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
- Dinner at 7pm (different locations)

Lecturers

- Kenny Wood general intro to MCRT, write a short scattered light code, photoionization code
- Jon Bjorkman theory of MCRT, radiative equilibrium techniques, error estimates, normalizing output results
- Tom Robitaille improving efficiency of MCRT codes, using HYPERION
- Tim Harries 3D gridding techniques, radiation pressure, time dependent MCRT, using TORUS

Lecturers

- Michiel Hogerheijde NLTE excitation, development of NLTE codes, using LIME
- Barbara Ercolano photoionization, using MOCASSIN
- Louise Campbell MCRT in photodynamic therapy of skin cancer

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?



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

Recap of radiation transfer basics

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

Specific Intensity
$$dE_{v} = I_{v} \cos\theta dA dt dv d\Omega$$

Units of I_v : J/m²/s/Hz/sr (ergs/cm²/s/Hz/sr) Function of position and direction Independent of distance when no sources or sinks



 \underline{s} is normal to dA

Mean Intensity
$$J_{\nu} = \frac{1}{4\pi} \int I_{\nu} d\Omega = \frac{1}{4\pi} \int_{0}^{2\pi} \int_{0}^{\pi} I_{\nu} \sin\theta \, d\theta \, d\phi$$

Same units as I_{v}

Function of position

Determines heating, ionization, level populations, etc



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

$$I = I_* \text{ for } 0 < \theta < \theta_* \quad (\mu_* < \mu < 1); \ \mu = \cos \theta$$
$$I = 0 \text{ for } \theta > \theta_* \quad (\mu < \mu_*)$$

$$J = \frac{1}{2} \int_{\mu_*}^{1} I \, \mathrm{d}\mu = \frac{1}{2} I_* (1 - \mu_*)$$
$$J = I_* \frac{1}{2} \left(-\sqrt{1 - R_*^2 / r^2} \right) = w I_*$$

w = dilution factorLarge $r, w = R^2/4r^2$

Monochromatic Flux

$$\mathcal{F}_{v} = \int I_{v} \cos\theta \,\mathrm{d}\Omega = \int_{0}^{2\pi} \int_{0}^{\pi} I_{v} \cos\theta \sin\theta \,\mathrm{d}\theta \,\mathrm{d}\theta$$

Energy passing through a surface. Units: J/s/m²/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 $I_v = B_v$ and integrate to get total luminosity:

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

Energy Density & Radiation Pressure

$$u_{v} = \frac{1}{c} \int I_{v} d\Omega \qquad \qquad p_{v} = \frac{1}{c} \int I_{v} \cos^{2} \theta d\Omega$$

 $u_v: J/m^3/Hz$ $p_v: N/m^2/Hz$

Isotropic radiation: $p_v = u_v/3$

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):

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

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

K related to radiation pressure:

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

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

$$\mathrm{d}E_{v} = j_{v}\,\mathrm{d}V\,\mathrm{d}t\,\mathrm{d}v\,\mathrm{d}\Omega$$

Energy, dE_v , added:stimulated emissionspontaneous emissionspontaneous emissionthermal emissionenergy scattered into the beam

Intensity contribution from emission along ds:

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

Extinction Coefficient

Energy removed from beam Defined per particle, per mass, or per volume

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

 $\sigma_v = \text{cross section per particle } (m^2)$ $n = \text{particle density } (m^{-3})$

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

 α_v : units of m⁻¹

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

$$κv: units m2 kg-1$$

 $ρ = density (kg m-3)$

Source Function

Same units as intensity:

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

Multiple processes contribute to emission and extinction:

$$S_{v}^{\text{tot}} = \frac{\sum j_{v}}{\sum \alpha_{v}}$$

e.g., a spectral line:

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

 $\eta_v = \alpha_v^l / \alpha_v^c$ = line-to-continuum extinction ratio; S_v^c, S_v^l are continuum and line source functions

Optical Depth
$$d\tau_{v} = \alpha_{v}(s) ds = \rho(s) \kappa_{v} ds$$

$$\tau_{v} = \int_{0}^{s} \alpha_{v} \, \mathrm{d}s = \int_{0}^{s} \rho \kappa_{v} \, \mathrm{d}s$$

Function of frequency via the opacity, and direction

Physically τ_v is number of photon mean free paths

Equation of Radiation Transfer

ERT along a ray:

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

Solution:
$$I_{\nu}(\tau_{\nu}) = I_{\nu}(0)e^{-\tau_{\nu}} + \int_{0}^{\tau_{\nu}} S_{\nu}(t_{\nu})e^{-(\tau_{\nu}-t_{\nu})} dt_{\nu}$$

Goal: Determine source function!

