2013 Summer Course

on Optical Oceanography, Remote Sensing, Radiative Transfer Theory, and HydroLight

Curtis Mobley

The Radiative Transfer Equation and Monte Carlo Simulation

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University of Maine
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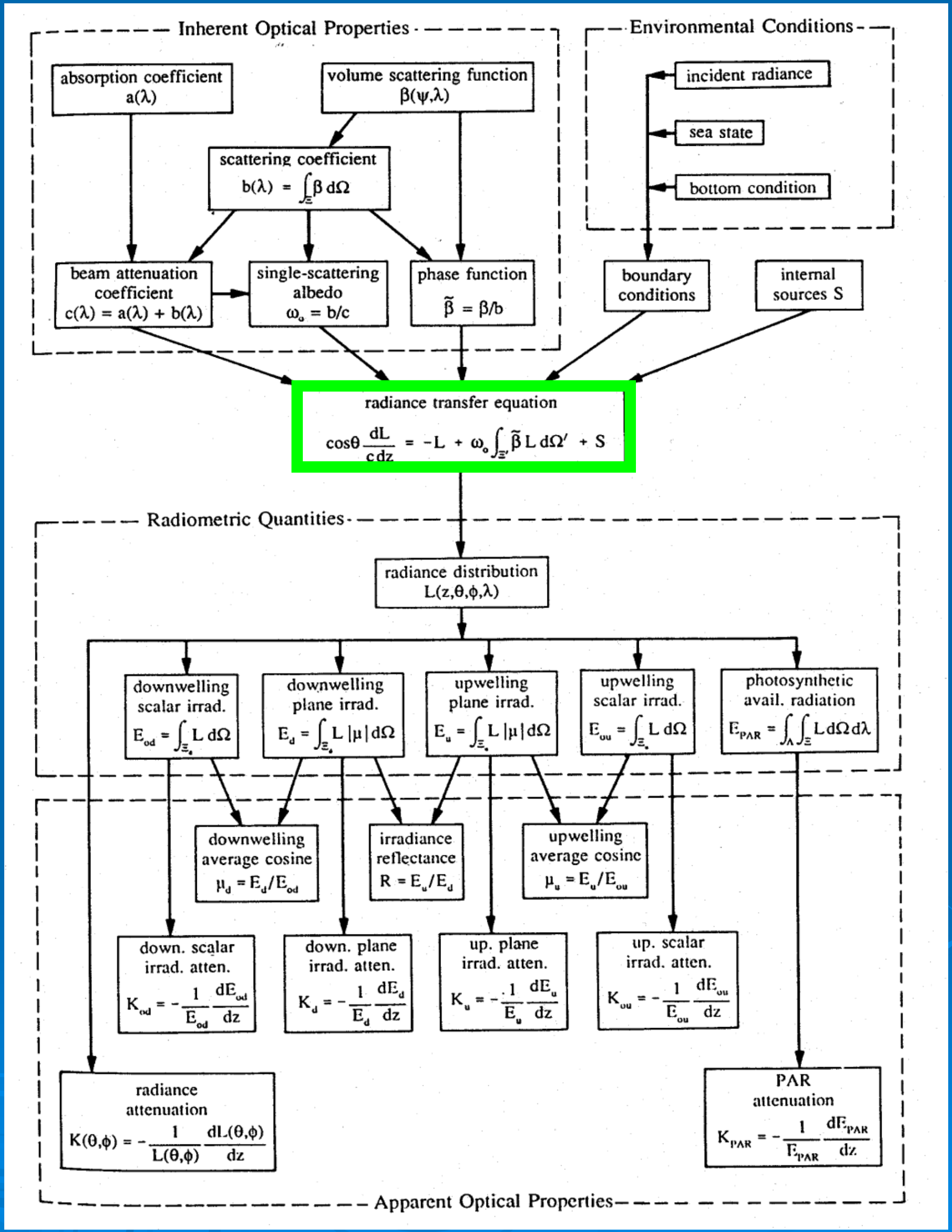
The Radiative Transfer Equation (RTE)

• expresses conservation of energy in terms of the radiance

• connects the IOPs, boundary conditions, and light sources to the radiance

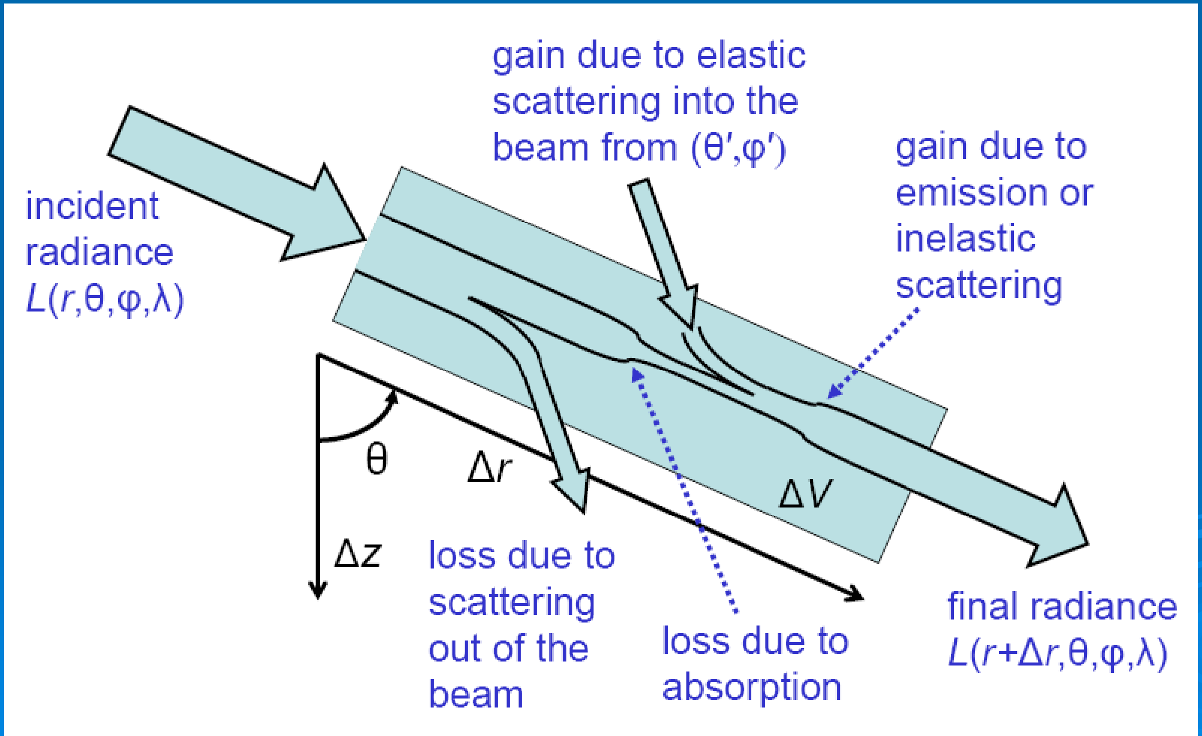
All other radiometric variables (irradiances) and AOPs can be derived from the radiance.

If you know the radiance, you know everything there is to know about the light field



Derivation of the RTE

To derive the time-independent RTE for horizontally homogeneous water, we consider the radiance at a given depth *z*, traveling in a given direction (θ, ϕ), at a given wavelength λ. We then add up the various ways the radiance *L*(*z*,θ,ϕ,λ) can be created or lost in a distance *Δr* along direction (θ, ϕ), going from depth *z* to *z+Δz*



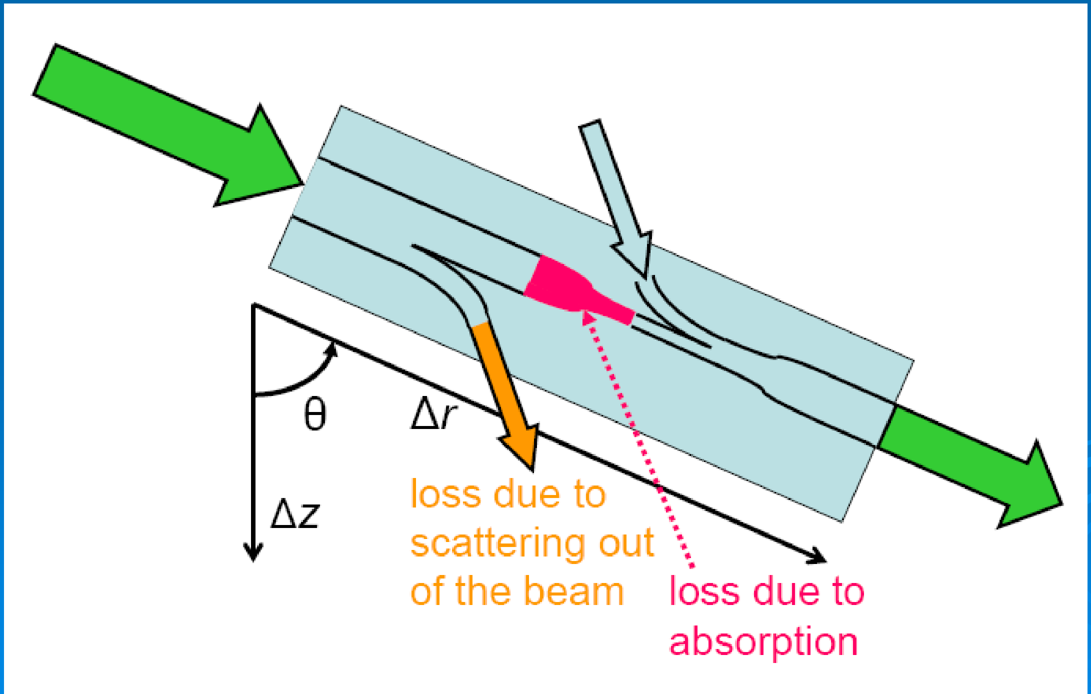
Losses of Radiance

The loss due to absorption is proportional to how much radiance there is:

$$\frac{dL(z,\theta,\phi,\lambda)}{dr} = - a(z,\lambda)\, L(z,\theta,\phi,\lambda)$$

Likewise for loss of radiance due to scattering out of the beam:

$$\frac{dL(z,\theta,\phi,\lambda)}{dr} = - b(z,\lambda)\, L(z,\theta,\phi,\lambda)$$

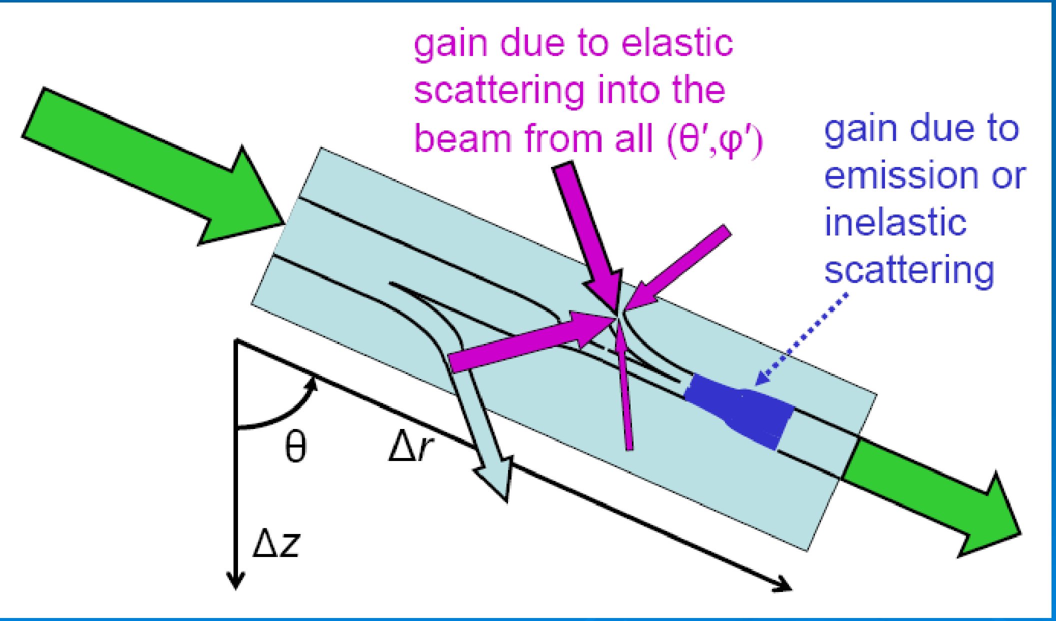


Sources of Radiance

Scattering into the beam from all other directions increases the radiance:

$$\frac{dL(z,\theta,\phi,\lambda)}{dr} = \int_{4\pi} L(z,\theta',\phi',\lambda)\,\beta(z;\,\theta',\phi' \rightarrow \theta,\phi\,;\lambda)\,d\Omega'$$

See www.oceanopticsbook.info/view/radiative_transfer_theory/deriving_the_radiative_transfer_equation for more detail



There can be internal sources of radiance $S(z,\theta,\phi,\lambda)$, such as bioluminescence

$$\frac{dL(z,\theta,\phi,\lambda)}{dr} = S(z,\theta,\phi,\lambda)$$

Add up the Losses and Sources

$$\frac{dL(z,\theta,\phi,\lambda)}{dr} = - a(z,\lambda)\, L(z,\theta,\phi,\lambda)$$

$$- b(z,\lambda)\, L(z,\theta,\phi,\lambda)$$

$$+ \int_{4\pi} L(z,\theta',\phi',\lambda)\, \beta(z;\, \theta',\phi' \rightarrow \theta,\phi;\, \lambda)\, d\Omega'$$

$$+ S(z,\theta,\phi,\lambda)$$

Finally, note that $a + b = c$ and that $dz = dr \cos\theta$ to get

The 1D RTE, Geometric-depth Form

$$\cos\theta \, \frac{dL(z,\theta,\phi,\lambda)}{dz} = - c(z,\lambda)\, L(z,\theta,\phi,\lambda)$$

$$+ \int_{4\pi} L(z,\theta',\phi',\lambda)\, \beta(z;\, \theta',\phi' \rightarrow \theta,\phi;\, \lambda)\, d\Omega'$$

$$+ S(z,\theta,\phi,\lambda)$$

This is the RTE that HydroLight solves.

The VSF $\beta(z;\, \theta',\phi' \rightarrow \theta,\phi;\, \lambda)$ is usually written as $\beta(z, \psi, \lambda)$ in terms of the scattering angle ψ, where

$$\cos\psi = \cos\theta' \cos\theta + \sin\theta' \sin\theta \cos(\phi' - \phi)$$

The 1D RTE, Optical-depth Form

Define the increment of dimensionless optical depth ζ as $d\zeta = c\,dz$ and write the VSF as *b* times the phase function, $\tilde{\beta}$, and recall that $\omega_o = b/c$ to get

$$\cos\theta \frac{dL(\zeta,\theta,\phi,\lambda)}{d\zeta} = - L(\zeta,\theta,\phi,\lambda) + \omega_o \int_{4\pi} L(\zeta,\theta',\phi',\lambda)\, \tilde{\beta}(\zeta;\theta',\phi' \to \theta,\phi;\lambda)\, d\Omega' + S(\zeta,\theta,\phi,\lambda)/c(\zeta,\lambda)$$

Can specify the IOPs by *c* and the VSF β, or by ω_o and the phase function $\tilde{\beta}$ (and also *c*, if there are internal sources)

Note that a given geometric depth *z* corresponds to a different optical depth $\zeta(\lambda) = \int_0^z c(z',\lambda)\, dz'$ at each wavelength

The 1D RTE, Geometric-depth Form

$$\cos\theta \, \frac{dL(z,\theta,\phi,\lambda)}{dz} = - c(z,\lambda)\, L(z,\theta,\phi,\lambda)$$

$$+ \int_{4\pi} L(z,\theta',\phi',\lambda)\, \beta(z;\, \theta',\phi' \rightarrow \theta,\phi;\, \lambda)\, d\Omega'$$

$$+ S(z,\theta,\phi,\lambda)$$

NOTE: The RTE has the TOTAL *c* and TOTAL VSF. Only oceanographers (not light) care how much of the total absorption and scattering are due to water, phytoplankton, CDOM, minerals, etc.

The RTE is a linear (in the unknown radiance), first-order (only a first derivitive) integro-differential equation. Given the green (plus boundary conditions), solve for the red. This is a two-point (surface and bottom) boundary value problem.

