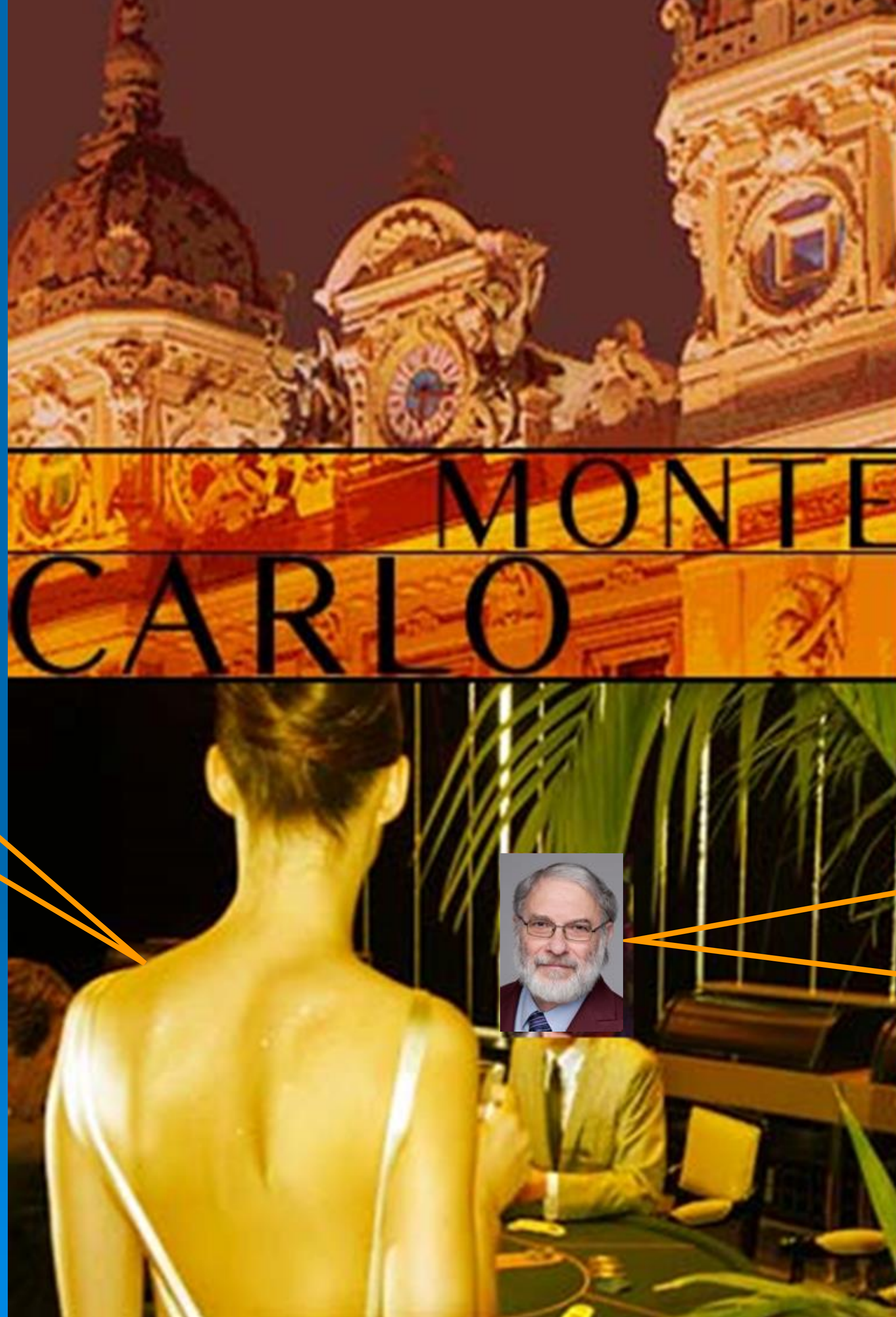
2021 Summer Course

on Optical Oceanography and Ocean Color Remote Sensing

Curtis Mobley

Monte Carlo Simulation

Schiller Coastal Studies Center


MONTE CARLO
Hey Curt, wanna go to my place and, uh, talk about radiative transfer theory?
Not tonight. I'm still debugging my new 3D Monte Carlo code

Example 3D Radiative Transfer Problems

(which can't be solved by the 1D HydroLight)

