Introduction to Monte Carlo Radiation Transfer

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1 Introduction

The purpose of this booklet is to introduce the reader to the basic concepts and techniques of radiation transfer using the Monte Carlo method. We will deal with the propagation of "photon packets" and their interaction with matter within a medium. For readers familiar with the traditional radiation transfer nomenclature, we will show how counting photons, weighted by their directions of travel, yields the source function and intensity moments of the radiation field throughout the medium.

First of all we wish to convey the conceptual simplicity of radiation transfer: a photon is emitted, it travels a distance, and then something happens to it. The difficulties arise in determining the source and direction of emission, the distance travelled, and what happens to the photon after this point.

Having been introduced to and trained in radiation transfer techniques using specific intensities, source functions, and intensity moments (which at times can appear rather abstract and removed from the basic physics) our outlook to the physical processes behind radiation transfer changed when we began to work with photons and the probabilistic nature of their interactions. In order to determine the paths and fates of photons we must understand the concepts of optical depths, albedos, absorption and scattering cross sections and phase functions. Since these are all based on probability distribution functions, this brings us to the crux of all Monte Carlo methods, random numbers. Photon paths and interactions are simulated by sampling randomly from the various probability distribution functions that determine the interaction lengths, scattering angles, and absorption rates.

The first chapter of this book lays out the basic algorithm for Monte Carlo radiation transfer and introduces cross sections, optical depths, scattering phase functions, and the various methods for sampling randomly from their probability distribution functions. These techniques are then applied to radiation transfer in a plane parallel, homogeneous, isotropic scattering slab. A computer program is presented that calculates the emergent energy and intensity as a function of viewing angle of the slab. These results may be compared with the classical solution of this problem. We also demonstrate how the counting of photons and their directions of travel leads to a determination of the source function and intensity moments throughout the atmosphere — thus relating the results of the Monte Carlo radiation transfer to traditional techniques.

Subsequent chapters extend these techniques to axisymmetric and inhomogeneous media, thus exploiting the fully three dimensional nature of the Monte Carlo technique. Codes are developed that include scattering, absorption, and re-emission from extended regions. In addition to unresolved spectral applications, we show how it is straightforward to extend these codes to produce images of the systems being simulated. These techniques are applicable to many diverse areas of astronomy such as circumstellar disks, bipolar outflows, the local interstellar medium, reflection nebulae, molecular clouds, and external galaxies. We hope that this book will provide the reader with the basic tools necessary to pursue their own particular research interests in the study of radiation transfer in a variety of situations.

2 Basic Concepts and Definitions

As we stated in the introduction, radiation transfer is easy: a photon is emitted, it travels a distance, and something happens to it. In this chapter we start with the assumption that a photon has been emitted and determine how far it will travel in a medium. Once this distance has been reached we discuss what can happen next. First of all we define a few basic terms that are central to any study of radiation transfer — photons, intensities, fluxes, cross sections and optical depths.

2.1 Photon Packets, Cross Sections, Optical Depths

In simulating the transfer of radiation we follow photon packets as they are scattered and absorbed within a medium. We start with a given total energy and split this equally among the photon packets that we follow. Each packet, which has a dircetion of travel, then posseses a definite total energy (and partial polarization) and these packets are related to the specific intensity, I_ν. The specific intensity of the radiation field is defined as the radiant energy dE_ν passing through a unit surface area dA at an angle θ to the surface normal within a solid angle $d\Omega$ in a frequency range $d\nu$ in time dt, viz

$$I_\nu = \frac{dE_\nu}{\cos\theta \, dA \, dt \, d\nu \, d\Omega} \ . \tag{1}$$

The units of specific intensity are [ergs cm^{-2} s^{-1} Hz^{-1} sr^{-1}]. Thus the photon packet (hereafter referred to as a photon) represents the energy dE_ν. Another quantity is the flux

$$F_\nu = \int I_\nu \cos\theta \, d\Omega \ , \tag{2}$$

which is the rate of energy flow across dA per unit time per unit frequency interval and has units [ergs cm^{-2} s^{-1} Hz^{-1}].