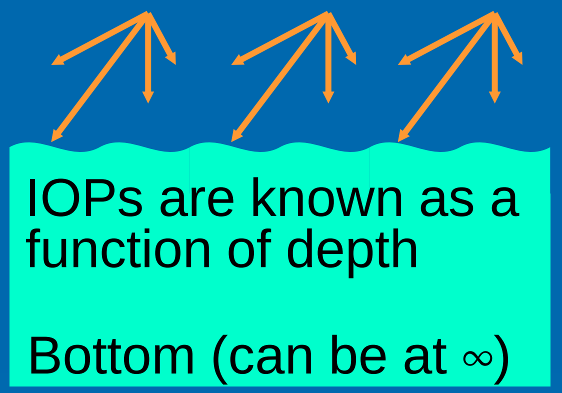
Solving the RTE

A unique solution of the RTE requires:

Radiance incident onto all boundaries from outside the region is known

Stretch out the region to make a horizontally homogeneous ocean

Radiance incident onto sea surface is known



A 3-D problem

A 1-D problem

Given the IOPs within the region and the incident radiances, we can solve for the radiance within and leaving the region

Solving the RTE: The Lambert-Beer Law

A trivial solution:

- Homogeneous water (IOPs do not depend on z)
- No path radiance : Either no scattering (VSF β = 0, so c = a + b = a), or no light other than the initial beam.
- No internal sources (S = 0)
- Infinitely deep water (no radiance coming from the bottom boundary, so L → 0 as z → ∞)
- Incident radiance *L*(z=0) is known just below the sea surface

$$\cos\theta \frac{dL(z,\theta,\phi,\lambda)}{dz} = -c(\lambda)L(z,\theta,\phi,\lambda)$$

$$\int_{L(z=0,\theta,\phi,\lambda)}^{L(z,\theta,\phi,\lambda)} \frac{dL}{L} = \int_0^z \frac{c(\lambda)\,dz}{\cos\theta}$$

$$L(z,\theta,\phi,\lambda) = L(z=0,\theta,\phi,\lambda)e^{-c(\lambda)z/\cos\theta}$$

Note that this *L* satisfies the RTE, the surface boundary condition, and the bottom boundary condition *L*(z=∞) = 0.

Solving the RTE: Gershun's Law

Start with the 1D, source-free, RTE.

$$\begin{aligned}\cos\theta\frac{dL(z,\theta,\phi,\lambda)}{dz} &= -\,c(z,\lambda)\,L(z,\theta,\phi,\lambda) \\ &+ \int_0^{2\pi}\int_0^{\pi} L(z,\theta',\phi',\lambda)\,\beta(z,\theta',\phi'\rightarrow\theta,\phi,\lambda)\sin\theta'\,d\theta'\,d\phi'\end{aligned}$$

Integrate over all directions. The left-hand-side becomes

$$\begin{aligned}\int_0^{2\pi}\int_0^{\pi}\cos\theta\frac{dL(z,\theta,\phi)}{dz}d\Omega(\theta,\phi) &= \frac{d}{dz}\int_0^{2\pi}\int_0^{\pi} L(z,\theta,\phi)\cos\theta\, d\Omega(\theta,\phi) \\ &= \frac{d}{dz}[E_{\mathrm{d}}(z) - E_{\mathrm{u}}(z)]\end{aligned}$$

Solving the RTE: Gershun's Law

The – *cL* term becomes

$$\iint -c(z)L(z,\theta,\phi)d\Omega(\theta,\phi) \;=\; -\,c(z)\iint L(z,\theta,\phi)d\Omega(\theta,\phi)$$

$$=\; -\,c(z)E_{\mathrm{o}}(z)$$

The elastic-scatter path function becomes

$$\iint\left[\iint L(z,\theta',\phi')\,\beta(z,\theta',\phi'\to\theta,\phi)d\Omega(\theta',\phi')\right]d\Omega(\theta,\phi)$$

$$=\iint L(z,\theta',\phi')\left[\iint \beta(z,\theta',\phi'\to\theta,\phi)d\Omega(\theta,\phi)\right]d\Omega(\theta',\phi')$$

$$=b(z)\iint L(z,\theta',\phi')d\Omega(\theta',\phi')$$

$$=b(z)E_{\mathrm{o}}(z)$$

Solving the RTE: Gershun's Law

Collecting terms,

$$\frac{d}{dz}\left[E_{\mathrm{d}} - E_{\mathrm{u}}\right] = -cE_{\mathrm{o}} + bE_{\mathrm{o}}$$

or

$$a(z,\lambda) = -\frac{1}{E_{\mathrm{o}}(z,\lambda)}\frac{d}{dz}\left[E_{\mathrm{d}}(z,\lambda) - E_{\mathrm{u}}(z,\lambda)\right]$$

Gershun's law can be used to retrieve the absorption coefficient from measured in-water irradiances (at wavelengths where inelastic scattering effects are negligible).

This is an example of an explicit inverse model that recovers an IOP from measured light variables.

Gershun's law is a "solution of the RTE," but in terms of irradiances. We haven't solved for the radiance $L(z,\theta,\phi,\lambda)$, which is what we really want.

Water Heating and Gershun's Law

The rate of heating of water depends on how much irradiance there is and on how much is absorbed:

$$\frac{\partial T}{\partial t} = \frac{1}{\rho c_v}\overline{aE_o} = -\frac{1}{\rho c_v}\frac{d(\bar{E}_d - \bar{E}_u)}{dz} \qquad \left[\frac{\text{deg C}}{\text{sec}}\right]$$

$$\text{where } \bar{x} = \int_0^\infty x(\lambda)\, d\lambda$$

c_v = 3900 J (kg deg C)$^{-1}$ is the specific heat of sea water
ρ = 1025 kg m^{-3} is the water density

This is how irradiance is used in coupled physical-biological-optical ecosystem models to couple the biological variables (which, with water, determine the absorption coefficient and the irradiance) to the hydrodynamics (heating of the upper ocean water)

Solving the RTE

Exact analytical (i.e., pencil and paper) solutions of the RTE can be obtained only for very simple situations, such as no scattering. There is no function (that anyone has ever found) that gives

$L(z,\theta,\phi,\lambda) = f(a, VSF$, sun angle, bottom reflectance, etc.)

even for very simple situations such as homogenous water with isotropic scattering. Even the extremely simple geometry of an isotropic point light source in an infinite homogeneous ocean is unsolved (a very complicated solution for $E_o(r)$ around a point source with isotropic scattering does exist). This is because of the complications of scattering (which don't exist for problems like the gravitational field around a point mass).

Solving the RTE

Approximate analytical solutions can be obtained for idealized situations such as single scattering in a homogeneous ocean. (This is where $R_{rs} = b_b/(a + b_b)$ comes from.)

See
www.oceanopticsbook.info/view/radiative_transfer_theory/level_2/the_singlescattering_approximation for a discussion of the single-scattering approximation (SSA), and see
www.oceanopticsbook.info/view/radiative_transfer_theory/level_2/the_quasisinglescattering_approximation
for the related quasi-single scattering approximation.

We don't have time to discuss these approximate solutions, and they are not very useful anyway.

Solving the RTE

The solution of the RTE for any realistic conditions of scattering or geometry must be done numerically. Three widely used exact numerical methods are seen in the literature (in RT theory, “exact” means that we don’t make approximations such as single scattering. Given accurate inputs and enough computer time, you can get the correct answer as closely as you wish.)

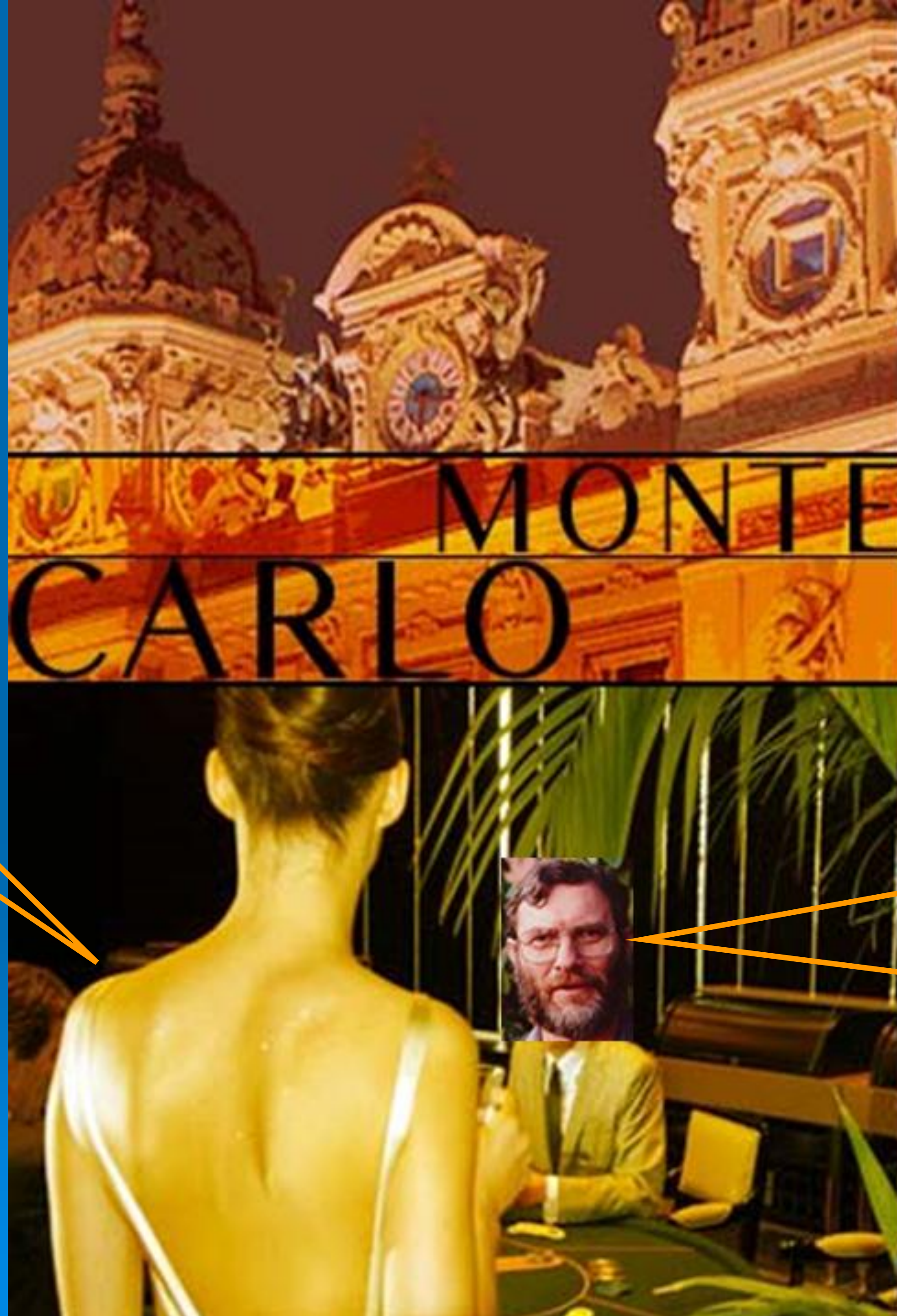
- Discrete ordinates: often used in atmospheric optics
    - highly mathematical
    - difficult to program
    - doesn’t handle highly peaked phase functions well
    - most codes need a level sea surface
    - models the medium as homogeneous layers
    - fast for irradiances and homogeneous systems
    - slow for radiances and inhomogeneous systems
    - therefore, not much used in oceanography