sloping or patchy bottoms

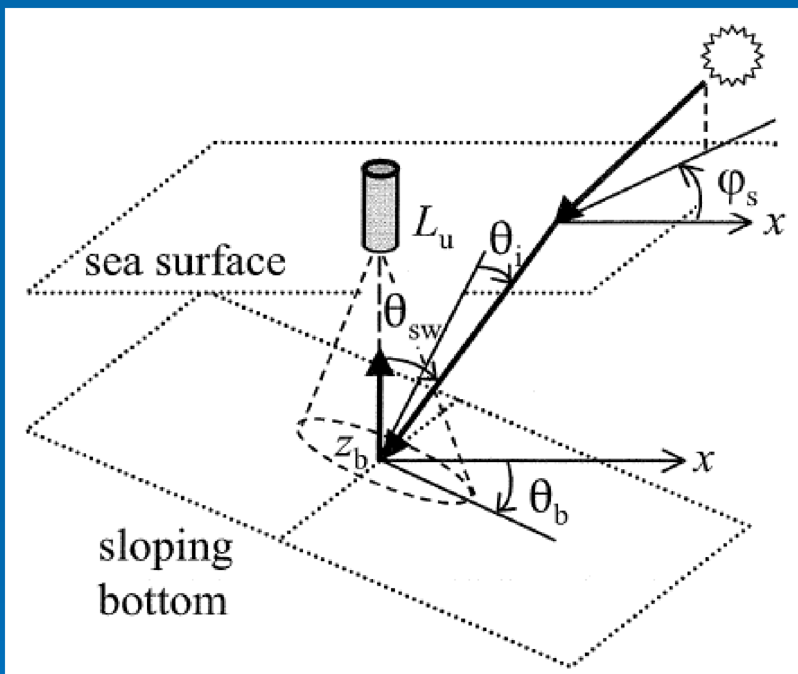
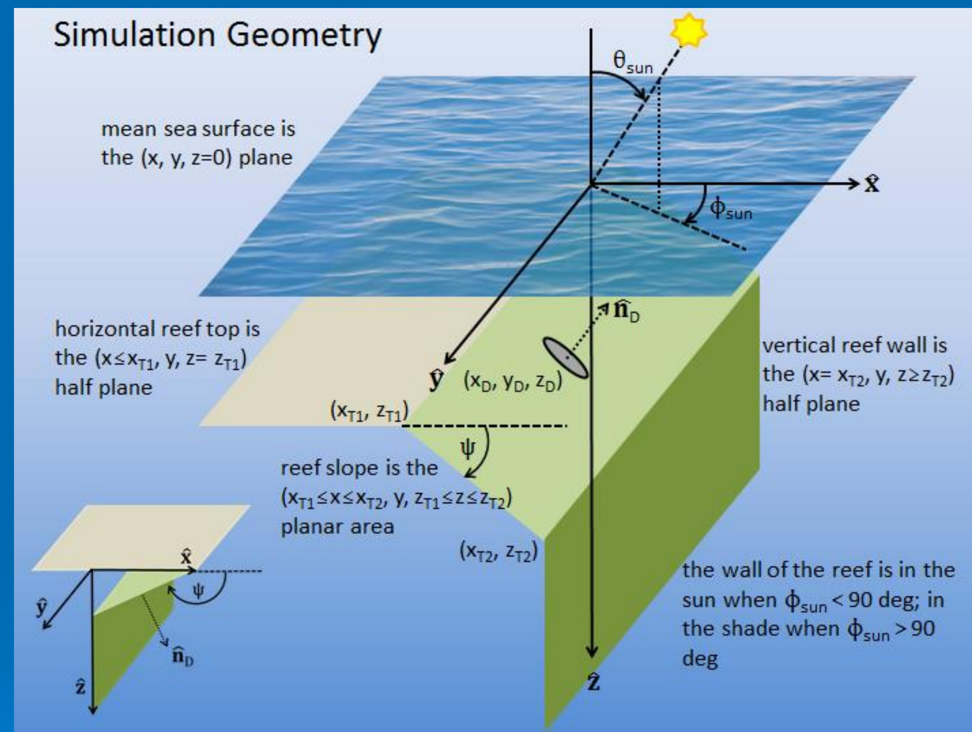


Fig. 5. Geometry for simulation of a sloping bottom.



