2017 Summer Course

on Optical Oceanography and Ocean Color Remote Sensing

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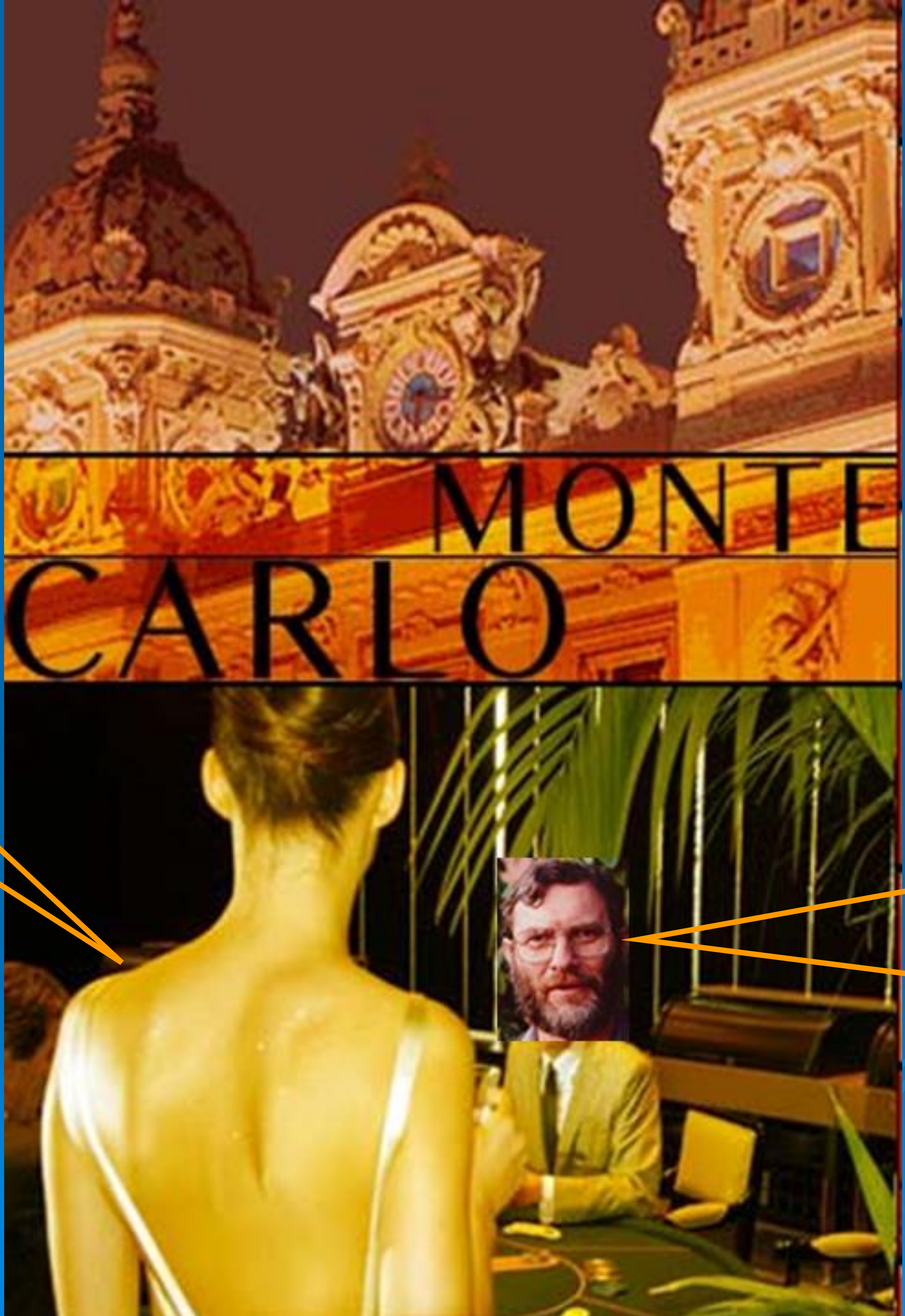
Monte Carlo Simulation

Delivered at the Darling Marine Center,
University of Maine
July 2017

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

Monte Carlo techniques refer to algorithms that use **probability theory** and **random numbers** to simulate a physical process.

An essential feature of Monte Carlo simulation is that **the known probability of occurrence of each separate event in a sequence of events is used to estimate the probability of the occurrence of the entire sequence.**

In the optics setting, the known probabilities that a "photon" (i.e, a packet of radiant energy) will travel a certain distance, be scattered through a certain angle, reflect off a surface in a certain direction, etc., are used to estimate the probability that a photon emitted from a source at one location will travel through the medium and eventually be recorded by a detector at a different location.

Averages over ensembles of large numbers of simulated photon trajectories give statistical estimates of radiances, irradiances, and other quantities of interest.

Monte Carlo Techniques for Solving the RTE

The basic idea:

- Mimic nature in the generation and propagation of photons, which are modeled as discrete particles
- 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

Monte Carlo Techniques for Solving the RTE

Topics to be covered:

- Probability distribution functions (PDFs) and cumulative distribution functions (CDFs)

- Random number generators

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

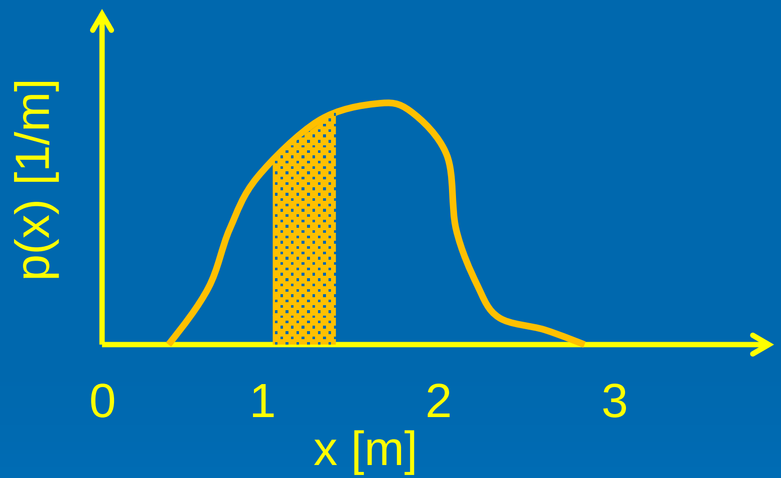
- Monte Carlo noise

There are web book pages on Monte Carlo techniques starting at www.oceanopticsbook.info/view/monte_carlo_simulation/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 adult humans