Solving the RTE

- Invariant Imbedding: what Hydrolight uses
  - highly mathematical (see *Light and Water*, Chaps 7 and 8; causes cosmic dissolution of brain cells for polarization)
  - difficult to program
  - 1D (depth dependence) problems only
  - run time increases linearly with optical depth
  - computes radiances accurately (no statistical noise)
  - extremely fast and accurate even for radiances and large depths

- Monte Carlo: widely used
  - simple math, easy to program
  - can solve 3D problems; polarization relatively easy
  - run time increases exponentially with optical depth
  - have to trace many photons to get accurate radiance estimates (solutions have statistical noise)
  - very long run times for radiances and/or great depths
  - more useful for irradiance computations and/or shallow depths

Hey Curt, wanna go to my place and, uh, talk about radiative transfer theory?



Not tonight. I'm still debugging my new Monte Carlo code

Monte Carlo Techniques for Solving the RTE

- The basic idea is to mimic nature in the generation and tracing of photons

- Build up a solution to the RTE one photon at a time

- The tools for doing this are basic probability theory and a random number generator

Points to be covered:

- PDFs and CDFs

- Random number generators

- Using CDFs to randomly select distances, angles, etc.

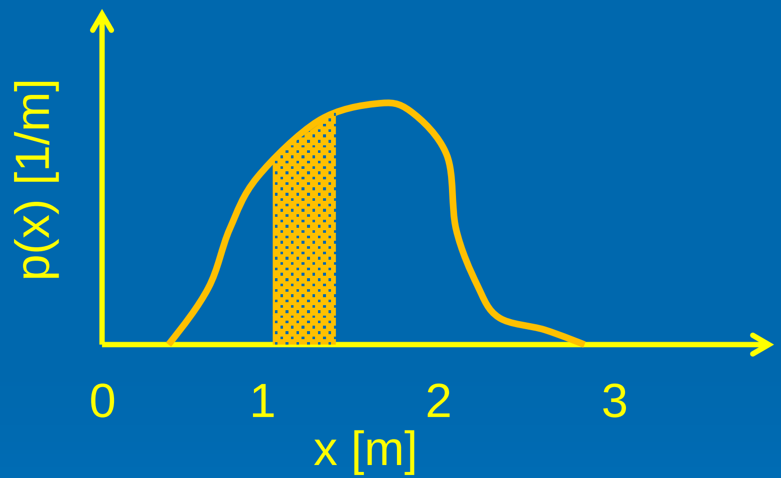
- Monte Carlo noise

There are web book pages on Monte Carlo techniques starting at http://www.oceanopticsbook.info/view/radiative_transfer_theory/level_2/monte_carlo_techniques_introduction

Probability Density Functions

A *probability density function* (PDF) is a non-negative function *p*(*x*) such that the probability that its variable *x* is between *x* and *x*+*dx* is *p*(*x*)*dx*.

Example: *x* = height of humans



Prob that a person selected at random from all humans is between 1.0 and 1.3 m tall is

$$\int_{1.0}^{1.3} p(x)dx$$

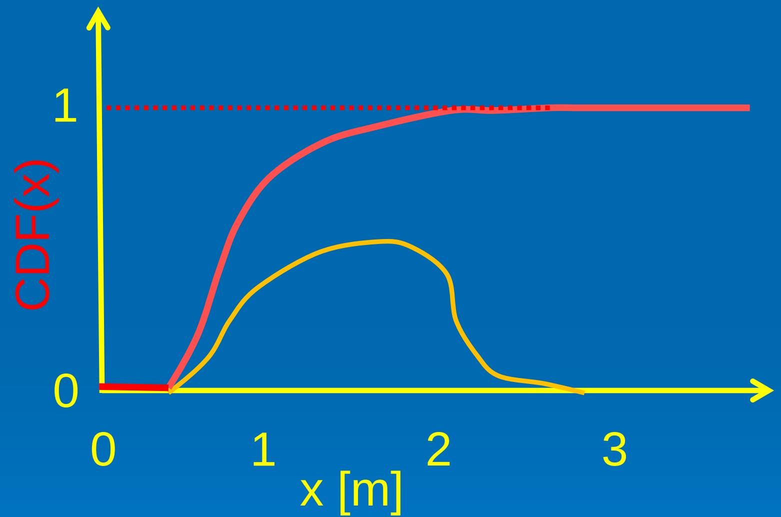
Normalization: $\int_0^\infty p(x)dx = 1$ That is, the prob is one that a person will have some height between 0 and ∞

Units of *p*(*x*) are always 1/[*x*]

Cumulative Distribution Functions

A *cumulative distribution function* (CDF) is a non-negative function *CDF*(*x*) such that the probability that its variable has a value <= *x* is CDF(*x*). For the human height example,

$$CDF(x) = \int_0^x p(x')dx'$$



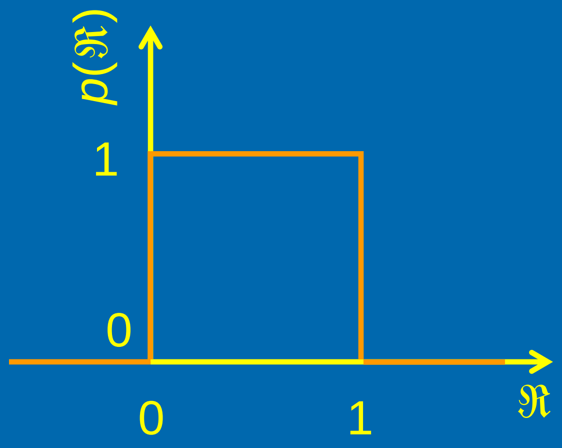
Prob that a person selected at random from all humans is between 1.0 and 1.3 m tall is

CDF(1.3) – CDF(1.0)

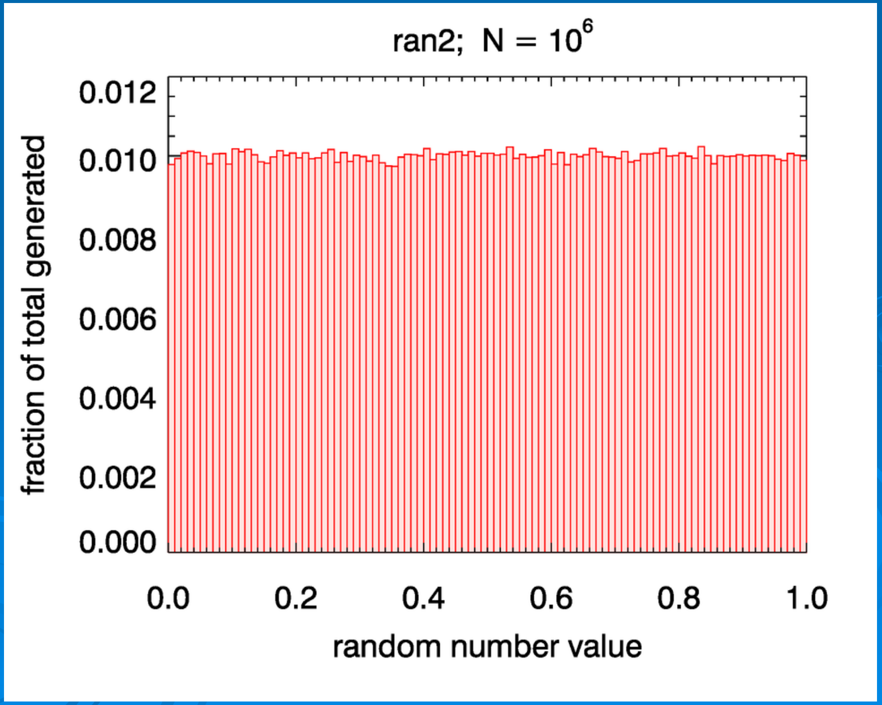
Note that CDF(∞) = 1. That is, the prob is one that a person will have some height less than ∞