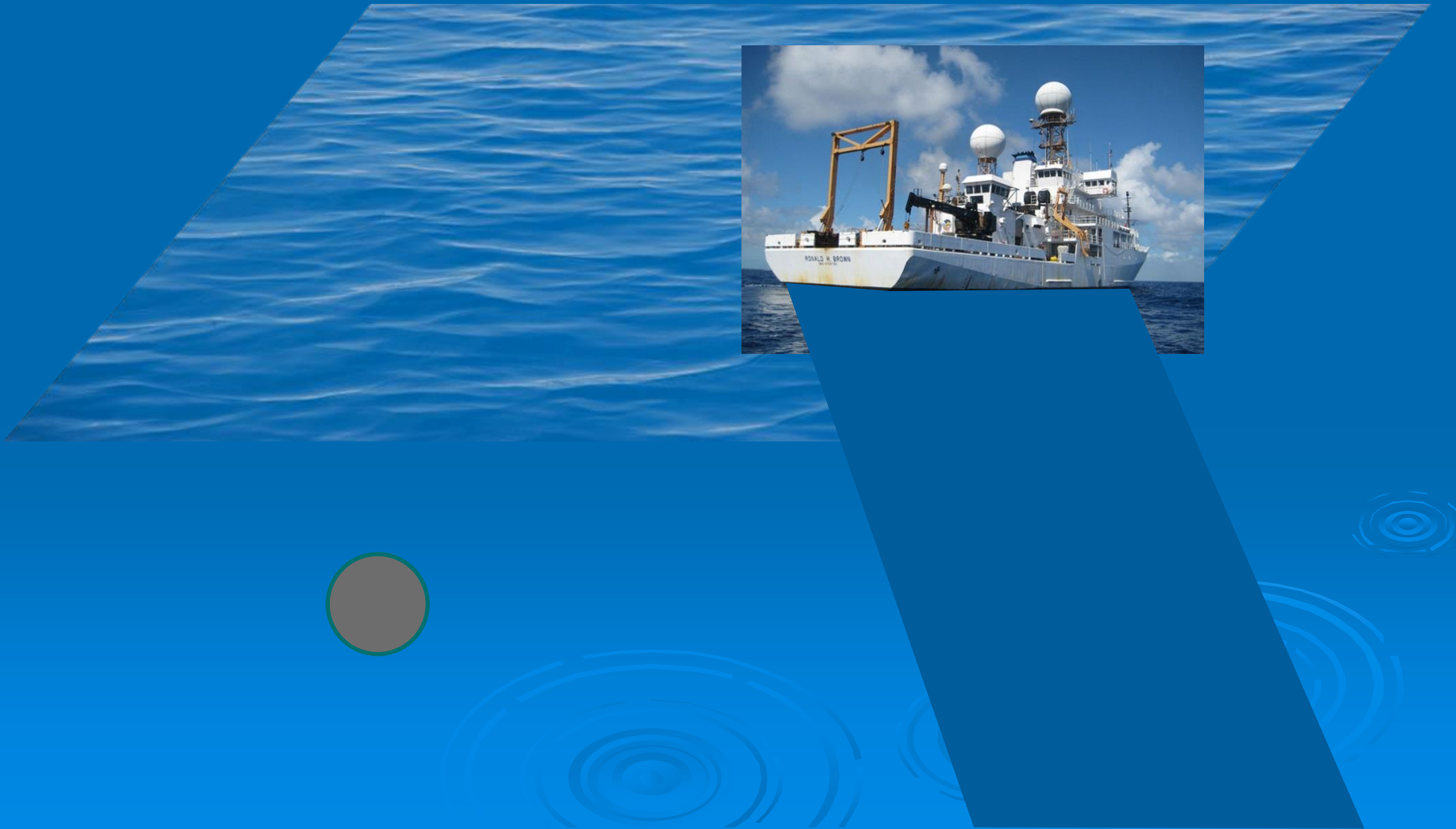
Mobley and Sundman, 2002

Mobley, 2018; Lesser et al., 2021

Example 3D Radiative Transfer Problems

(which can't be solved by the 1D HydroLight)

objects in the water, or instrument and ship shadow effects



Monte Carlo Techniques

Monte Carlo techniques refer to the use of **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 light ray (often called a "photon packet") 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 ray 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 ray 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 light rays
- Build up a solution to the RTE one ray 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:

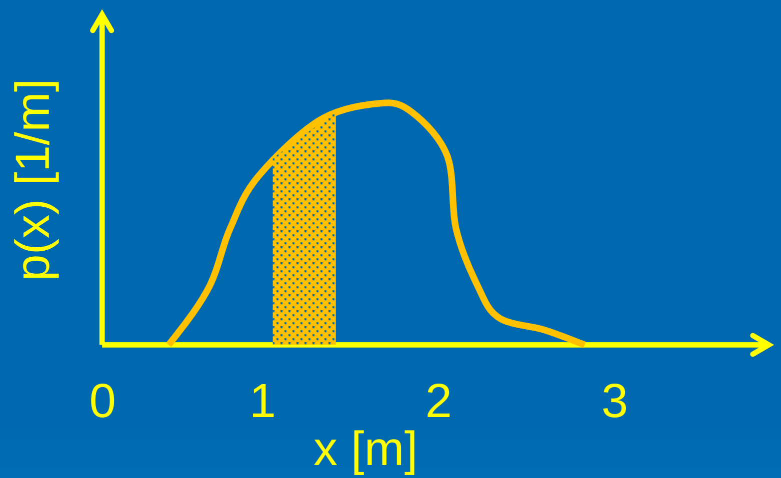
- Probability distribution functions (PDFs) and cumulative distribution functions (CDFs)
- Random number generators
- Using CDFs to randomly select distances, scattering angles, etc.
- Monte Carlo noise

There are web book pages on Monte Carlo techniques starting at https://www.oceanopticsbook.info/view/monte-carlo-simulation/introduction and see Chapter 12 of the OOB.

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



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

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

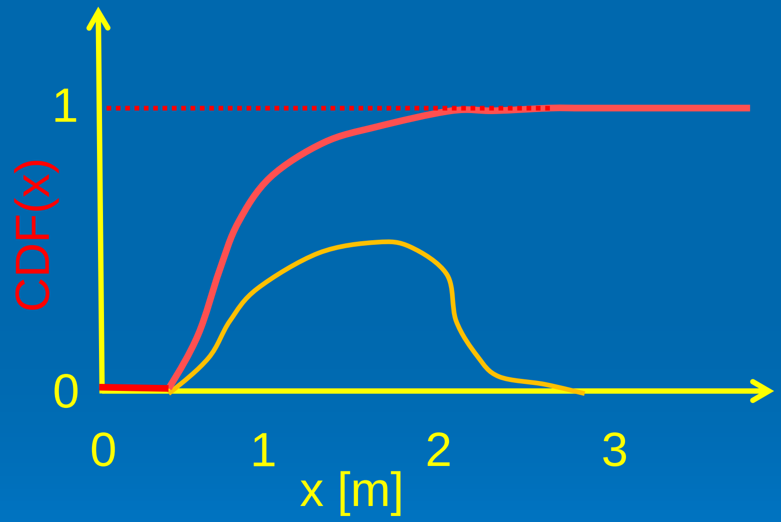
Normalization: $\int_{0}^{\infty} p(x)dx = 1$ that is, the prob is one that a person will have some height between 0 and ∞