The photons interact according to probabilistic interactions determined by the scattering and absorption cross sections of the particles within the medium. These cross sections are related to the difference between the incoming and outgoing energy (or number of photons) at a point. A cross section, σ is defined by the energy per second per frequency per solid angle (number of photons) that is removed from the direction of travel, by either scattering or absorption thus

$$\text{Energy removed per second per frequency} = I_\nu \, \sigma \ . \tag{3}$$

A cross section thus has dimensions of area [cm^2].

Consider now a homogeneous medium filled with scatterers or absorbers of number density, n, and cross section σ. The number of photons scattered per second by an infinitessimal volume is $I_\nu \, \sigma \, n \, A \, dl$, so the number of photons scattered per second per area is $I_\nu \, \sigma \, n \, dl$. Therefore the intensity differential along a length dl is

$$dI_\nu = -I_\nu \, n \, \sigma \, dl \ , \tag{4}$$

giving the familiar relation between the incident and outgoing intensity

$$I_\nu(l) = I_\nu(0) \, \mathrm{e}^{-n\sigma l} \ . \tag{5}$$

The fraction of photons scattered or absorbed per unit length is thus $n \, \sigma$ and this quantity is called the volume absorption coefficient. It is related to the opacity or mass absorption coefficient, κ, by

$$n\sigma = \rho\kappa \ , \tag{6}$$

where ρ is the mass density of scatterers or absorbers. A related quantity is the photon *mean free path*, $1/n\sigma$, which is the average distance a photon travels between interactions.

The probability that a photon interacts (is scattered or absorbed by the particles) over a length dl is thus $n\,\sigma\,dl$, so the probability of travelling dl without interacting is therfore $1 - n\,\sigma\,dl$. If we now divide a length L into N sections of equal length, the probability of travelling the distance L without an interaction occuring is

$$P(L) = (1 - n\,\sigma\,L/N)^N = e^{-n\,\sigma\,L} = e^{-\tau} \ , \tag{7}$$

where we have introduced the *optical depth* $\tau = n\,\sigma\,L$. Physically, the optical depth over a distance L in a given direction is the number of photon mean free paths over that distance. In general the optical depth is defined as

$$\tau = \int_0^L n\,\sigma\,ds \ . \tag{8}$$

The optical depth will in general be be wavelength dependent due to continuum and line opacity depending on the the absorbing and scattering species present.

2.2 I've travelled L, what happens now?

After the photon has travelled the interaction length one of two things can occur, it is either absorbed or scattered. The photon's fate is determined by the *albedo* which is the probability that the photon is scattered. The albedo is defined as

$$a = \frac{n_s\,\sigma_s}{n_s\,\sigma_s + n_a\,\sigma_a} \ , \tag{9}$$

where the subscripts refer to the number densities and cross sections of scatters and absorbers respectively.

There are several different types of absorption (continuous absorption, line absorption, resonance line scattering, etc.) and in general the photon will be absorbed at a certain frequency and will be re-emitted at another frequency in a different direction of travel. The frequency and angular redistribution functions associated with different absorption processes will be dealt with in more detail in later chapters. For the present we shall not concern ourselves with the photon's ultimate fate and will assume that if a photon is absorbed we will terminate it and emit a new photon from the source. In this way the absorbed photon will not contribute to the emergent flux, but it can contribute to the mean intensities as it scatters throughout the atmosphere until it is absorbed.

If a photon is scattered it then travels in a new direction that is determined by the angular phase function of the scattering particle. The phase function is the probability that a photon will be scattered from one direction to another, $P(\cos\chi)$, where χ is the scattering angle. Two of the most common phase functions used for modeling scattering atmospheres are the isotropic phase function, $P(\mu) = \frac{1}{2}$, and the Rayleigh phase function, $P(\mu) = \frac{3}{8}(1 + \mu^2)$, where $\mu = \cos\chi$. Note that, as with all phase functions, they are normalized over scattering angles such that

$$\int_{-1}^{1} P(\mu)\,d\mu = 1 \ , \tag{10}$$

that is, the probability that the photon is scattered into 4π steradians is unity.