U(0,1) Random Number Generators

A Uniform 0-1 random number generator is anything (usually a computer program) that when called returns a number ℜ between 0 and 1 with equal probability of returning any value 0 < ℜ < 1. ℜ ~ U(0,1)



0.6314325330
0.2641695440
0.7653187510
0.3009850980
0.9278188350
0.0138932914
0.3010187450
0.1198131440
0.3243462440
0.3493790630
0.1154079510
0.1382016390
0.1065650730



Random Determination of Photon Path Lengths

Recall Beer's law (collimated beam in a dark ocean):

$L(r) = L(0) \exp(-cr) = L(0) \exp(-\tau)$

The exponential decay of radiance can be explained if the individual photons have a probability of being absorbed or scattered out of the beam between τ and $\tau + d\tau$ that is

$p(\tau)d\tau = \exp(-\tau)\, d\tau \Rightarrow p(\tau) = \exp(-\tau)$

We want to use our U(0,1) random number generator to randomly determine photon path lengths τ that obey the pdf $p(\tau) = \exp(-\tau)$. Going from $\Re$ to τ is a change of variables:

$$p(\Re)d\Re = p(\tau)d\tau$$

$$\int_0^{\Re} p(\Re')d\Re' = \int_0^{\tau} p(\tau')d\tau'$$

$$\Re = \mathrm{CDF}(\tau) = 1 - \exp(-\tau)$$

Random Determination of Photon Path Lengths

Solving

$\Re = 1 - \exp(-\tau)$ for τ

gives

$\tau \;\; = -\ln(1- \Re) = -\ln \Re$

Draw a U(0,1) random number $\Re$, and then the corresponding photon path is

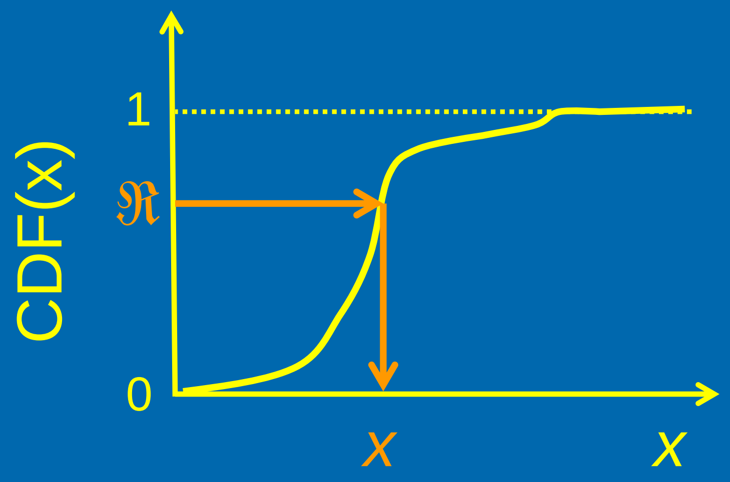
$\tau \;\; = -\ln \Re$

or

$r = -(1/c) \ln \Re$ for distances *r* in meters.

Fundamental Principle of MC Simulation

The equation $\Re$ = CDF(x) uniquely determines x such that x obeys the corresponding pdf p(x)



General procedure:

1. Figure out the pdf p(x) that governs the variable of interest, x
2. Compute the corresponding CDF(x)
3. Draw a U(0,1) random number $\Re$
4. Solve $\Re$ = CDF(x) for x
5. Repeat steps 3 and 4 many, many, many times to generate a sample of x values that reproduces the behavior of x in nature

Photon Mean Free Path

The pdf for the distance a photon travels is $p(\tau) = \exp(-\tau)$. What is the average distance $\langle \boldsymbol{\tau} \rangle$ that a photon travels? Called the mean free path.

$$\langle \tau \rangle \equiv \int_0^\infty \tau\, p(\tau) d\tau = \int_0^\infty \tau\, e^{-\tau}\, d\tau = 1$$

or, since τ = cr,

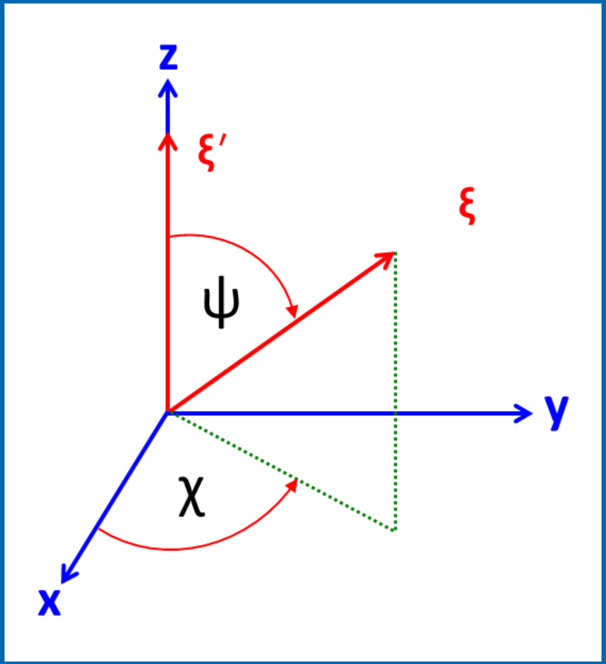
$\langle \boldsymbol{r} \rangle$ = 1/c (meters)

What is the variance about the mean distance traveled?

$$\sigma^2(\tau) \equiv \int_0^\infty [\tau - \langle \tau \rangle]^2 e^{-\tau} d\tau = 1$$

so the standard deviation is also 1/c (meters)

Random Determination of Scattering Angles



Scattering is inherently 3D:

ψ is polar scattering angle

χ is azimuthal scattering angle

$$\int_{4\pi} \tilde{\beta}(\psi', \chi' \rightarrow \psi, \chi)\, d\Omega(\psi, \chi) = 1$$

phase functions can be interpreted as pdfs for scattering from (ψ′, χ′) to (ψ, χ)

$$d\Omega(\psi, \chi) = \sin\psi\, d\psi\, d\chi$$

Random Determination of Scattering Angles

For isotropic media and unpolarzed light, ψ and χ are independent, so the bivariate pdf is the product of 2 pdfs:

$$\tilde{\beta}(\psi,\chi)\ \sin\psi\, d\psi\, d\chi = p_\Psi(\psi)\, d\psi\, p_X(\chi)\, d\chi$$

Any azimuthal angle $0 \le \chi < 2\pi$ is equally likely:

$$p_X(\chi) = 1/(2\pi); \quad CDF_X(\chi) = \chi/(2\pi); \quad \chi = 2\pi\mathfrak{R}$$

