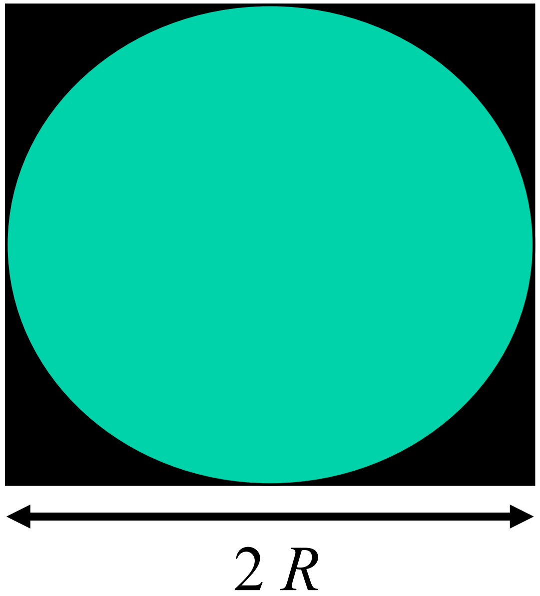


e.g., $P(x)$ can be complex function or tabulated

Multiply two random numbers:
uniform probability / area

Pick x_1 in range $[a, b]$: $x_1 = a + \xi(b - a)$, calculate $P(x_1)$
Pick y_1 in range $[0, P_{max}]$: $y_1 = \xi P_{max}$
If $y_1 > P(x_1)$, reject x_1. Pick x_2, y_2 until $y_2 < P(x_2)$: accept x_2
Efficiency = Area under $P(x)$

Calculate π by the Rejection Method



Pick N random positions (x_i, y_i):

x_i in range $[-R, R]$: $x_i = (2\xi - 1)\,R$

y_i in range $[-R, R]$: $y_i = (2\xi - 1)\,R$

Reject (x_i, y_i) if $x_i^2 + y_i^2 > R^2$

Number accepted / $N = \pi R^2 / 4R^2$

$$N_A / N = \pi / 4$$

Increase accuracy (S/N): large N

FORTRAN 77:

```
do i = 1, N
   x = 2.*ran – 1.
   y = 2.*ran –1.
   if ( (x*x + y*y) .lt. 1. ) NA = NA + 1
end do
pi = 4.*NA / N
```

Albedo

Photon gets to interaction location at randomly chosen τ, then decide whether it is scattered or absorbed. Use the ***albedo*** or ***scattering probability***. Ratio of scattering to total opacity:

$$a = \frac{\sigma_S}{\sigma_S + \sigma_A}$$

To decide if a photon is scattered: pick a random number in range [0, 1] and scatter if $\xi < a$, otherwise photon absorbed

Now have the tools required to write a Monte Carlo radiation transfer program for isotropic scattering in a constant density slab or sphere