2.3 Sampling from Probability Distribution Functions

We now have all the basics necessary to build a simple Monte Carlo radiation transfer code – we emit a photon, send it a distance L, then either absorb (terminate) it or scatter it into a new direction. However, the distances travelled and scattering angles are not uniformly chosen from all space $L\{0, \infty\}$ or all angles $\chi\{0, \pi\}$, since there are probability distribution functions associated with the interaction length and scattering angle as we described above. We must therefore sample the optical depths and scattering angles such that the chosen τs and χs "fill in" the respective $P(\tau)$ and $P(\chi)$. In order to sample a quantity (in our case τ and χ) randomly from a probablilty distribution function there are several techniques which will now be explained.

2.3.1 Sampling from the Cumulative Distribution Function

To sample a quantity x_0 from a probability distribution function $P(x)$, which is normalized over all x, we use the *fundamental principle* which is

$$\xi = \int_a^{x_0} P(x)\, dx = \psi(x_0) \ , \tag{11}$$

where ξ is a random number sampled uniformly from the range 0 to 1, a is the lower limit of the range over which x is defined, and ψ is the cumulative probability distribution function.

We need to sample how far a photon travels before being absorbed or scattered. The probability that a photon travels an optical depth τ without an interaction is $\mathrm{e}^{-\tau}$. The probability of scattering prior to τ is $1 - \mathrm{e}^{-\tau} = \psi(\tau)$. Therefore we can sample from the cumulative probability according to $\xi = 1 - \mathrm{e}^{-\tau}$, giving

$$\tau = -\log(1 - \xi) \ . \tag{12}$$

Having sampled a random optical depth in this manner we may then calculate the physical distance L that the photon travels from

$$\tau = \int_0^L n\, \sigma\, dl \ . \tag{13}$$

Finding L from the above equation accounts for the largest percentage of CPU time in most Monte Carlo codes. This is because in general L cannot be found analytically from equation 13 and we must use numerical techniques which can be computationally intensive. However, for certain densities we can find L analytically and this enables us to generate large numbers of photons in a fraction of the time required if we had to solve equation 13 numerically. Geometries which allow this include spherically symmetric ($1/r^2$) density laws, ellipsoidal envelopes, and any homogeneous (constant density) medium. In our initial investigations we shall adopt such geometries in order to obtain results with small statistical fluctuations in a short time.

2.3.2 The Rejection Method

The rejection method is used when equation 11 either cannot be solved easily or does not have an analytic solution for x_0. This method works for any probability distribution function if we know the peak value and is like throwing darts at a graph of the probability distribution.

To sample x_0 from $P(x)$ with peak P_{max} over the range $x[a, b]$, sample from a uniform distribution for x_0 between a and b, sample from a uniform distribution for y between 0 and P_{max}, then reject values of x_0 for which $y > p(x_0)$.

2.4 Random Numbers

It should be obvious by now that the Monte Carlo technique derived its name from the famous gambling town in southern France where fortunes are won and lost with the throw of a (presumably) random and fair dice. When simulating photon interactions we are constantly calling upon random number generators to choose optical depths and scattering angles and we hope that our dice are truly random and fair. Since our random numbers are generated by computers it is interesting to note John von Neumann's comment that "anyone wishing to produce random numbers with a computer is truly in a state of sin". This comment is based on the fact that all computers follow set algorithms and hence no output can truly be random. However, algorithms can be developed that produce sequences of numbers that pass tests for randomness. Such sequences generally have very long periods, thus minimizing the danger of repeating the same photons. There are many excellent articles on computer generated random numbers and we refer the reader to these in the supplemental reading section at the end of the book. For a quick introduction Chapter 7 of *Numerical Recipes* presents some of the more common algorithms and the random number generator that we use throughout this book is the *Numerical Recipes* routine ran2 presented in this chapter. Anywhere this routine is used the reader may substitute their own favourite random number generator in its place.