$$p_\Psi(\psi) = 2\pi\tilde{\beta}(\psi)\sin\psi$$

$$2\pi\int_0^\pi \tilde{\beta}(\psi)\sin\psi\, d\psi = 1$$ √

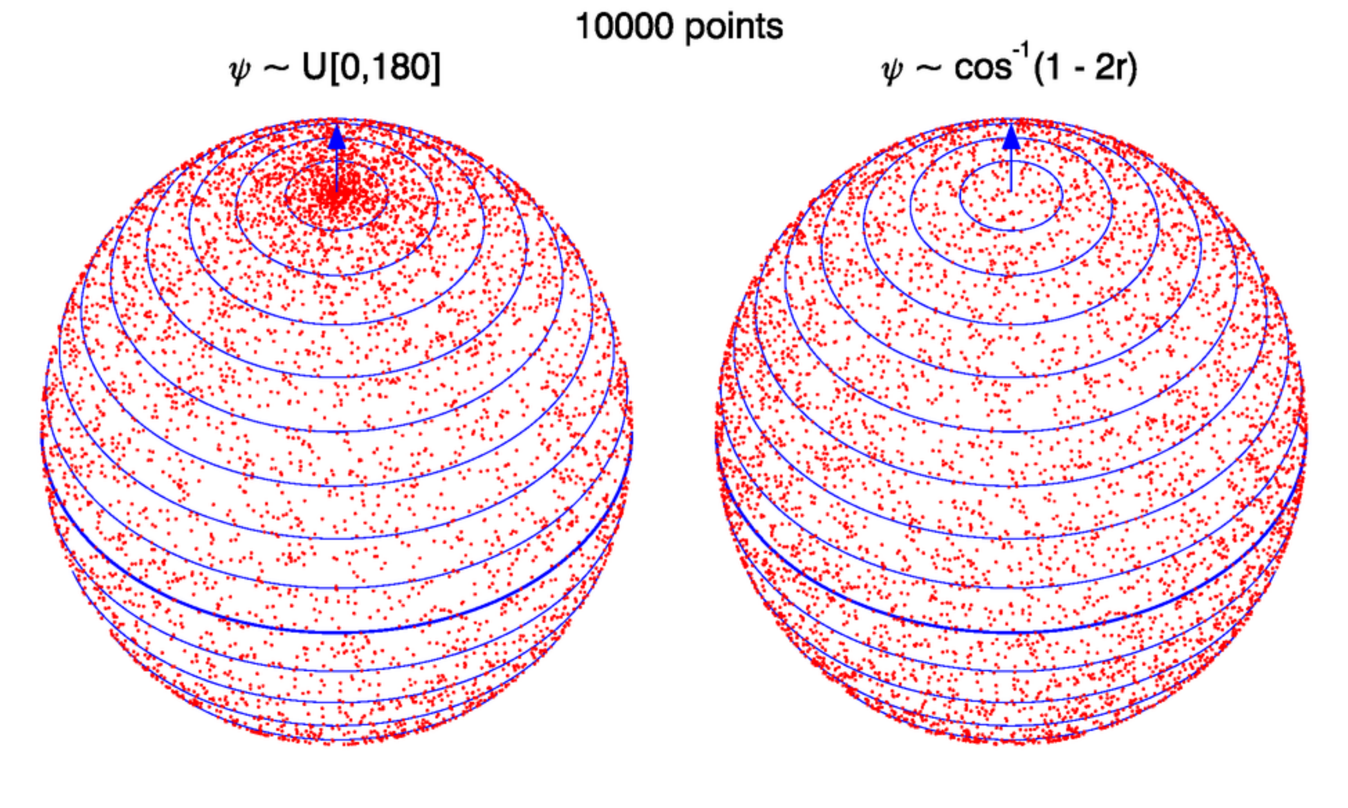
$$\mathfrak{R} = CDF(\psi) = 2\pi\int_0^\psi \tilde{\beta}(\psi')\ \sin\psi'\, d\psi'$$

solve for ψ (usually must solve numerically)

Isotropic Scattering

For isotropic scattering,

$$\tilde{\beta}(\psi) = \frac{1}{4\pi}$$ which gives $$\psi = \cos^{-1}(1 - 2\mathfrak{R})$$



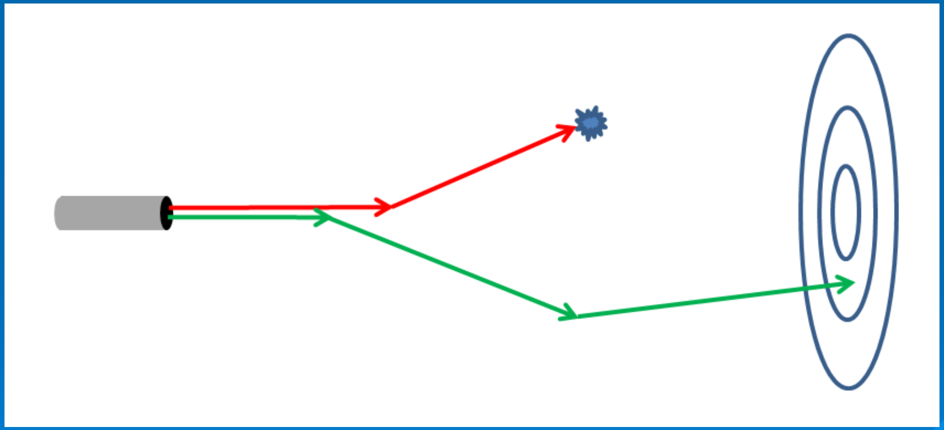
Isotropic means equally likely to scatter into any element of solid angle, not equally likely to scatter through any polar scattering angle ψ

Tracing Photon Packets

The albedo of single scattering, $\omega_o = b/c$, is the probability that a photon will be scattered, rather than absorbed in any interaction

What nature does:

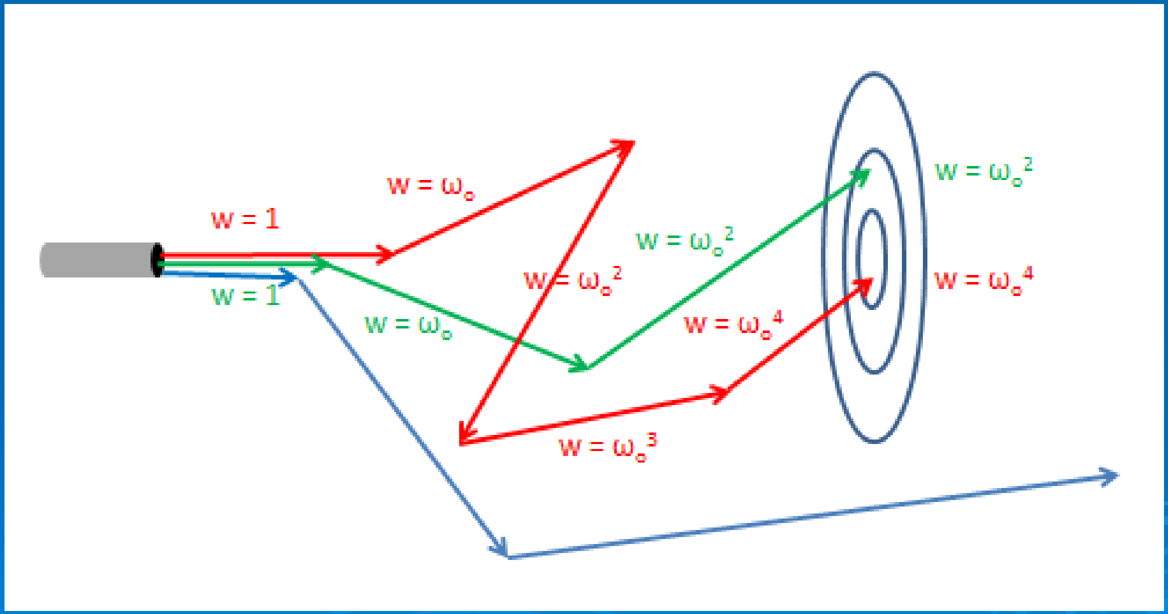
- draws a random number and gets the distance
- draws another random number and compares with ω_o :
  - if $\Re > \omega_o$ the photon is absorbed; start another one
  - if $\Re \leq \omega_o$ the photon is scattered; compute the scattering angles



Any photon that is absorbed never contributes to the answer and is wasted computation. Nature can afford to waste photons; scientists can't.