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

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

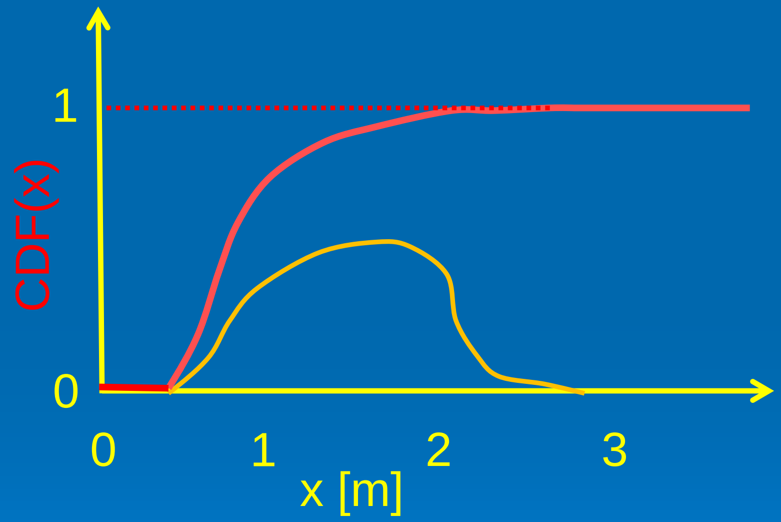
Normalization: $\int_0^\infty p(x)\,dx = 1$ That is, the prob is one that a person will have some height between 0 and ∞

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,

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



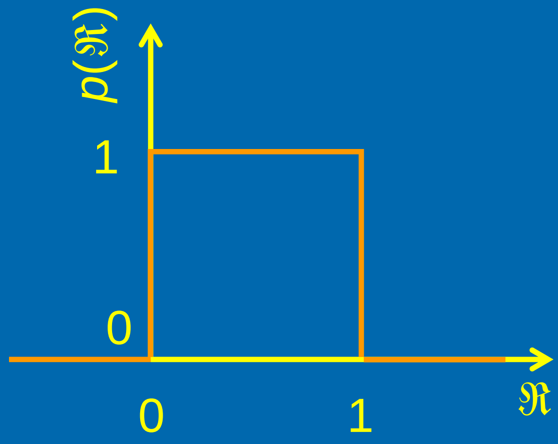
Prob that a person selected at random from all humans is between 1.0 and 1.3 m tall is

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 $\mathfrak{R}$ between 0 and 1 with equal probability of returning any value $0 < \mathfrak{R} < 1$. $\mathfrak{R} \sim U(0,1)$



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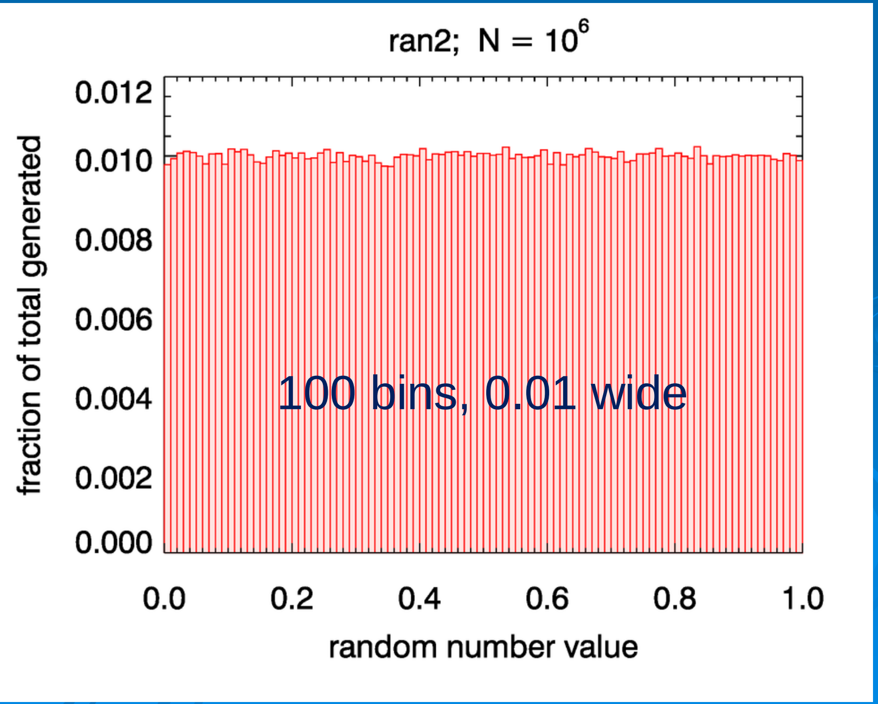
0.1065650730



Random Determination of Photon Path Lengths

Recall Beer's law (for a 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:

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

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

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

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

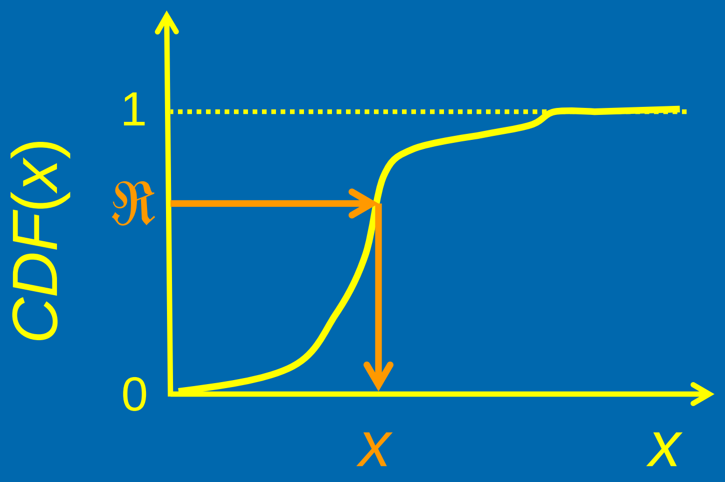
$\tau = -\ln \Re$

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,

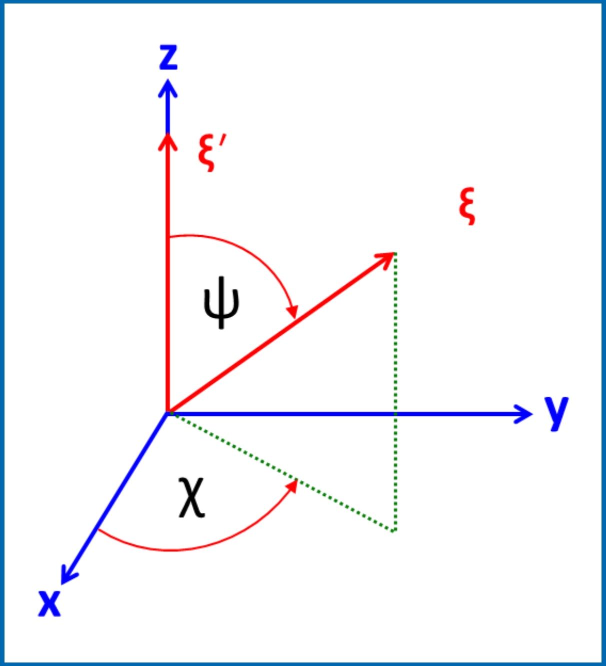
$\langle \boldsymbol{r} \rangle$ = 1/c (meters)