3 A Plane Parallel Atmosphere

We now apply the concepts and definitions presented in Chapter 1 to radiation transfer within a plane parallel isotropic scattering atmosphere. The solution for the angular dependence of the intensity and polarization of the emergent radiation from a semi-infinite slab was presented by Chandrasekhar (1960). In what follows we shall develop a code that determines the emergent energy and intensity from a slab illuminated from below, as well as the mean intensities of the radiation field within the slab.

3.1 Emitting New Photons

For a slab illuminated from below we need to inject photons from the origin such that the flux in any direction of emission is isotropic. To achieve this we must sample the angles such that

$$\xi = 2\int_0^{\mu} \mu\, d\mu \;, \tag{14}$$

where the specific intensity is independent of direction and the lower limit is 0 since we are injecting photons in only upward directions. This then gives

$$\mu = \cos\theta = \sqrt{\xi}\;, \qquad \phi = 2\,\pi\,\xi\;. \tag{15}$$

The initial photon position is the origin and the direction cosines of the photon are

$$n_x = \sin\theta\cos\phi\;, \quad n_y = \sin\theta\sin\phi\;, \quad n_z = \cos\theta\;. \tag{16}$$

3.2 Plane Parallel Geometry and Distances Travelled

We shall investigate the propagation of photons within a homogeneous planar slab of height $z_{max} = 1$. The slab may be parameterized by its total vertical optical depth $\tau_{max} = n\,\sigma\,z_{max} = n\,\sigma$, where σ is the scattering cross section. The distance L travelled by a photon along any ray is then simply

$$L = \frac{\tau}{n\,\sigma} = \frac{\tau}{\tau_{max}}\;, \tag{17}$$

where the optical depth is sampled from $\tau = -\log\xi$. The photon's position is then updated according to

$$x = x + L\sin\theta\cos\phi\;, \quad y = y + L\sin\theta\sin\phi\;, \quad z = z + L\cos\theta\;. \tag{18}$$

At this point the photon may be absorbed, scattered, or escape from the atmosphere (i.e., $z > z_{max}$ or $z < 0$). Since we are considering a pure scattering atmosphere the albedo $a = 1$ and every interaction will be a scattering event.

3.3 Isotropic Scattering

In an isotropic scattering atmosphere the photons are scattered uniformly into 4π steradians. We generate the new direction by sampling uniformly for ϕ in the range 0 to 2π and μ in the range -1 to 1, thus

$$\phi = 2\pi\,\xi\;, \qquad \mu = 2\xi - 1\;, \tag{19}$$

where ξ is a random number in the range 0 to 1, as before.

3.4 Binning Photons

Once the photon exits the slab we must place it into a "bin" depending on its direction of travel. We are trying to measure continuous distributions such as the emergent flux or intensity using a discrete set of events. In other words we are sampling (in the statistical sense) the distribution function we wish to measure. We do this by binning the photons to produce histograms of the distribution function. For resolved objects we can make images by noting also the final position of the photon before it exited the medium (see Chapter 4). For unresolved objects we choose to place the photon into (μ, ϕ) bins. Binning in $\cos\theta$ and ϕ ensures that each bin is of equal solid angle since $d\Omega = \sin\theta d\theta d\phi = d\mu d\phi$. The number of bins depends on the symmetry of the radiation source and the scattering medium, and for fully three dimensional systems we must choose enough bins to give resolution on scales of the smallest variation with solid angle. In the case of the plane parallel slab, each ϕ direction of exit is equally probable (the system is axisymmetric) so we need only bin in μ. In addition, since we are interested in the radiation emerging from the top of the slab, we bin the photons in the range $0 < \mu < 1$ (i.e., $0^\circ < \theta < 90^\circ$).

3.5 Flux Normalization

We wish to compute the output flux or intensity. Other radiation transfer methods work in intensity to solve the problem and then compute flux when comparing to observations. Monte Carlo naturally works in flux/energy units and so we only need to compute intensity when comparing to other radiation transfer methods.