Monte Carlo II
Scattering Codes

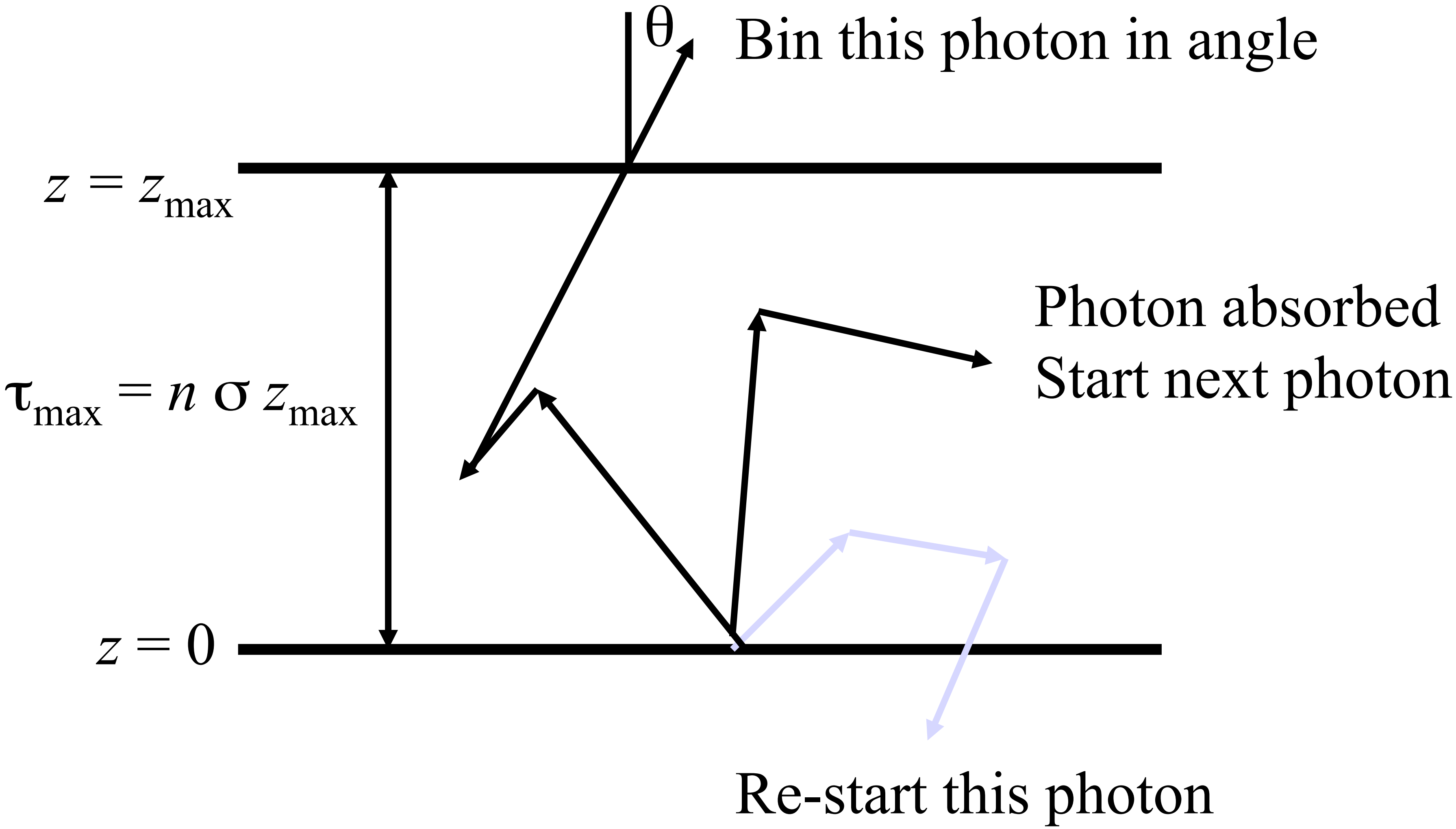
- Plane parallel scattering atmosphere
- Optical depths & physical distances
- Emergent flux & intensity
- Internal intensity moments

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

Emit photons
Photon scatters in slab until:

absorbed: terminate, start new photon
$z < 0$: re-emit photon
$z > 1$: escapes, "bin" photon

Loop over photons
Pick optical depths, test for absorption, test if still in slab


θ
Bin this photon in angle
$z = z_{max}$
$\tau_{max} = n\,\sigma\,z_{max}$
Photon absorbed
Start next photon
$z = 0$
Re-start this photon

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

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

$$I_\nu(\mu) = \frac{dE}{\mu\, dA\, dt\, d\nu\, d\Omega} \quad \Rightarrow \frac{dE}{dA\, dt\, d\nu\, d\Omega} \propto \frac{dN}{d\Omega} \propto \mu I_\nu(\mu)$$

Sample μ from $P(\mu) = \mu\, I\,(\mu)$ using cumulative distribution. Normalization: emitting outward from lower boundary, so $0 < \mu < 1$

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

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

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

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

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

Absorb or Scatter: Scatter if $\xi < a$, otherwise photon absorbed, exit "do while in slab" loop and start a new photon.

Structure of FORTRAN 77 program:

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

Intensity Moments

The moments of the radiation field are:

$$J_\nu = \frac{1}{4\pi}\int I_\nu \, \mathrm{d}\Omega \quad H_\nu = \frac{1}{4\pi}\int I_\nu \, \mu \, \mathrm{d}\Omega \quad K_\nu = \frac{1}{4\pi}\int I_\nu \, \mu^2 \, \mathrm{d}\Omega$$

Compute these moments throughout the slab. First split the slab into layers, then tally number of photons, weighted by powers of their direction cosines to obtain *J*, *H*, *K*. Contribution to specific intensity from a single photon is:

$$\Delta I_\nu = \frac{\Delta E}{|\mu| \Delta A \, \Delta t \, \Delta\nu \, \Delta\Omega} = \frac{F_\nu}{|\mu| N_0 \, \Delta\Omega} = \frac{\pi B_\nu}{|\mu| N_0 \, \Delta\Omega}$$