Interconnectedness

Moments $(J_{\nu}, H_{\nu}, K_{\nu})$ depend on I_{ν} Need to solve ERT to get I_{ν}

 I_{v} (and hence J_{v}) depends on position and direction I_{v} depends on S_{v} , hence on emissivity and opacity Opacity depends on temperature and ionization Temperature and ionization depends on J_{v}

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

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

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

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

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_{v}
 - Solve for ionization structure, some regions neutral
- 2nd iteration:
 - new opacity structure,
 - different solution for ERT, different J_v 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 $N_{\gamma} = E_i / hv_i$ MC photon packet moving in direction θ contributes to the specific intensity:



 I_{v} 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



 ν (spectrum) θ (phase function)



Energy removed from beam per particle /t / v / d $\Omega = I_v \sigma$

Intensity differential over dl is $dI_v = -I_v n \sigma dl$. Therefore $I_v (l) = I_v (0) \exp(-n \sigma l)$ Fraction scattered or absorbed / length = $n \sigma$ $n \sigma$ = volume absorption coefficient = $\rho \kappa$ Mean free path = 1 / n σ = 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 / Nbability of traveling L before interacting i

Probability of traveling L before interacting is

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

= $(1 - n \sigma L / N)^{N} = \exp(-n \sigma L)$ (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

$$CDF = Area under PDF = \int P(x) dx$$

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

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

$$\xi = \int_{a}^{X} P(x) \, \mathrm{d}x \Longrightarrow X \qquad \int_{a}^{b} P(x) \, \mathrm{d}x =$$

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



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

 $P(\tau) = \exp(-\tau)$, 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:

$$\tau = \int_{0}^{L} n \sigma \, \mathrm{d}s$$

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 $[0, 2\pi]$:

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

Using fundamental principle from above:

$$\xi = \int_{0}^{\theta} P(\theta) d\theta = \frac{1}{2} \int_{0}^{\theta} \sin \theta d\theta = \frac{1}{2} (1 - \cos \theta)$$

$$\xi = \int_{0}^{\phi} P(\phi) d\phi = \frac{1}{2\pi} \int_{0}^{\phi} d\phi = \frac{\phi}{2\pi}$$

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

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. P(x)



Calculate π by the Rejection Method



FORTRAN 77:

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

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 photonsPhoton 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



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)

$I_v(\mu) =$	dE	\Rightarrow	dE	$\propto \frac{dN}{d\Omega}$	dN	\sim	$\mu I(\mu)$
	$\mu dA dt dv d\Omega$		$dA dt dv d\Omega$		$\sim \mu I_{v}($	$\mu_v(\mu)$	

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

$$\xi = \frac{\int_{0}^{\mu} P(\mu) d\mu}{\int_{0}^{0} P(\mu) d\mu} = \mu^{2} \implies \mu = \sqrt{\xi}$$
$$\int_{0}^{\mu} P(\mu) d\mu$$

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
       call emit photon
1
       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:

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

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:

$$\Delta I_{\nu} = \frac{\Delta E}{\mid \mu \mid \Delta A \,\Delta t \,\Delta \nu \,\Delta \Omega} = \frac{F_{\nu}}{\mid \mu \mid N_{0} \,\Delta \Omega} = \frac{\pi \, B_{\nu}}{\mid \mu \mid N_{0} \,\Delta \Omega}$$

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)

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



Net displacement of a single photon from starting position after *N* 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 :

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

Each squared term averages to the square of the free path of a photon l^2 . Thus, $\langle \mathbf{r}_1^2 \rangle = l^2$ where $l \sim$ the mean free path. 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 $l_*^2 = N l^2 \implies l_* = l \sqrt{N}$

- i.e., the root mean square net displacement of a photon after *N* scatterings is $\sqrt{N} \times l$ where l^2 = mean square free path of a photon.
- Worked example: How many scatterings does it take a photon to escape from a region of size *L* and optical depth τ ?

If the medium is optically thick, then a typical photon will random walk until $l_* \sim L$.

Using
$$l_* = \sqrt{Nl}$$
, we find: $N \approx L^2 / l^2$

Since *l* is approximately the mean free path, $\tau \approx \alpha_v L \approx L/l$

Thus $N \approx \tau^2, \tau >> 1$

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

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

If needed, saying $N \approx \tau + \tau^2$ 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. 3D Monte Carlo Scattering Codes

3D linear cartesian grid – limitations

Point sources and diffuse emission

Scattering – Heyney-Greenstein phase function

Forced first scattering (good S/N for optically thin cases)

Peeling off photons – high res images from one viewing angle

Subroutines commented and described in on-line booklet

To get going – params.par, density.f, sources.f, emit.f





Circumbinary disk





Disk galaxy

```
nphotons=1000000,
iseed=-1556.
kappa=66.,
albedo=0.4,
hgg=0.41,
pl=0.51,
pc=0.0,
sc=1.,
xmax=800.,
ymax=800.,
zmax=800.,
rimage=800.,
viewthet=85.,
viewphi=0.
```

Scattered light code: Point Sources

Modify the following...

- Parameter file params.par
- Source locations sources.txt & sources.f
- Density structure density.f

Try this....

- Change number of photons
- Viewing angles
- Source locations and luminosities
- Disk flaring and inner edge

```
subroutine sources(xsource,ysource,zsource,lsource,lumtot)
   implicit none
   include 'sources.txt'
   integer i
c**** Set photon locations and luminosities
   xsource(1)=-50.
   ysource(1)=0.
   zsource(1)=0.
   lsource(1)=2.25
   xsource(2)=50.
   ysource(2)=0.
   zsource(2)=0.
   lsource(2)=1.
c**** Calculate total luminosity of all sources
   lumtot=0.
   do i=1,nsource
    lumtot=lumtot+lsource(i)
   end do
   return
   end
```

subroutine density(x,y,z,rho) implicit none real x,y,z,rho real w,w2,r,r2,h0,h

w2=x*x+y*y w=sqrt(w2) r2=w2+z*z r=sqrt(r2)

h0=7.

if((r.gt.200.).and.(r.lt.800.)) then

h=h0*(w/100.)**1.25

```
rho=exp(-0.5*z*z/(h*h))/w2*2.4e-11 ! rho in g/cm^3
```

else

rho=0.

endif

return end