The outgoing energy in the ith bin, normalized to the total energy, is just

$$\frac{dE_i}{dE} = \frac{N_i}{N_0} \; , \tag{20}$$

where N_i is the number of photons in the ith bin and N_0 is the total number of photons. In order to calculate the emergent intensity from the top of our slab we note that the energy per area through the slab surface is

$$\frac{dE}{dA} = F_\nu = \pi B_\nu \; , \tag{21}$$

where πB_ν is the physical flux. Suppose the energy in the ith bin is $dE_i = N_i \, dE/N_0$, then taking equation 1 relating the energy per area per solid angle we then get the intensity in the ith bin as

$$I_\nu = \frac{dE_i}{\mu \, d\Omega \, dA} = \frac{N_i \, \pi B_\nu}{N_0 \, \mu \, d\Omega} \; . \tag{22}$$

For our plane parallel slab our elemental solid angle is $d\Omega = 2\pi d\mu$ and $d\mu = 1/N_\mu$, with N_μ being the number of μ bins. This then gives,

$$\frac{I_\nu}{B_\nu} = \frac{N_i \, N_\mu}{2 \, N_0 \, \mu_i} \; , \tag{23}$$

where μ_i is the μ value at the center of the ith bin.

3.6 Errors

Since the Monte Carlo method employs a stochastic approach, the results for the emergent energies in each bin contain random sampling errors. Consequently, in all Monte Carlo simulations, a large number of events (i.e., photons) must be generated until the physical properties under investigation (in our case the emergent energy) have small statistical fluctuations. It is therefore necessary to estimate the errors on the results stored in each bin. In our investigation we calculate the total energy, E, for each direction bin. The number of photons in each bin obeys Poisson statistics, so the error in the total energy in each direction bin is simply $\sigma_E = E_i/\sqrt{N_i}$, where E is the energy and N_i is the number of photons in the bin.

3.7 Intensity Moments

One of the criticisms we have frequently heard levelled at Monte Carlo radiation transfer is that it is a "black box" and it is difficult to "get at" the physics. This criticism may stem from Monte Carlo's feature that there are no output equations and we simulate individual situations. However, while not intending to be critical, glancing through current theoretical radiation transfer papers based on traditional techniques, does the physics jump out at you ? Alternatively, read Chandrasekhar (pp 233-248) on the solution of the semi-infinite atmosphere — physical, black box?!

As we have outlined in the previous sections, the Monte Carlo technique tracks each and every photon packet as it propagates through an atmosphere. Clearly the black box criticism can be removed to any desired level (depending on memory storage) by tabulating quantities of interest throughout the medium. Astrophysically important quantities are the intensity moments J, H, and K that measure the mean intensity, flux, and radiation pressure at points throughout the medium.

$$J = \frac{1}{4\pi}\int I\,d\Omega\ , \quad H = \frac{1}{4\pi}\int I\,\mu\,d\Omega\ , \quad K = \frac{1}{4\pi}\int I\,\mu^2\,d\Omega\ . \tag{24}$$

These intensity moments are used in heating and force calculations, and in the equations of statistical equilibrium (see later chapters).

Keeping with the plane parallel slab, we may compute the intensity moments as a function of optical depth through the slab. First of all we split the slab into layers of equal width, then tally the number of photons, weighted by powers of their direction cosines, to obtain the three moments. We note that the contribution to the specific intensity from a single photon is

$$\Delta I = \frac{\Delta E}{|\mu|\ \Delta A\,\Delta\Omega} = \frac{F_\nu}{|\mu|\ N_0\,d\Omega} = \frac{\pi B_\nu}{|\mu|\ N_0\,d\Omega}\ , \tag{25}$$

which may be substituted into the intensity moment equations. Converting the integral to a summation we then get

$$J = \frac{B_\nu}{4\,N_0}\sum_i \frac{1}{|\mu_i|}\ , \quad H = \frac{B_\nu}{4\,N_0}\sum_i \frac{\mu_i}{|\mu_i|}\ , \quad K = \frac{B_\nu}{4\,N_0}\sum_i \frac{\mu_i^2}{|\mu_i|}\ . \tag{26}$$

Note that the mean flux, H, is simply the net energy (number of photons travelling up minus the number travelling down) passing each level. These summations may be implemented in the Monte Carlo code and this demonstrates how Monte Carlo techniques return the same quantities as the more traditional methods.