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

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

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 $0 \leq \chi < 2\pi$ is equally likely:

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

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

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

√

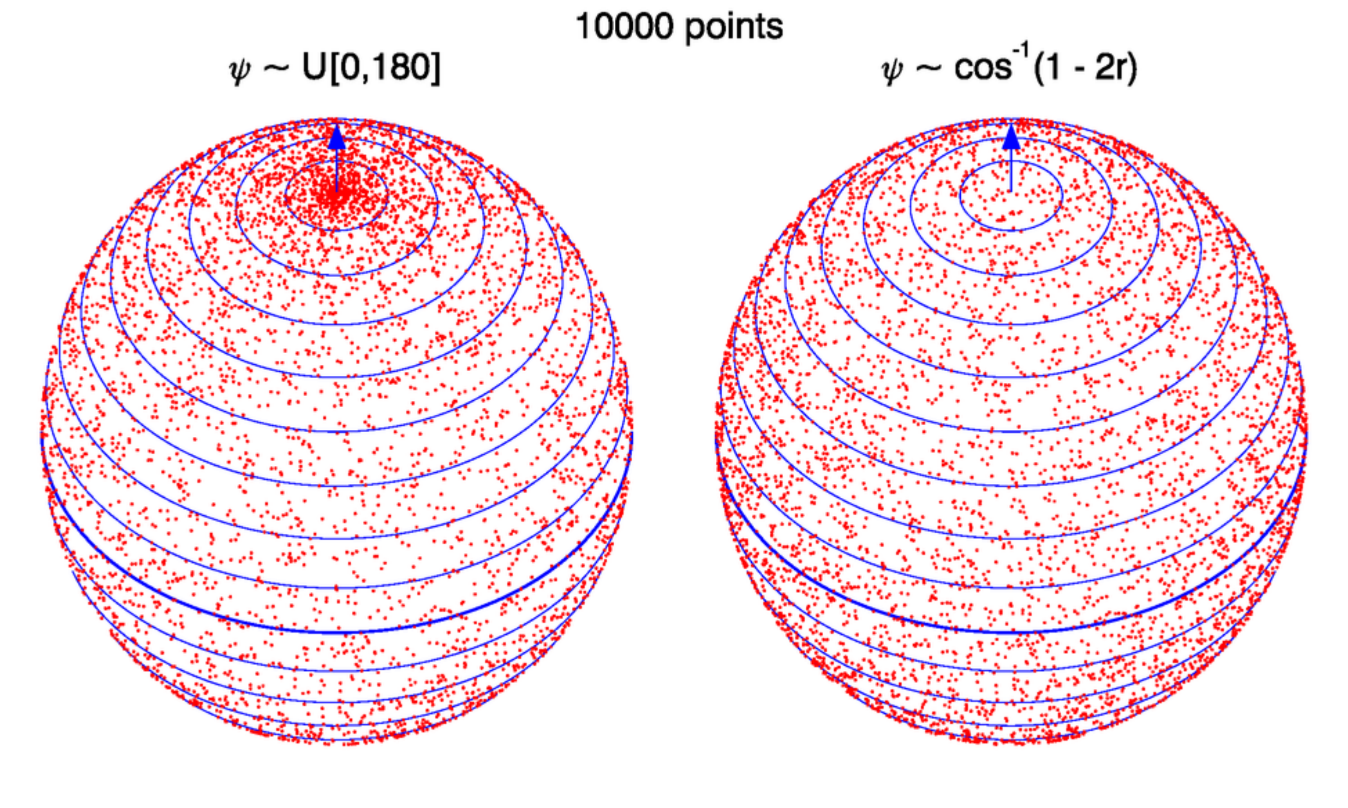
$$\mathfrak{R} = CDF(\psi) = 2\pi \int_0^\psi \tilde{\beta}(\psi')\ \sin\psi'\, d\psi'$$

solve for ψ (usually must solve numerically)

Example: Isotropic Scattering

For isotropic scattering,

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



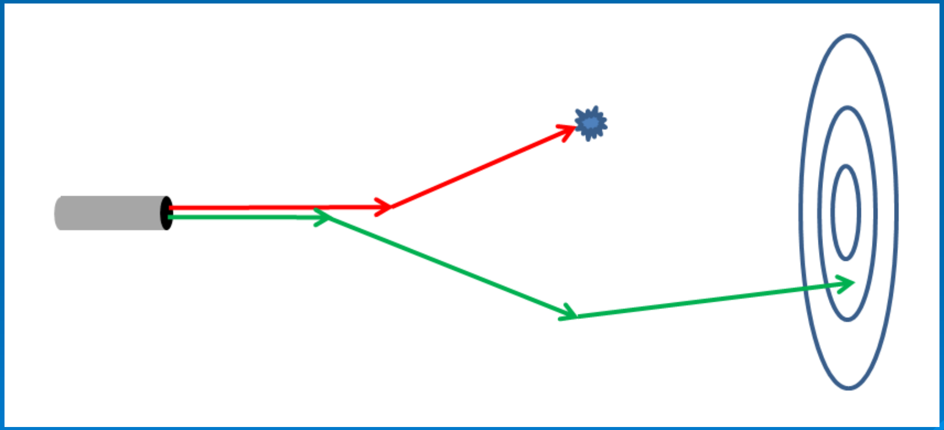
Isotropic means equally likely to scatter into any element of *solid angle*, not equally likely to scatter through any polar scattering angle ψ

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:

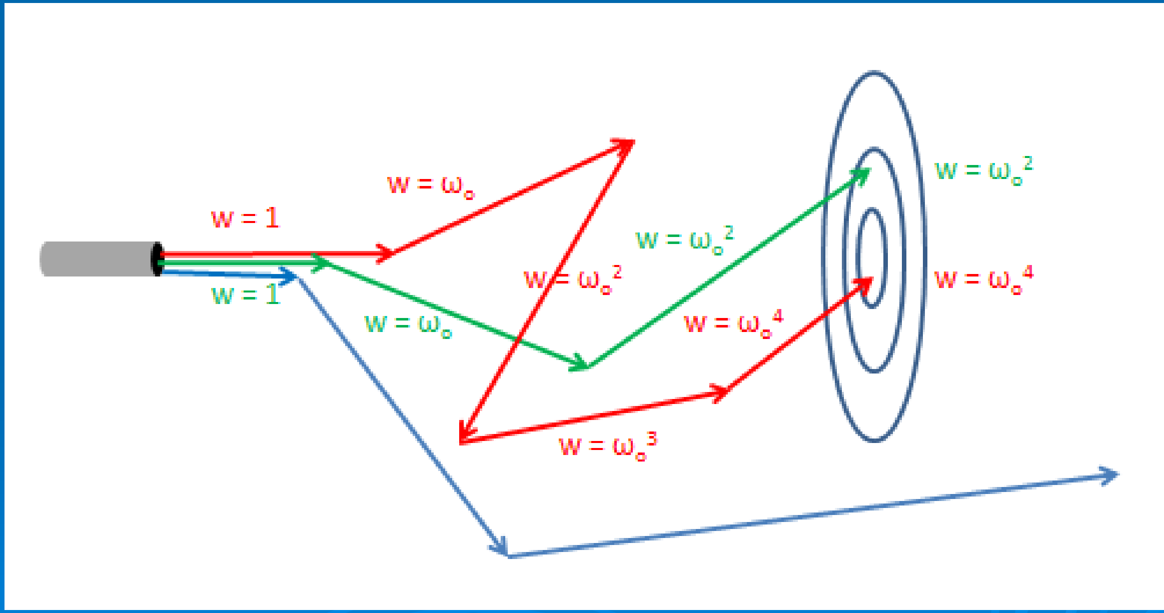
- draws a random number and gets the distance
- draws another random number and compares with ω_o :
  - if $\Re > \omega_o$ the photon is absorbed; start another one
  - if $\Re \leq \omega_o$ the photon is scattered; compute the scattering angles