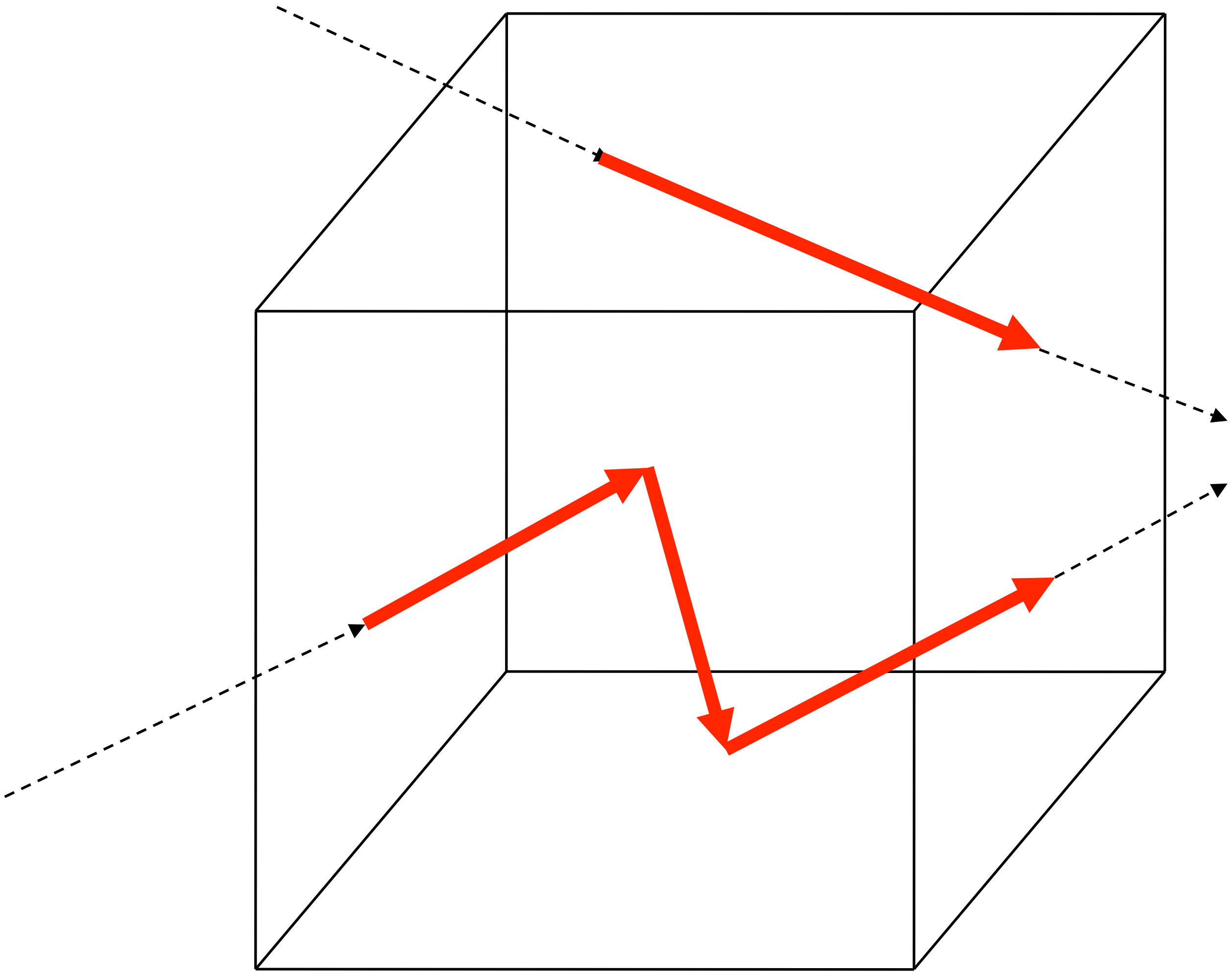
Substitute into intensity moment equations and convert the integral to a summation to get:

$$J_\nu = \frac{B_\nu}{4N_0}\sum_i \frac{1}{|\mu_i|} \quad H_\nu = \frac{B_\nu}{4N_0}\sum_i \frac{\mu_i}{|\mu_i|} \quad K_\nu = \frac{B_\nu}{4N_0}\sum_i \frac{\mu_i^2}{|\mu_i|}$$

Note the mean flux, *H*, is just the net energy passing each level: number of photons traveling up minus number traveling down.