3.8 A Plane Parallel, Isotropic Scattering Monte Carlo Code

As will become apparent, implementing a plane parallel, isotropic scattering code is a straightforward task. The files can be obtained by anonymous ftp to cfa-ftp.harvard.edu in the directory outgoing/kwood/mc-code. The driver program which tracks the photons is planepar.f. This program calls various subroutines to generate new photons, intensity moments, scattering angles, and finally the emergent energy and intensity. The input parameters for the code are supplied in the parameter file slab.par. This contains the total number of photons (nphotons), the random number seed (i1) required by ran2.f, the number of μ bins (mubins), the number of levels (nlevel) at which the intensity moments are to be calculated, the albedo (set equal to one for pure isotropic scattering), and the total vertical optical depth (taumax) of the slab. The steps in the program are as follows:

1. Having read in these parameters, we then initialize the energy, and intensity arrays to zero with iarray.f. Here we also calculate the angle θ_i at the centre of each μ bin.

2. We then proceed with the loop over all photons. The routine newphot.f initializes the photon position to be at the origin and assigns the photon a direction isotropically according to equation 15.

3. An optical depth is generated via $\tau = -\log\xi$. This optical depth corresponds to a physical distance $L = \tau/\tau_{\max}$ within the slab and then the photon position is updated according to equation 18. Note that in

a plane parallel slab we only need to know the z coordinate of the photon, but we have left in x and y to demonstrate that the code truly is three dimensional.

4. Once the photon position has been updated we calculate the intensity moments with the subroutine moments.f. This calculates how many levels the photon crosses and updates the intensity moments in these levels according to the summations in equation 26, note that we calculate the moments in the upward and downward directions.

5. We then determine whether to scatter or absorb the photon. Since we are simulating a pure scattering atmosphere we call the subroutine isoscatt.f which generates a random scattering direction for the photon from 4π steradians.

6. We then repeat steps 3 through 5 until the photon exits the slab, i.e. $z > z_{\max}$ or $z < 0$. If $z > z_{\max}$ then the photon exits the top of the slab and we place it into the relevant μ bin. If the photon exits the bottom of the slab, we re-emit a new photon isotropically from the origin. In this way we match the lower boundary condition that the photon number flux is given by N_0.

7. Finally when all photons have exited the slab we calculate the intensity and write out the files as energy.dat and moments.dat.

Yes folks, a few calls to a random number generator, a wee bit of geometry, and you're doing three dimensional radiation transfer. Now who said Monte Carlo was a mystery?

3.9 Output Results

In Figure 1 we show results of a run of the code for a slab of optical depth $\tau_{\max} = 10$. The diamonds in the left panel show the intensity as a function of exit angle, the solid line is Chandrasekhar's result for a semi-infinite slab. We see that at an optical depth of 10, our slab model very closely approximates the semi-infinite solution. In the middle panel we show the intensity moments as a function of optical depth measured from the top of the slab. The right panel shows the Eddington factors ($f = K/J$, $g = H/J$), note that deep in the atmosphere $J = 3K$ as expected.