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

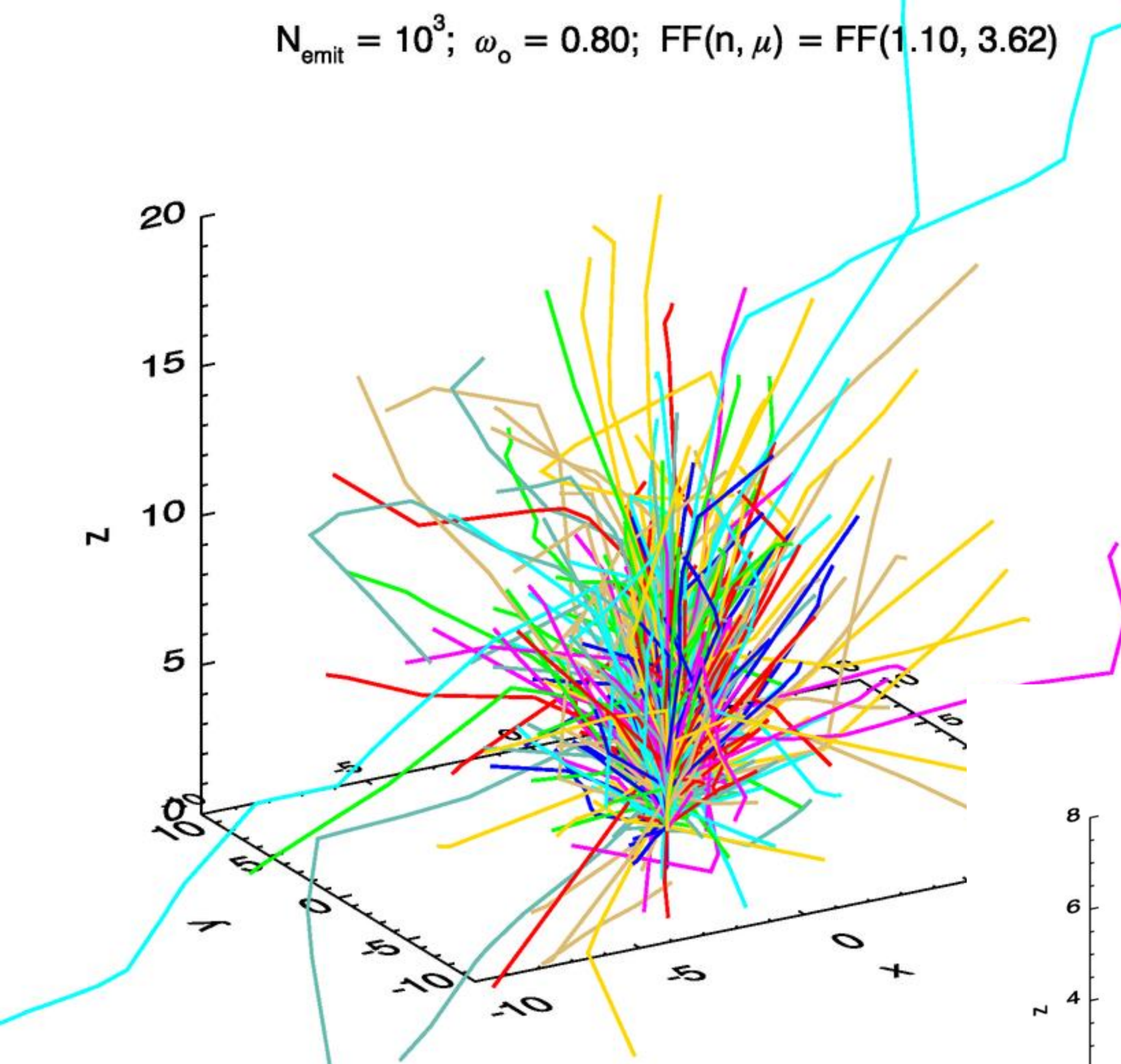
Tracing Photon Packets

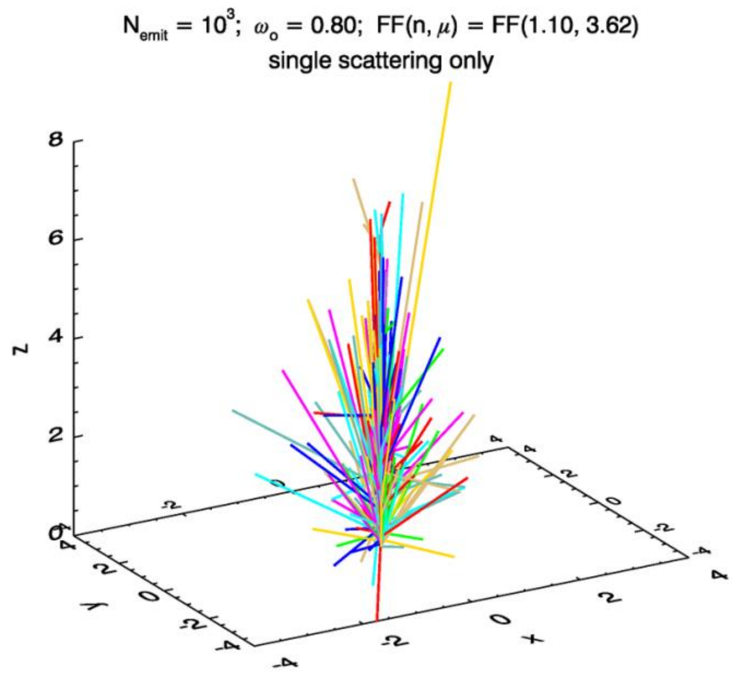
Rather that lose some photons to absorption, consided each “photon” to be a packet of many photons starting with power w = 1 W. At each interaction, multiply the current packet weight w by ω_o to account for loss of some of the original power to absorption. This increases the number of photon packets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



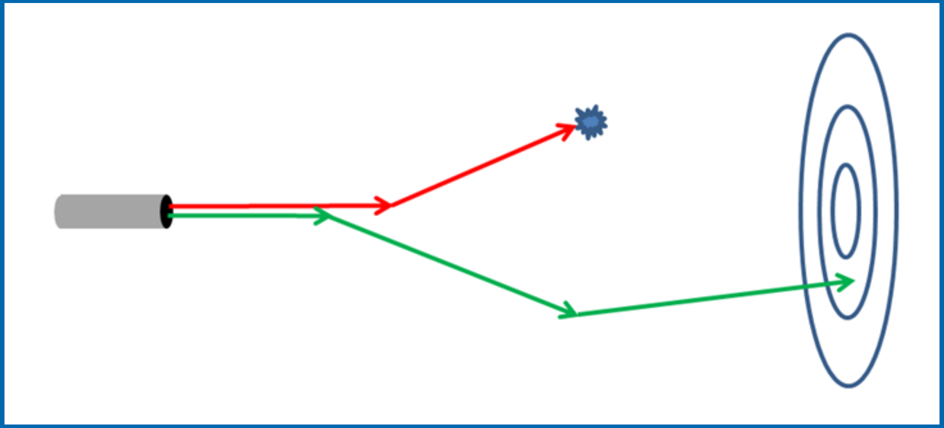
Usually kill the photon packet when w < 10^{-8}, for example, if it hasn't hit the target.