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,

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



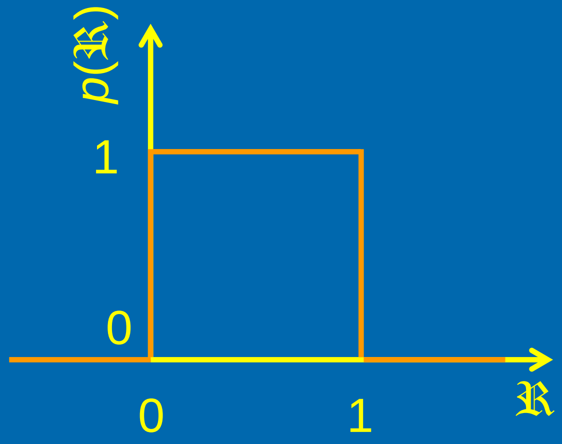
Probability that a person selected at random from all humans is between 1.0 and 1.3 m tall is

CDF(1.3) – CDF(1.0)

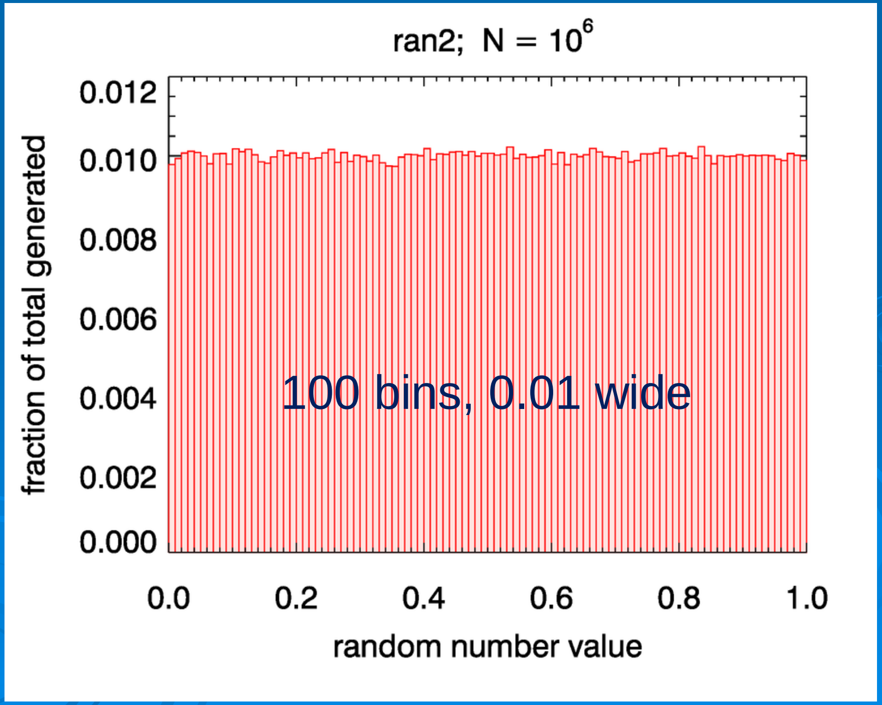
Note that CDF(∞) = 1. That is, the probability is one that a person will have some height less than ∞