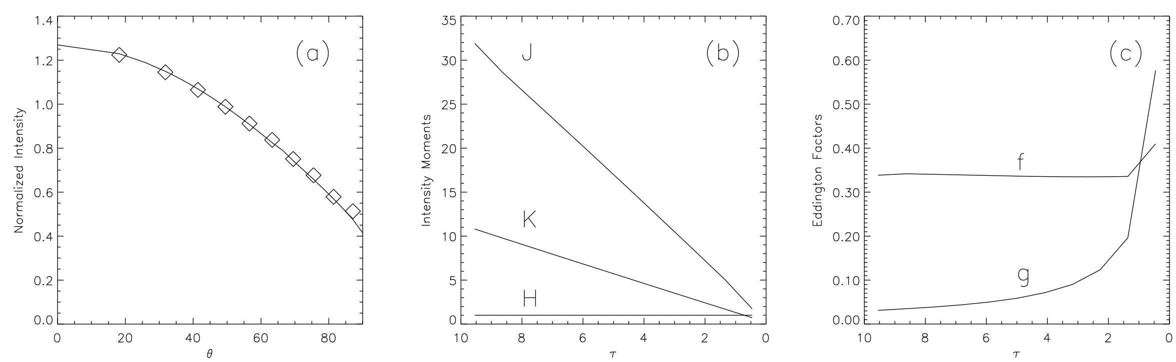

Figure 1: Plane parallel slab, $\tau_{\max} = 10$. (a) Emergent intensity, diamonds are Monte Carlo results, solid line is Chandrasekhar's result for a semi-infinite atmosphere. (b) Internal intensity moments. (c) Eddington factors.

4 Making Images

Up until now we have investigated spatially unresolved systems, that is we only concerned ourselves with the photon exit direction and not the position from where it came. For most stellar applications this is sufficient, since stars are essentially point sources and we observe their spectra and polarization, which depend on viewing angle (i.e., photon direction). However, the growing number of high resolution images that are being returned from *HST* make an imaging code desirable. With the information available on individual photons from the Monte Carlo technique, generating images is a straightforward task — we note the position and direction of exit of the photon, and project this onto a plane, with the positioning of the plane depending on the photon's direction. By placing planes around the object through which the radiation transfer is being simulated, we may build up 2D images of it from all viewing angles. The number of images required depends on the degree of symmetry of the system.

In the previous chapter we binned the photons according to their angle of exit. Now we must also bin the exiting photons into x and y bins on the viewing plane. Having determined the viewing angle via μ and ϕ binning, we calculate the x and y coordinates of the photon on the image plane according to

$$x_{\rm image} = z\,\sin\theta - y\,\cos\theta\sin\phi - x\,\cos\theta\cos\phi\ , \quad y_{\rm image} = y\,\cos\phi - x\,\sin\phi\ , \tag{27}$$

where (x, y, z) is the final position of the photon prior to exiting the medium, (θ, ϕ) is the direction of travel, and $(x_{\rm image}, y_{\rm image})$ is the position on the plane centered on (θ, ϕ) that the photon will hit. By generating many photons and projecting them onto planes we will build up an image, the same principle behind taking a picture.

5 Monte Carlo Radiative Equilibrium

We wish to develop a method to calculate the temperature distribution throughout an extended dusty environment for use with Monte Carlo simulations of the radiation transfer. The radiation transfer technique we employ has been described in previous chapters, so we only summarize it here. The basic idea is to divide the luminosity of the radiation source into equal-energy, monochromatic "photon packets" (hereafter photons) that are emitted stochastically by the source. These photons are followed to random interaction locations, determined by the optical depth, where they are either scattered or absorbed with a probability given by the albedo. If the photon is scattered, a random scattering angle is obtained from the scattering phase function (differential cross section). If instead the photon is absorbed, its energy is added to the envelope, raising the local temperature, and to conserve energy the photon is reemitted at a new frequency determined by the envelope temperature. These reemitted photons comprise the diffuse radiation field. After either scattering or absorption plus reemission, the photon continues to a new interaction location. This process is repeated until all the photons escape the dusty environment, whereupon they are placed into frequency and direction-of-observation bins that provide the emergent spectral energy distribution. Since all the injected photons eventually escape (either by scattering or absorption followed by reemission), this method implicitly conserves total energy. Furthermore it automatically includes the diffuse radiation field when calculating both the temperature structure and the emergent spectral energy distribution.

We now describe in detail how we calculate the temperature structure and emergent spectral energy distributions of dusty environments illuminated by a radiation source. This radiation can come from any astrophysical source — either internal or external, point-like or extended.