Visualizing Photon Paths

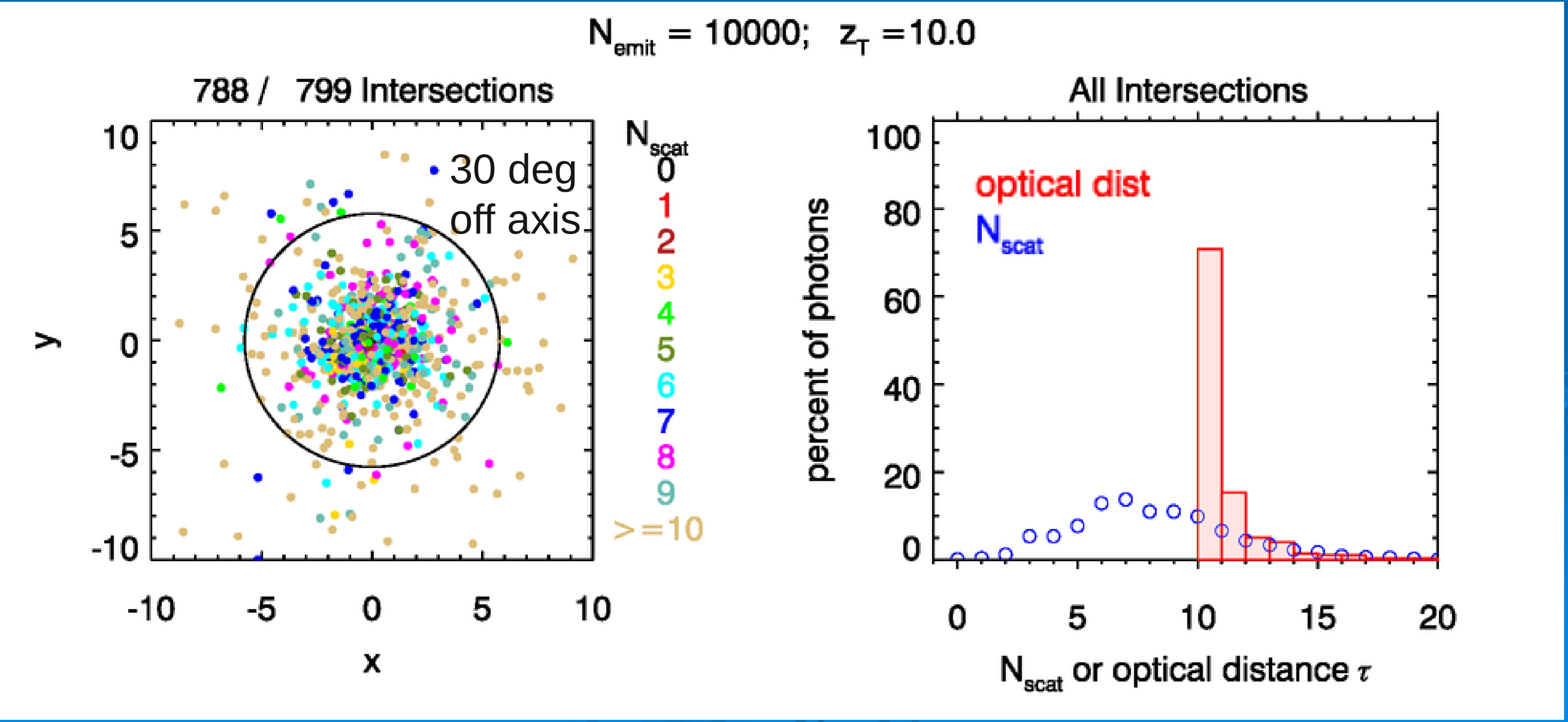




Visualizing Photon Paths

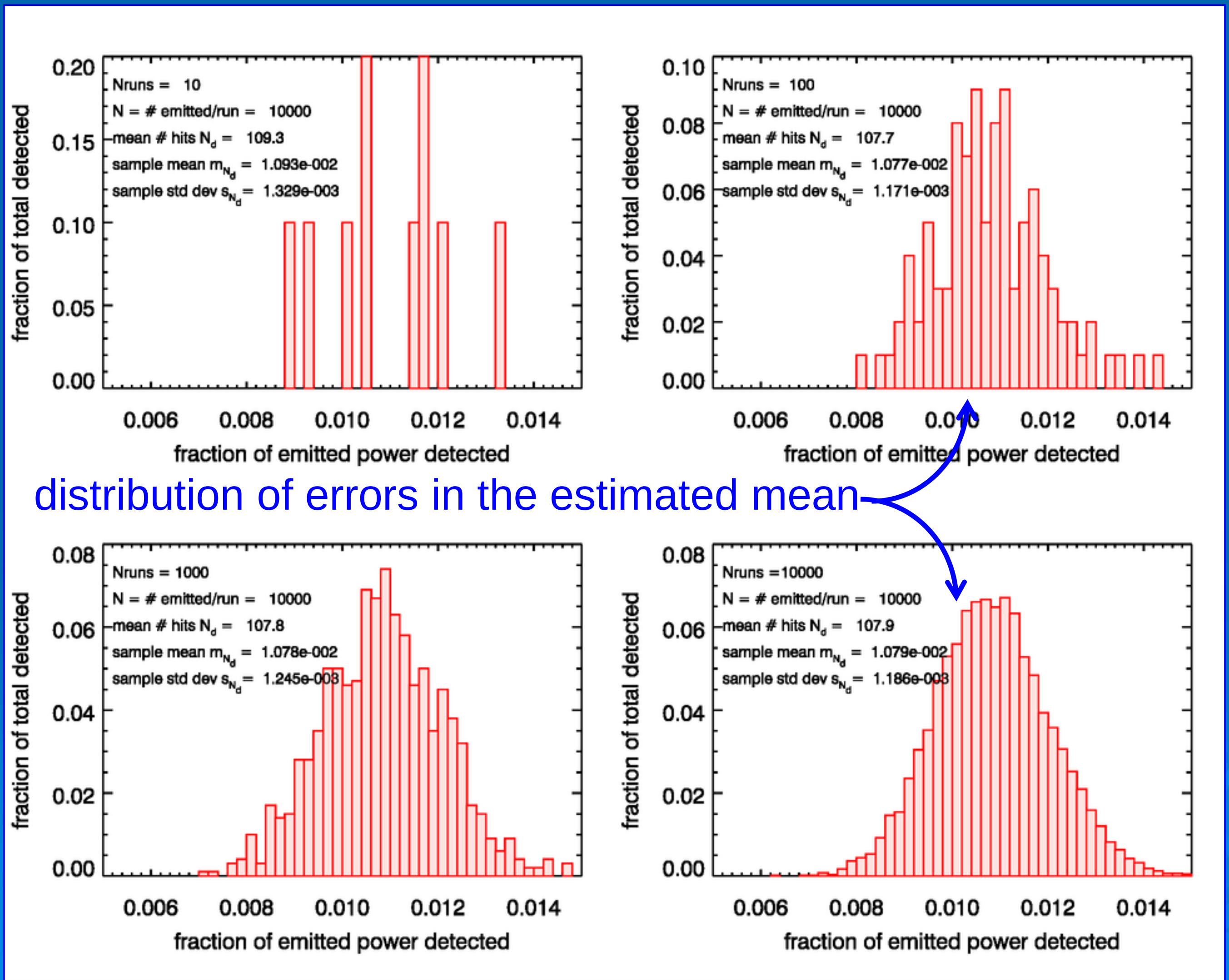


Monte Carlo simulation gives understanding at the photon level, which can't be obtained from radiance (e.g., from HydroLight)