Pathlength formula (Lucy 1999)
Long history of use in neutronics

$$J_i = \frac{L}{4\pi N_0 \Delta V_i}\sum l$$



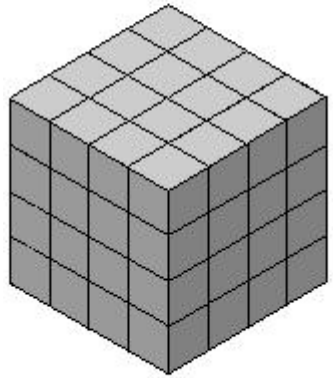
$$J_i = \frac{L}{4\pi \, N \, \Delta V_i} \sum l$$

Some Monte Carlo photon packets may pass through a cell without interacting (scatter or absorbed), but the path length estimator ensures they still contribute to the estimates for mean intensity, absorbed energy, radiation pressure, etc

Summing path lengths gives better estimates for intensities, absorbed energy, radiation pressure, etc. More photons pass through a cell than interact with a cell

Mean intensity, *J*, related to photon energy density, *u*, via

$$u_\nu = 4\pi J_\nu / c$$



u related to time photon spends in a cell, $t = l/c$, so can form Monte Carlo estimator:

$$u_\nu = \frac{1}{c\,\Delta t\,\Delta V_i} \sum \varepsilon_\nu\, l$$

Where ε_ν = MC packet energy = $L\,\Delta t / N$. Hence, get estimator for *J* which will be accurate in optically thin regions:

$$J_i = \frac{L}{4\pi N \Delta V_i} \sum l$$

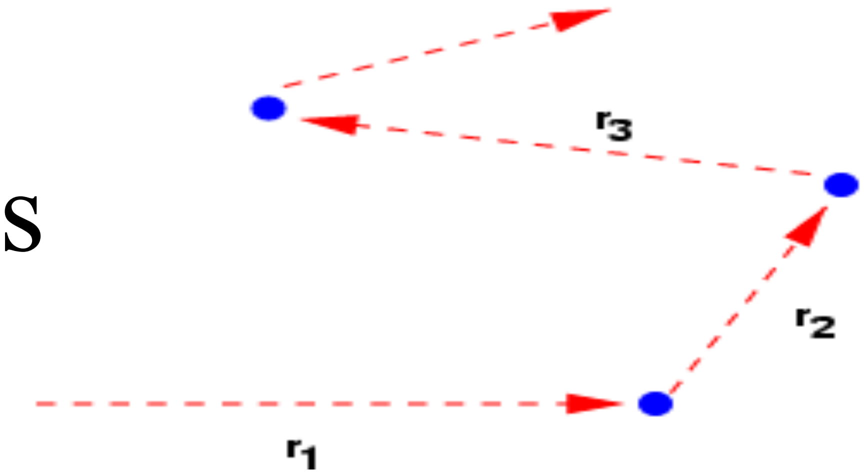
How much energy absorbed in a cell? Could count number of absorption events in each cell, but this is inaccurate for optically thin systems. We know the change in intensity for radiation passing through a medium with absorbing particles is

$$\mathrm{d}I = - I\, n\, \sigma_{\mathrm{abs}}\, \mathrm{d}l = - I\, \mathrm{d}\tau_{\mathrm{abs}}$$

Hence, a Monte Carlo estimator for absorbed energy:

$$\boxed{E_i^{\mathrm{abs}} = \frac{L}{4\pi\, N\, \Delta V_i} \sum n\, \sigma_{\mathrm{abs}}\, l}$$

Random walks



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

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

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

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

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 we have

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

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

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

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

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

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

Therefore $N \approx \tau + \tau^2 / 2$ will be roughly correct for any optical depth

Student exercises: write codes to…

- Calculate pi via rejection method

- Sample random optical depths and produce histogram vs tau

- Monte Carlo isotropic scattering code for uniform density sphere illuminated by central isotropic point source. Compute average number of scatterings vs radial optical depth of sphere.

- Make scattered light images for uniform sphere using "peeling off" technique ("next event estimator")