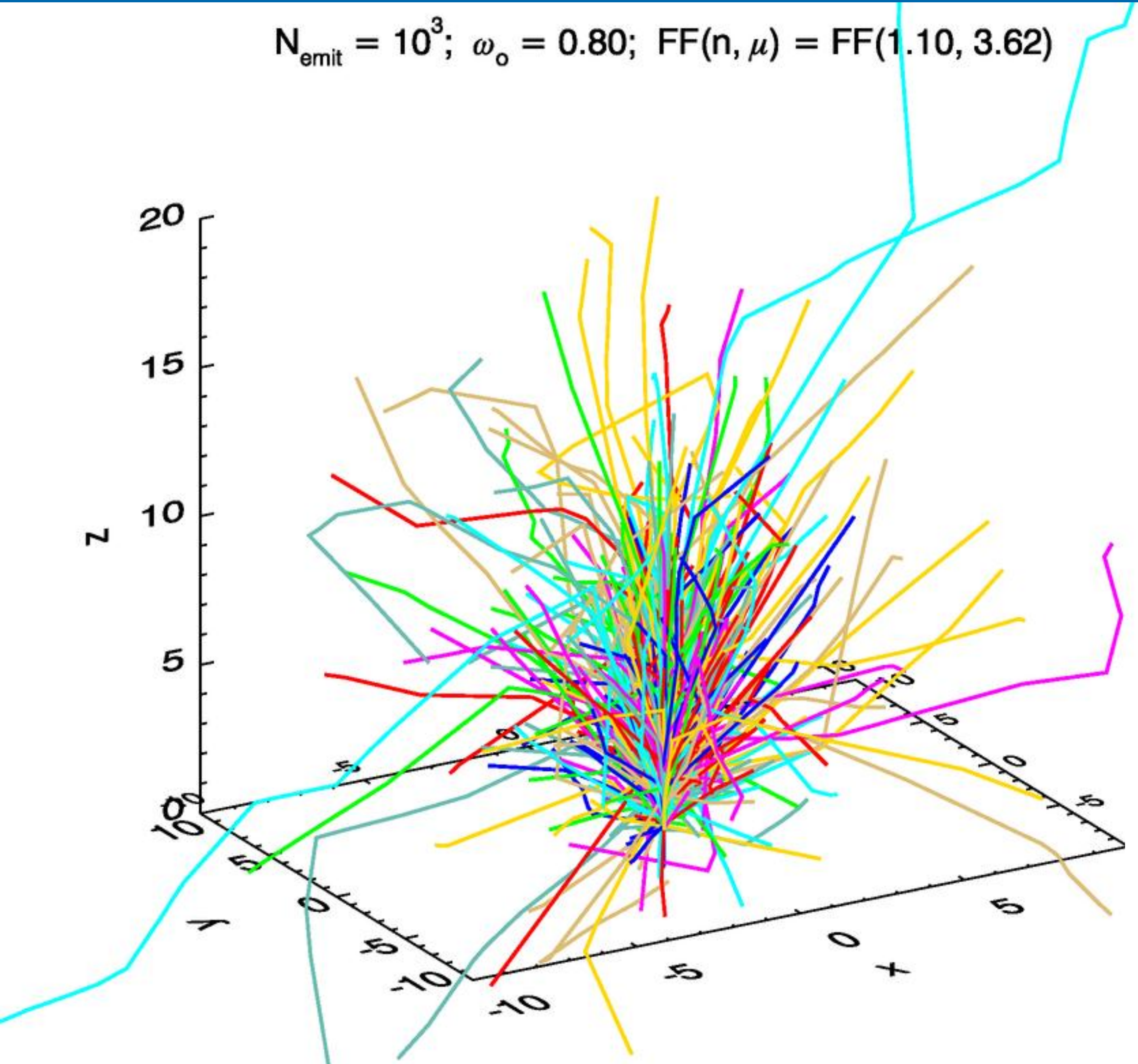
Tracing Photon Packets

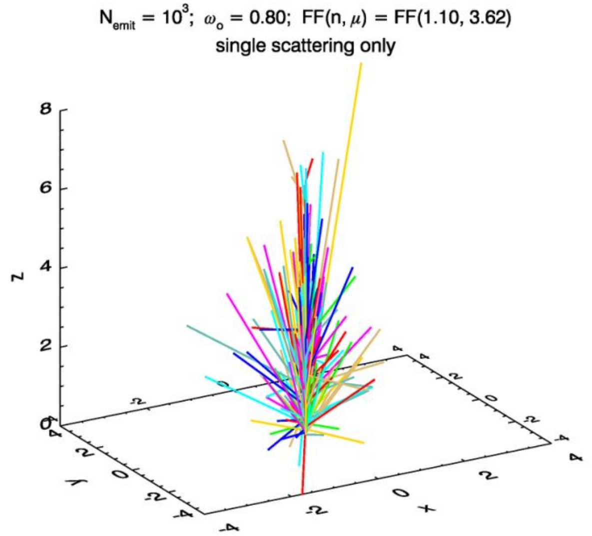
Rather that lose some photons to absorption, consided each "photon" to be a packet of many photons starting with power *w* = 1 W. At each interaction, multiply the current packet weight *w* by ω_o to account for loss of some of the original power to absorption. This increases the number of photon packets that contribute to the answer (although some may still miss the target).



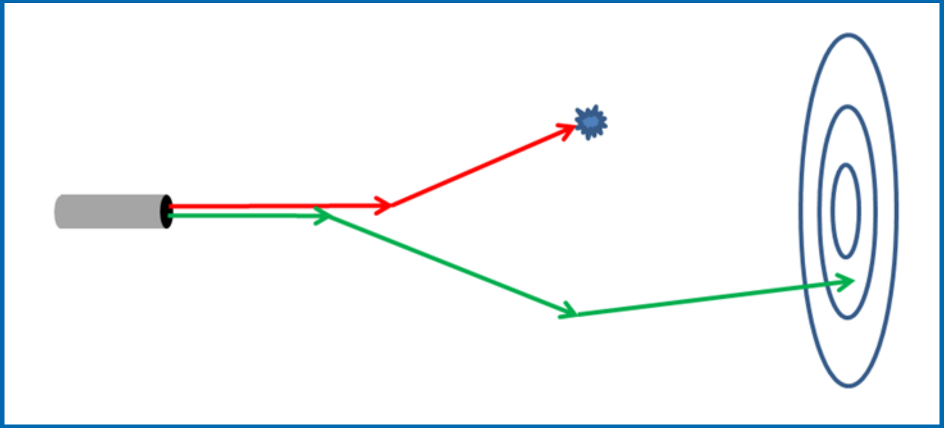
Usually kill the photon packet when w < 10^{-8}, for example, if it hasn't hit the target.