Statistical Noise

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



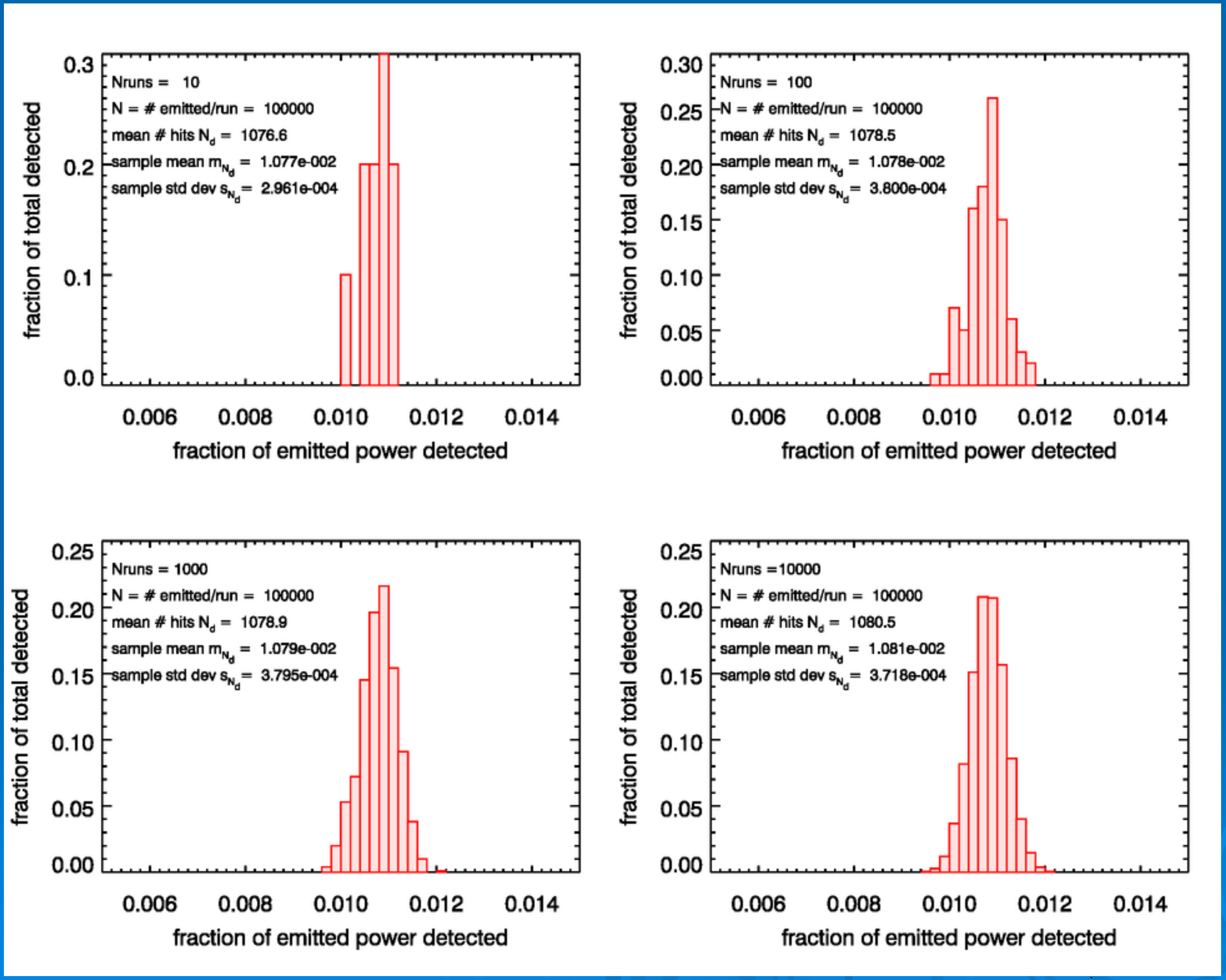
Repeated runs (different sequences of random numbers) with the same number of photons per run.

Note that as more runs are done, the distribution of computed values (errors) 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

You now know enough to do the Monte Carlo lab.

However, before writing your own a MC code to do extensive simulations, read about other ways to get more photons onto the target without more computer time (see the Web Book Monte Carlo chapter). 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

Variance Reduction: Backward Monte Carlo

Emit photos from the *detector* with weight $w = 1$ and the angular distribution of the detector, and trace to the source. Then weight the "detected" photons at the source to apply the correct source weight. Only photons paths conecting the true source and the true detector are then traced.

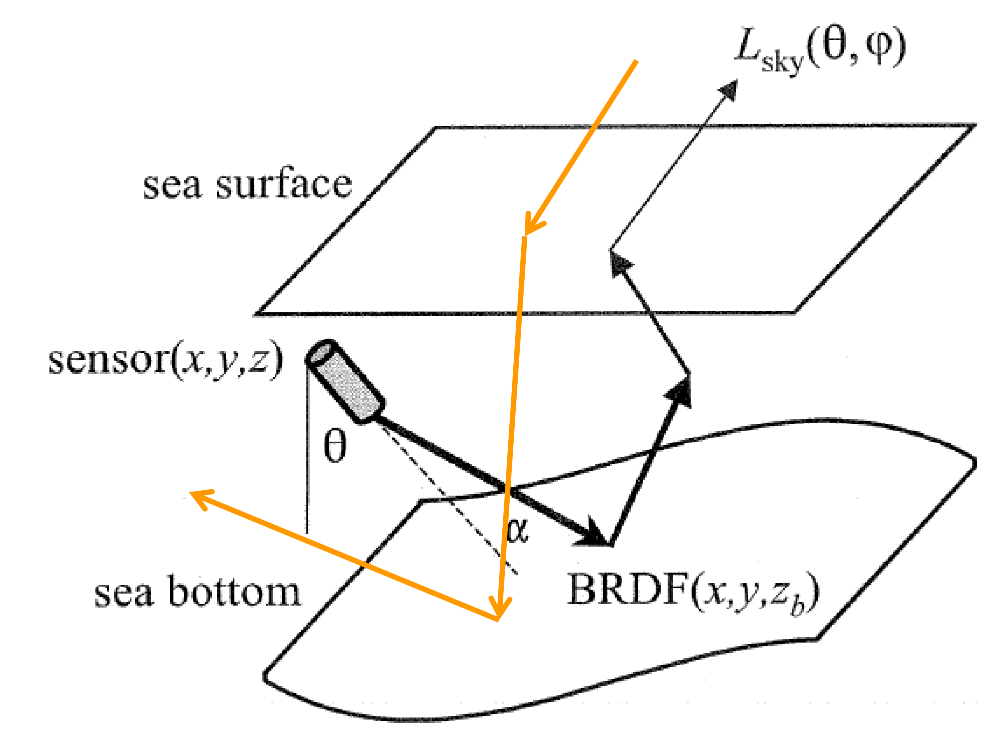


Fig. 1. Illustration of backward Monte Carlo ray tracing. The photon packets are traced from the sensor to the sky, rather than from the sky to the sensor.