5.1 Radiative Equilibrium Temperature

Initially we divide the source luminosity, L, into N photon packets. Each photon packet has the same energy, E_γ, so

$$E_\gamma = L/N \ . \tag{28}$$

Similarly, the envelope is divided into spatial grid cells. When the monochromatic photon packet is injected into the envelope, it will be assigned a random frequency chosen from the spectral energy distribution of the source. This frequency determines the dust opacity (per mass), κ_ν, and scattering parameters for the ensuing random walk of the photon through the envelope. We inject source photons and maintain a running total of how many are absorbed in the $i^{\rm th}$ grid cell, N_i. Whenever a photon is absorbed in a grid cell, we deposit its energy in the cell and recalculate the cell's temperature. The total energy absorbed in the cell is

$$E_i^{\rm abs} = N_i E_\gamma \ . \tag{29}$$

We assume that the dust particles are in local thermodynamic equilibrium (LTE) and for simplicity we adopt a single average dust temperature, T, independent of grain size. Note that although we use dust for the continuous opacity source, we could replace the dust by any continuous LTE opacity source. In radiative equilibrium, the absorbed energy, $E_i^{\rm abs}$, must be reradiated. The thermal emissivity of the dust $j_\nu = \kappa_\nu \rho B_\nu(T)$, where B_ν is the Planck function, so the emitted energy is

$$\begin{aligned} E_i^{\rm em} &= 4\pi \int \kappa_\nu \rho B_\nu(T)\, d\nu\, dV_i \\ &= 4\pi \int \kappa_P(T) B(T) \rho\, dV_i \ , \end{aligned} \tag{30}$$

where κ_P is the Planck mean opacity and $B = \sigma T_i^4/\pi$ is the frequency integrated Plank function. If we adopt a temperature that is constant throughout the grid cell, T_i, then

$$E_i^{\rm em} = 4\pi \kappa_P(T_i) B(T_i) m_i \ , \tag{31}$$

where m_i is the mass of the cell. Equating the absorbed (29) and emitted (31) energies, we find that after absorbing N_i photons, the dust temperature is given by

$$\sigma T_i^4 = \frac{N_i L}{4N\kappa_P(T_i) m_i} \ . \tag{32}$$

The Planck mean opacity is a weak function of temperature, so we solve this equation by iteration. To do so efficiently, we pre-tabulate the Planck mean opacities for a large range of temperatures and evaluate $\kappa_P(T_i)$ by interpolation, using the temperature from the previous iteration. Upon convergence, we have the temperature, T_i, from heating by the cumulative photon absorption.

5.2 Temperature Correction

Now that we know the temperature after absorbing an additional photon within the cell, we must reradiate this energy so that the heating always balances the cooling. Prior to absorbing this photon, the cell already has emitted photons that carried away an energy given by the cell's emissivity $j_\nu = \kappa_\nu B_\nu(T_i - \Delta T)$, where ΔT is the change in temperature arising from the absorption of this photon. The total energy that should be radiated at the new temperature is $\kappa_\nu B_\nu(T_i)$, so the additional energy to be carried away is given by

$$\Delta j_\nu = \kappa_\nu \left[B_\nu(T_i) - B_\nu(T_i - \Delta T) \right] \tag{33}$$

As long as E_γ is not too large, the temperature change ΔT is small, so

$$\Delta j_\nu \approx \kappa_\nu \Delta T \frac{dB_\nu}{dT} \ . \tag{34}$$

Therefore, to correct the previously emitted spectrum to that of the new temperature, T_i, we reemit the photon with a frequency chosen from the normalized probability distribution

$$\frac{dP_i}{d\nu} = \frac{\kappa_\nu}{K} \left(\frac{dB_\nu}{dT} \right)_{T=T_i} \ , \tag{35}$$

where the normalization constant $K = \int_0^\infty \kappa_\nu (dB_\nu/dT)\, d\nu$.

Now that the photon's frequency has changed, we change the opacity and scattering parameters accordingly and continue with scattering, absorption, temperature correction, and re-emission until all source photons finally escape from the system, which automatically conserves energy. When completed, the scheme described above yields the temperature structure throughout the envelope, the emergent spectral energy distribution as a function of viewing angle, and it automatically accounts for the diffuse envelope emission.

In principle we could also account for back-warming of the source. Whenever a photon hits the source, the source must reradiate this new energy. This will change the temperature of the source and the new source photons can be emitted using a difference spectrum similar to equation (35).