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



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

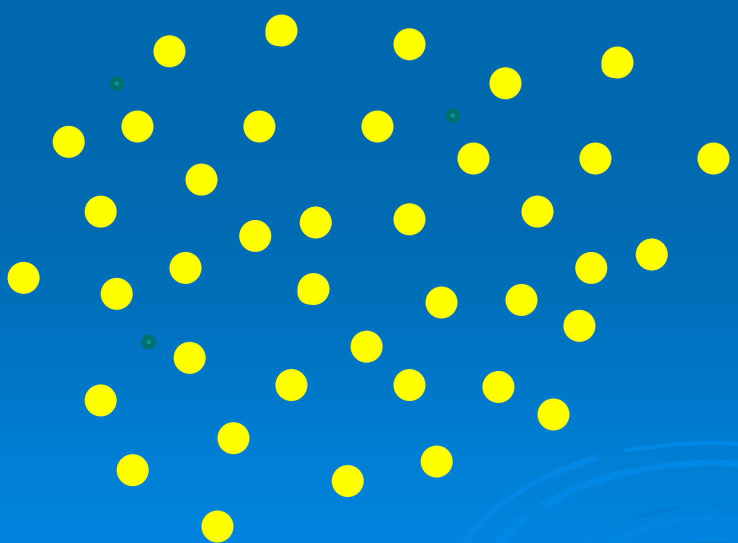


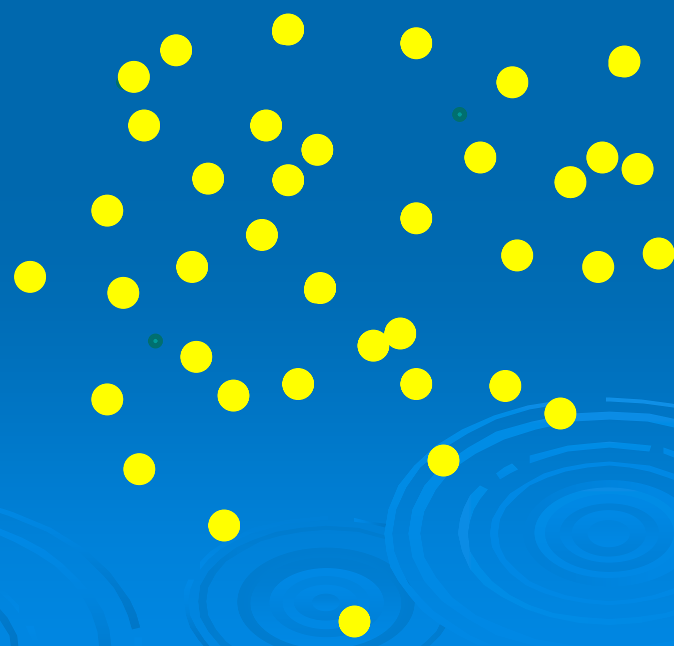
Which Sequence of Numbers is Probably NOT Random?

452878231035972340523765091082725314057609439765120372140674….

142983211983496178801321756333339673012007362876201847772190….

Which Arrangement of Dots is Probably NOT Random?



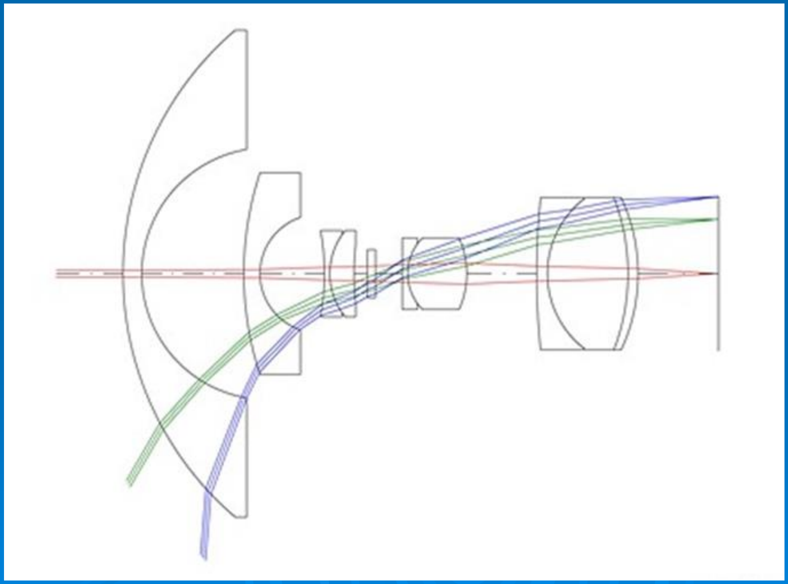


Light Rays

A light ray is a hypothetical construct that indicates the direction of the propagation of light at any point in space.

This idea is based on the every-day observation that light travels in straight lines (in a homogeneous medium).

Geometric optics is an approximate model of light propagation that holds when the scattering particles (or lenses, mirrors, etc.) are much, much larger than the wavelength, so that diffraction and interference can be ignored. Light rays are the basic “objects” of geometrical optics. Geometric optics and very sophisticated ray tracing programs are used to design camera lenses.



Random Determination of Ray Path Lengths

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

$$L(r) = L(0)e^{-cr} = L(0)e^{-\tau}$$

The exponential decay of radiance can be explained if the individual rays have a probability of being absorbed or scattered out of the beam between τ and τ+dτ that is

$$p(\tau)d\tau = e^{-\tau}d\tau \implies p(\tau) = e^{-\tau}$$

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

$$p(\mathfrak{R})d\mathfrak{R} = U(\mathfrak{R})d\mathfrak{R} = p(\tau)d\tau$$

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

$$\mathfrak{R} = CDF(\tau) = 1 - e^{-\tau}$$

Random Determination of Ray Path Lengths

Solving

$$\mathfrak{R} = 1 - e^{-\tau} \quad \text{for} \quad \tau$$

gives

$$\tau = -\ln(1 - \mathfrak{R}) \quad \text{or} \quad \tau = -\ln(\mathfrak{R}) \quad \text{since} \quad \mathfrak{R} \sim U[0,1]$$