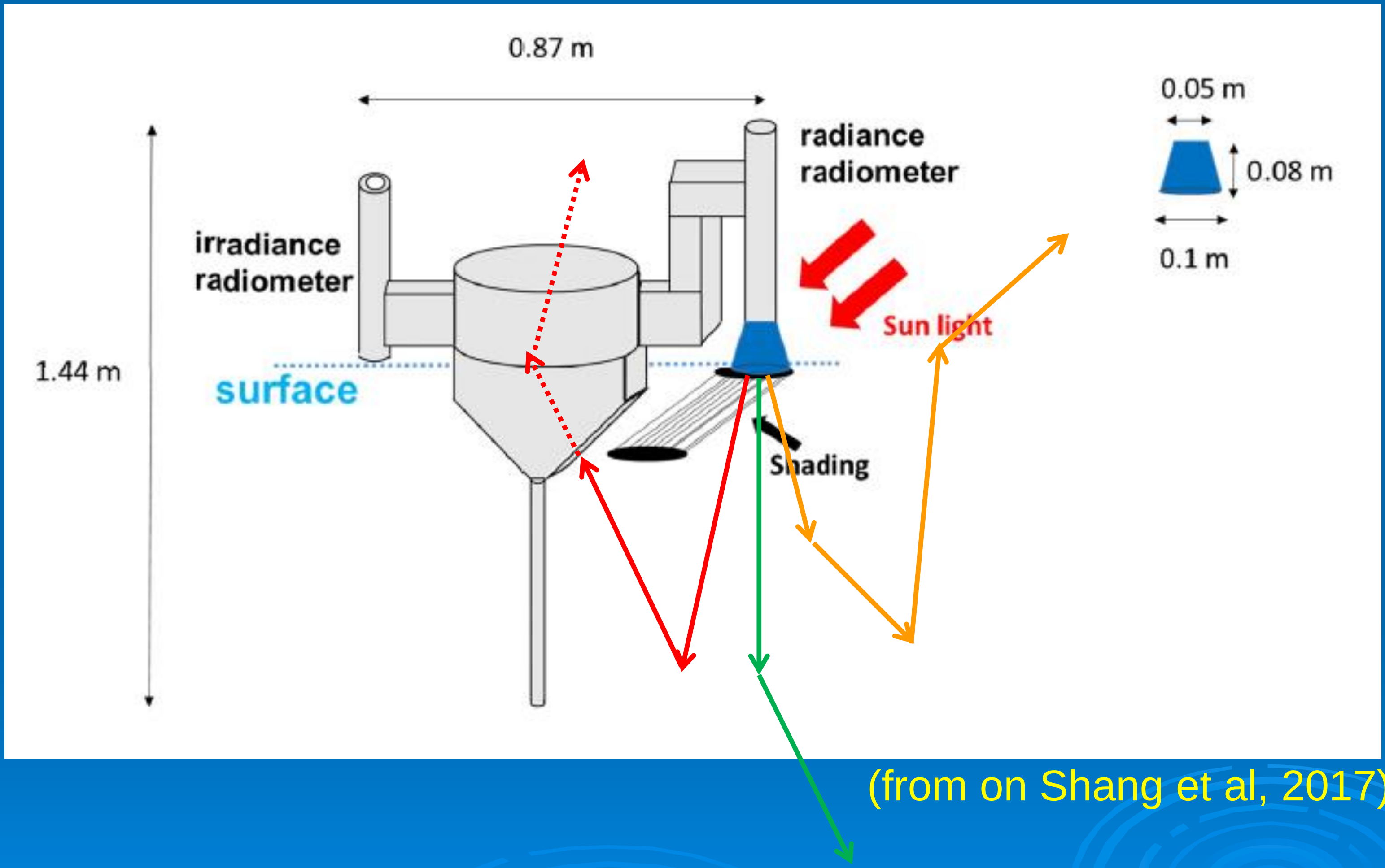
Each photon reaching the sky is weighted by the sky radiance in the photon direction.

BMC is most useful for an extended source (like the sky) and a or small (even point) detector (such as a radiance sensor)

Mobley and Sundman, L&O, 2003

Example: Backward Monte Carlo

Developing a shadow correction for the Lee method.

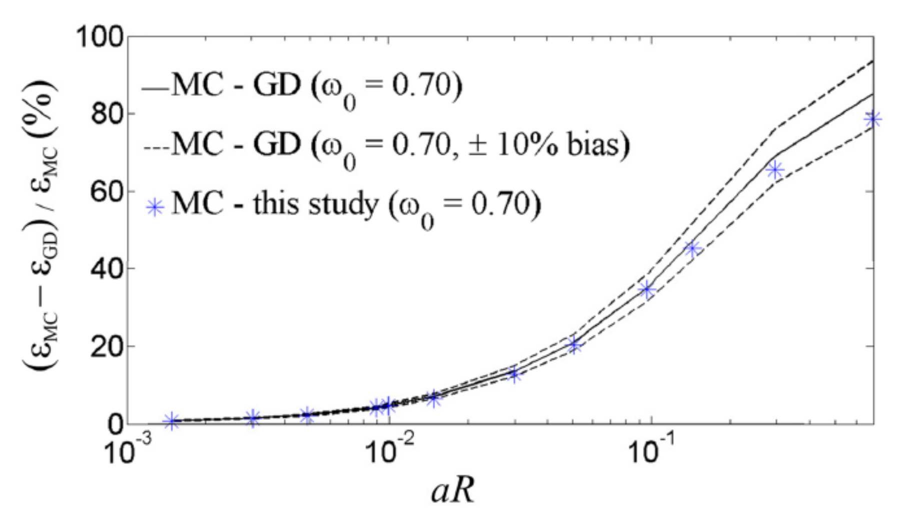


(from on Shang et al, 2017)

Example: Backward Monte Carlo

First they compared their BMC code with HydroLight, for no instrument present (1 D geometry); agree to within 1%

Then they compared their BMC results with Gordon and Ding (1992) for the geometry of GD92 (cylindrical instrument, didn't study backscatter effects)



Then they did simulations on a super computer for their instrument geometry and developed a shading correction for their specific instrument as a funtion of *a*, b_b, sun zenith angle.

Monte Carlo Strengths

- **They are conceptually simple.** The methods are based on a straightforward mimicry of nature.

- **They are very general.** Monte Carlo simulations can be used to solve problems for any geometry (e.g., 3D volumes with imbedded objects), incident lighting, scattering phase functions, etc. It is relatively easy to include polarization and time dependence.

- **They are instructive.** The solution algorithms highlight the fundamental processes of absorption and scattering, and they make clear the connections between the photon-level and the energy-level formulations of radiative transfer theory.

- **They are simple to program.** The resulting computer code can be very simple, and the tracing of photons is well suited to parallel processing.

Monte Carlo Weaknesses

- **They can be computationally very inefficient.** Monte Carlo simulation is a “brute force” technique. If care is not taken, much of the computational time can be expended tracing photons that never contribute to the solution, e.g., because they never intercept a simulated detector.

- **They are not well suited for some types of problems.** For example, computations of radiance at large optical depths can require unacceptably large amounts of computer time because the number of solar photons penetrating the ocean decreases exponentially with the optical depth. Likewise, the simulation of a point source and a point (or very small) detector is difficult.

- **They provide no insight into the underlying mathematical structure of radiative transfer theory.** The simulations simply accumulate the results of tracing large numbers of photons, each of which is independent of the others.

Following Marco Polo Along the Silk Road in Western China

If you want to see more trip photos:

https://ann-and-curt.smugmug.com/

There is a video of my Jerlov talk on my public Dropbox at

https://dl.dropboxusercontent.com/u/20040892/Jerlov_Mobley_highres.mp4

(the good part ;-) starts at ~10 min)