Visualizing Photon Paths

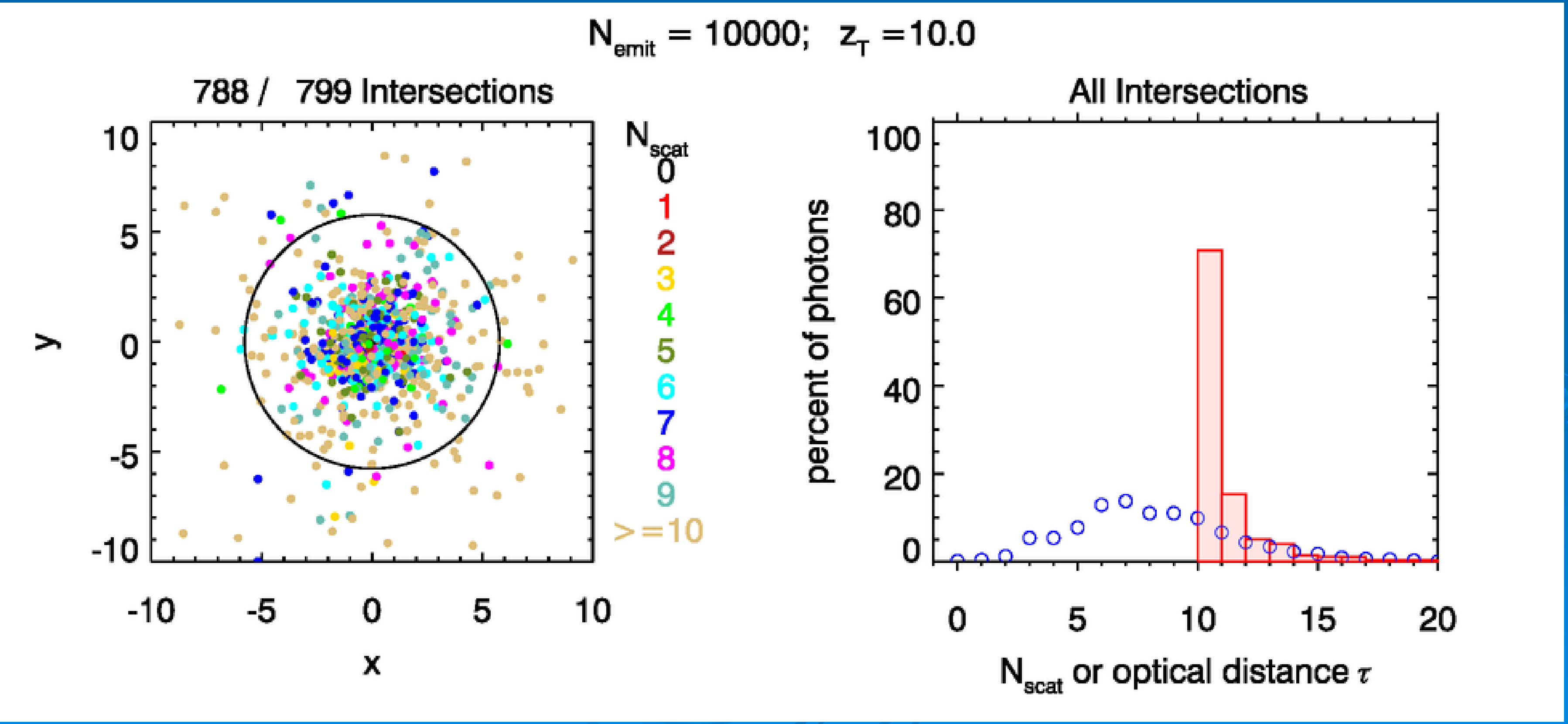




Visualizing Photon Paths

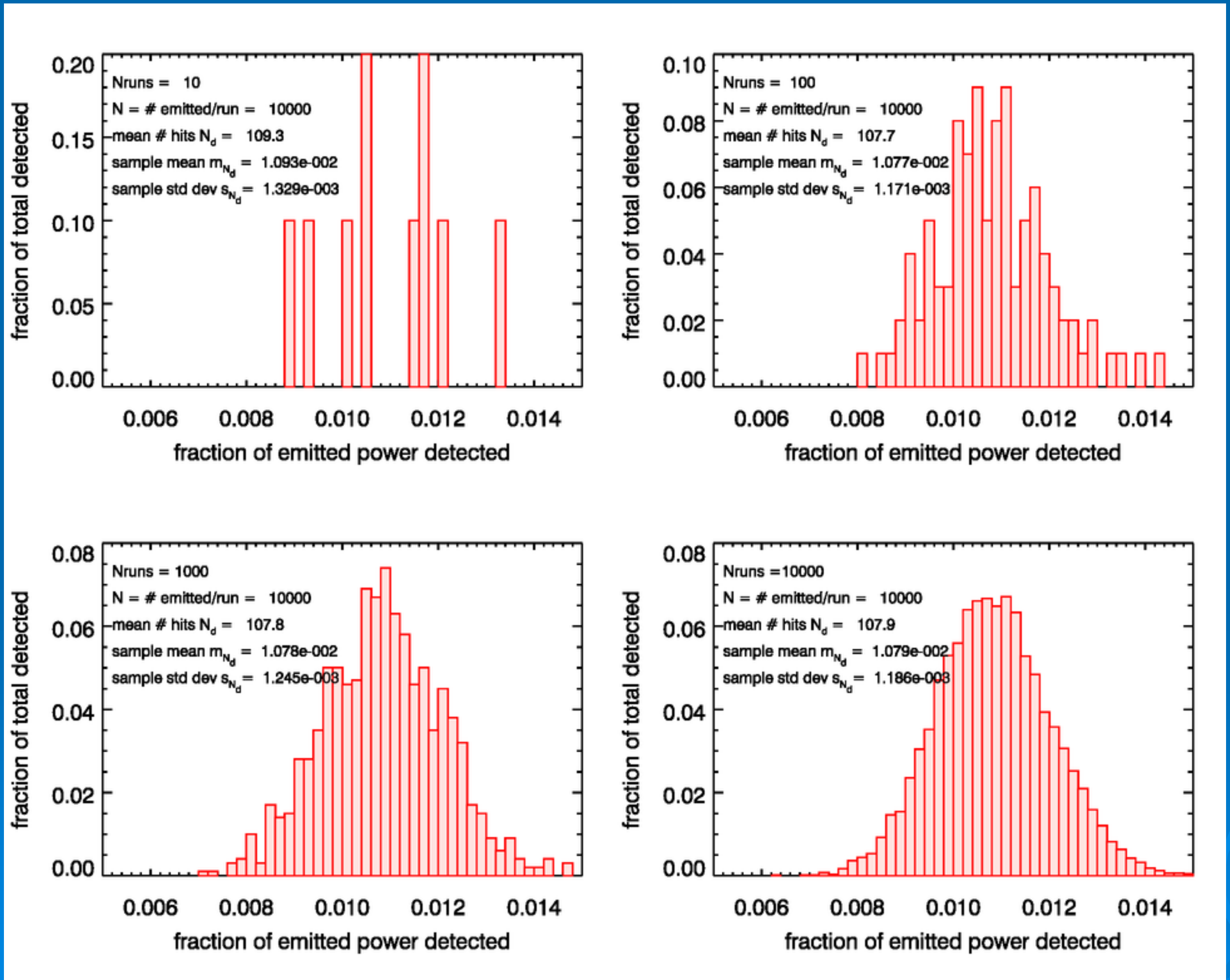


Monte Carlo simulation gives understanding at the photon level, which can't be obtained from radiance (e.g., from HydroLight)



Statistical Noise

The answer you get depends on random numbers and on the number of photons collected, so has statistical noise, aka Monte Carlo noise.



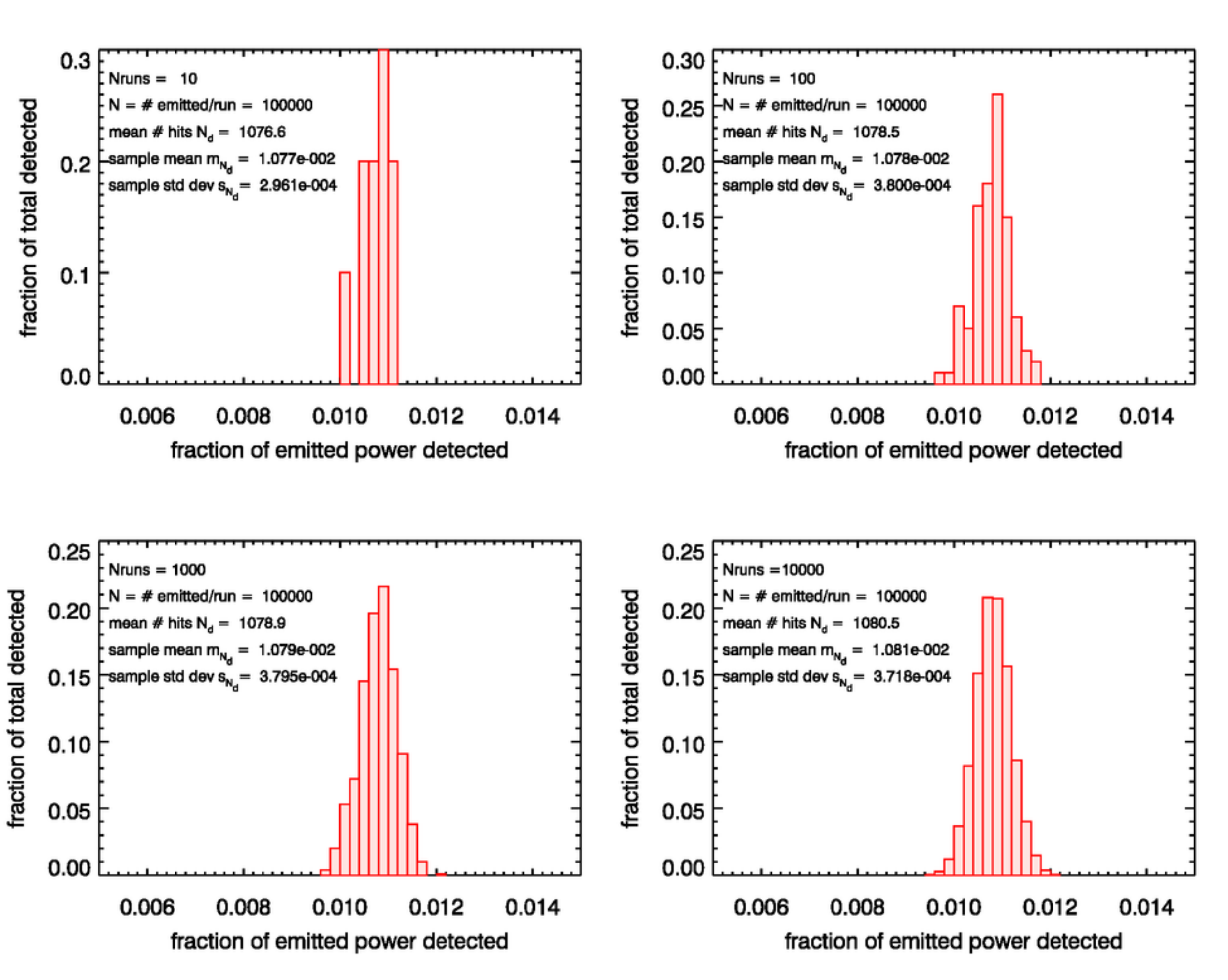
Repeated runs (different sequences of random numbers) with the same number of photons per run.

Note that as more runs are done, the distribution of computed values approaches a Gaussian:

The Central Limit Theorem in action

Statistical Noise

Standard error of the mean too large? Trace more photons...



The same numbers of runs , but with more photons per run.

The variance in the computed values is $\propto 1/N$, N = number of photons *detected*

std dev $\propto 1/\text{sqrt}(N)$

To reduce the std dev of the estimate by a factor of 10, must detect 100 times more photons

Variance Reduction

We now know enough to do the Monte Carlo lab.

However, before writing a MC code to do extensive simulations, read about other ways to get more photons onto the target without more computer time. These are generally called "variance reduction" techniques, and there are many ("Importance sampling," "Backward ray tracing", "forced collisions",...)

In general:

- First, figure out how to simulate what nature does
- Then figure out how to redo the calculations to maximize the number of photons detected (i.e., solve a different problem that has the same answer as the original problem—variance reduction)
- The goal (seldom attained) is to Never Waste a Photon

Sea Kayaking in SE Greenland, 2005

photo by Curtis Mobley