Draw a U[0,1] random number $\mathfrak{R}$, and then the corresponding ray path length is

$$\tau = -\ln(\mathfrak{R})$$

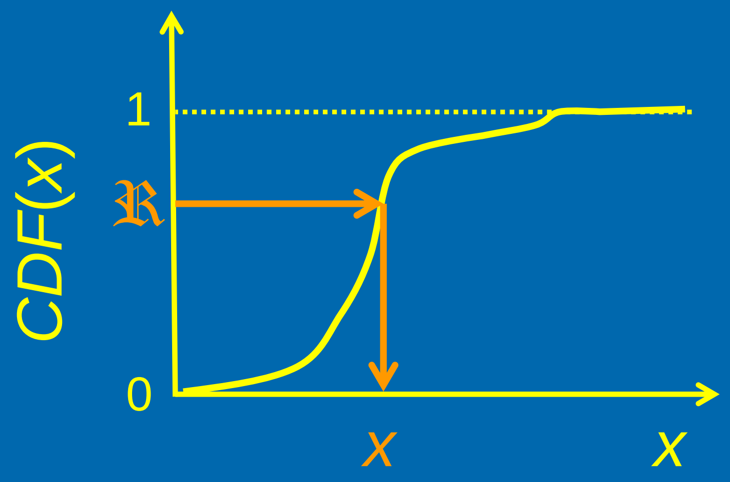
or

$$r = -\frac{1}{c}\ln(\mathfrak{R})$$

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

Mean Free Path

The pdf for the distance a ray travels is $p(\tau) = \exp(-\tau)$.
What is the average distance $<\tau>$ that a ray 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 $\tau = cr$,

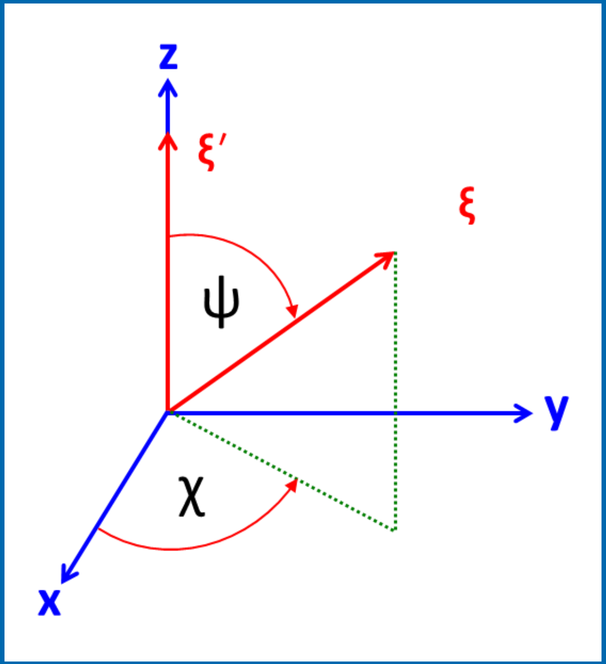
$<r> = 1/c$ (meters)

What is the variance about the mean distance traveled?

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

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 $0 \le \chi < 2\pi$ 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)

Example: Isotropic Scattering

$$\Re = CDF(\psi) = \int_0^{\psi} PDF(\psi')\, d\psi'$$

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

$$\text{for } \tilde{\beta}(\psi') = \frac{1}{4\pi} \text{ we get}$$

$$\Re = \frac{1}{2} \int_0^{\psi} \sin\psi'\, d\psi'$$

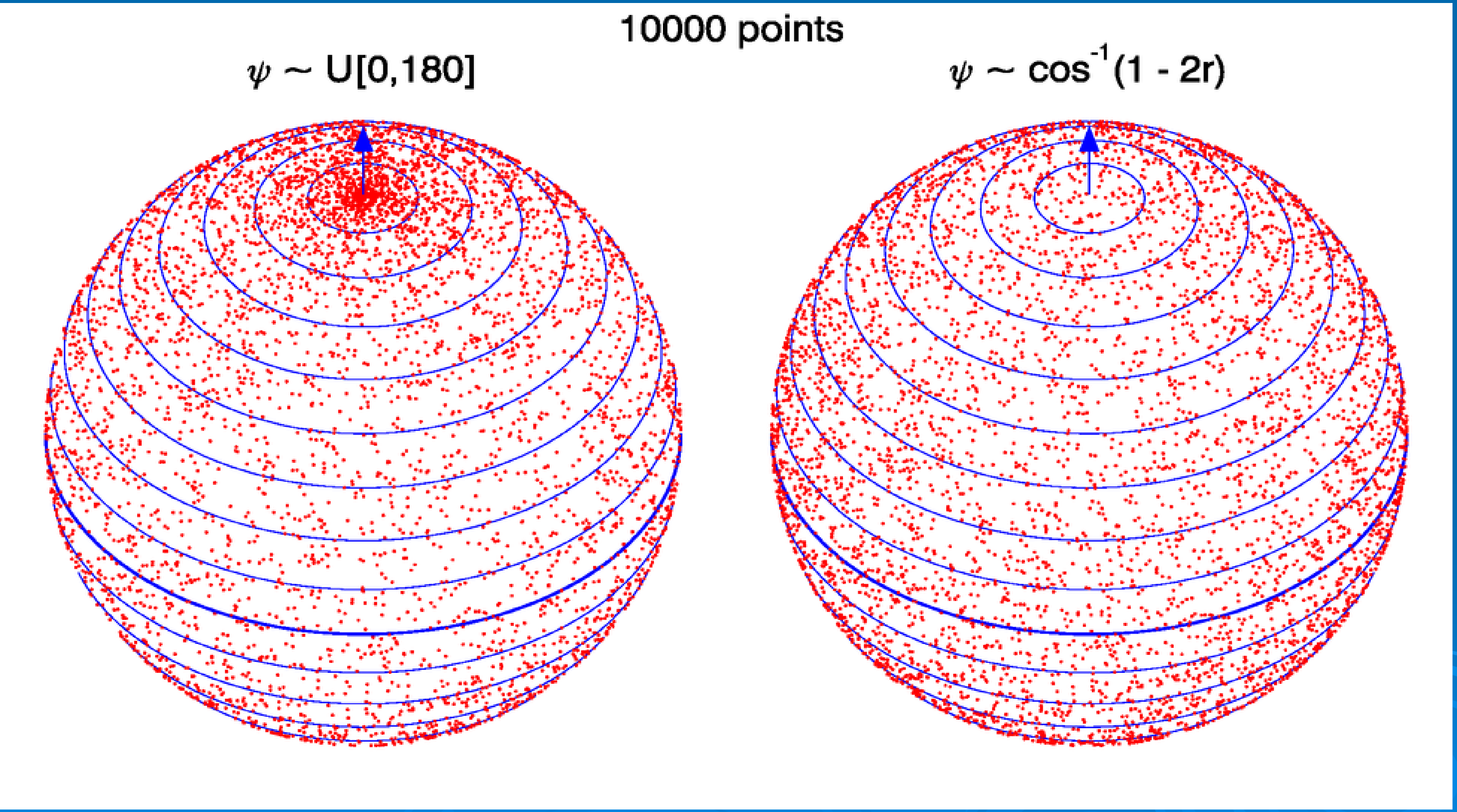
$$= \frac{1}{2}(1 - \cos\psi)$$

$$\psi = \cos^{-1}(1 - 2\Re)$$

Example: Isotropic Scattering

For isotropic scattering,

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



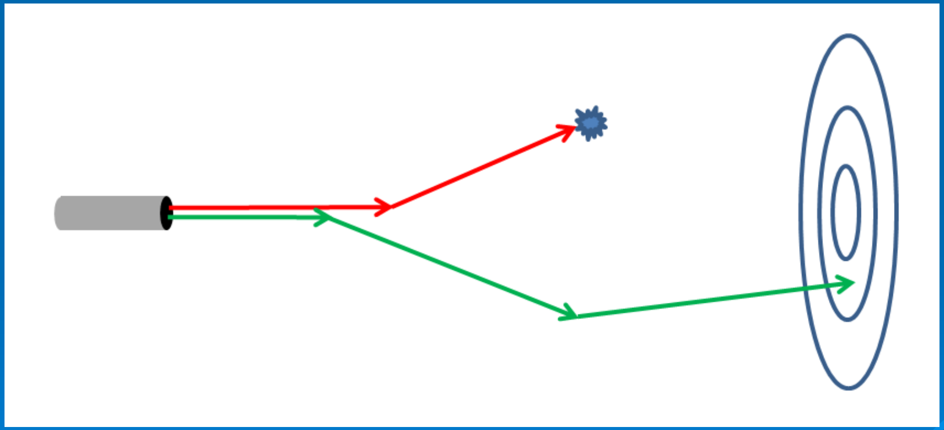
Isotropic means equally likely to scatter into any element of *solid angle*, not equally likely to scatter through any polar scattering angle ψ

Tracing Rays

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

What nature does:

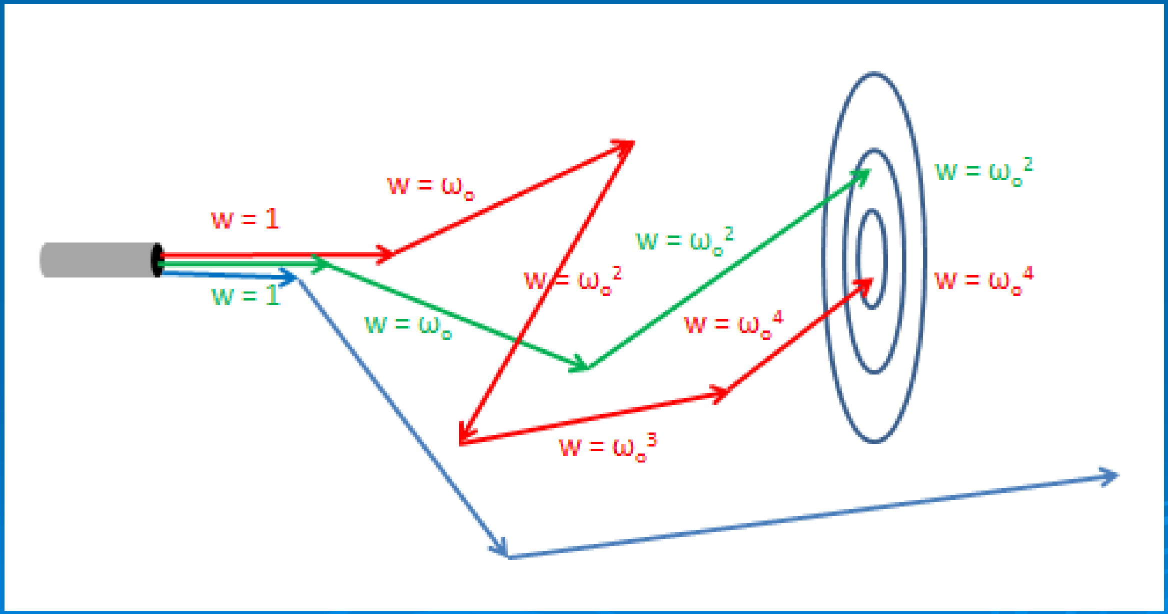
- draws a random number and gets the distance
- draws another random number and compares with ω_o :
    - if $\Re > \omega_o$ the ray (photon) is absorbed; start another one
    - if $\Re \leq \omega_o$ the ray (photon) is scattered; compute the scattering angles



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

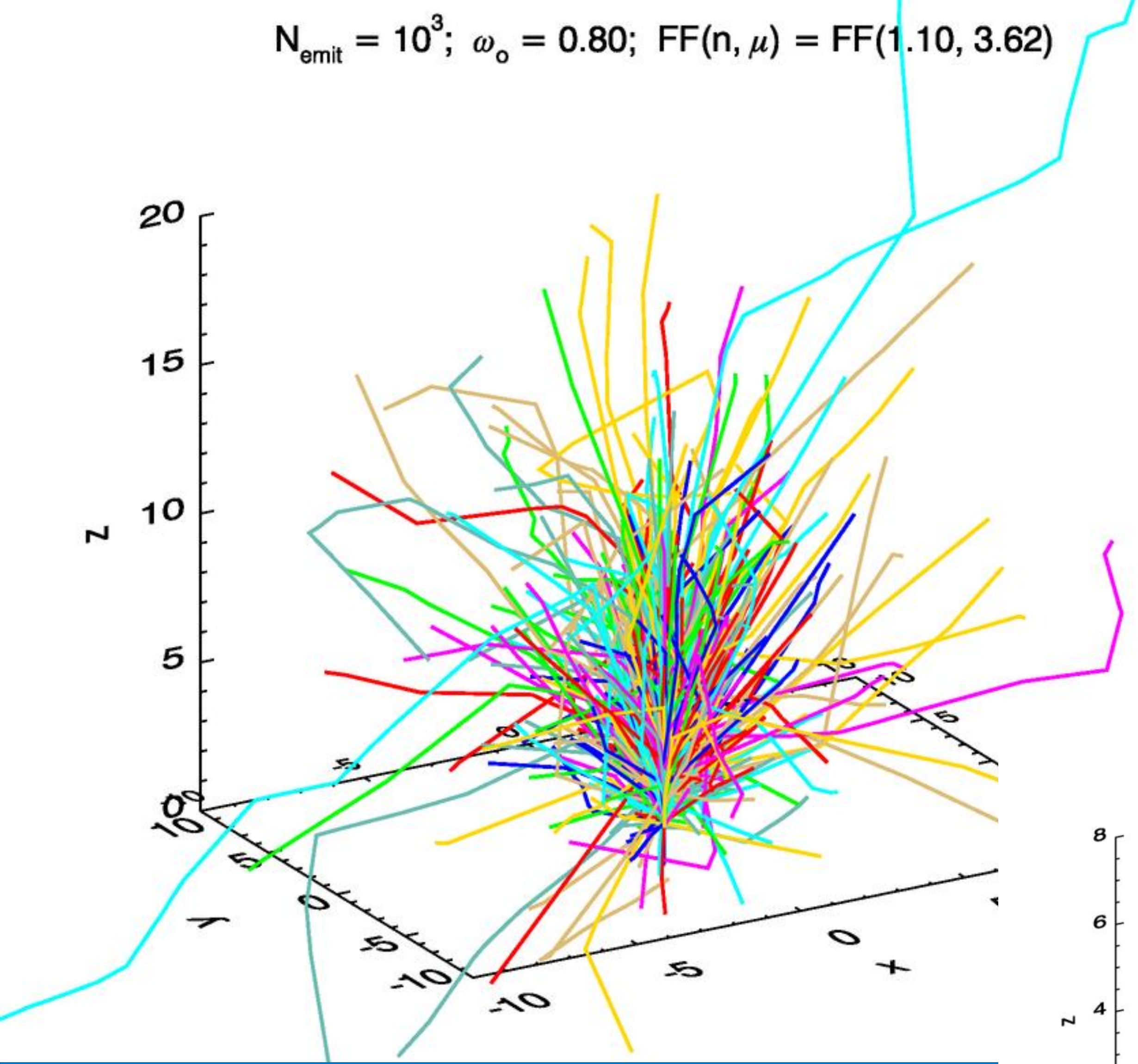
Tracing Ray Bundles

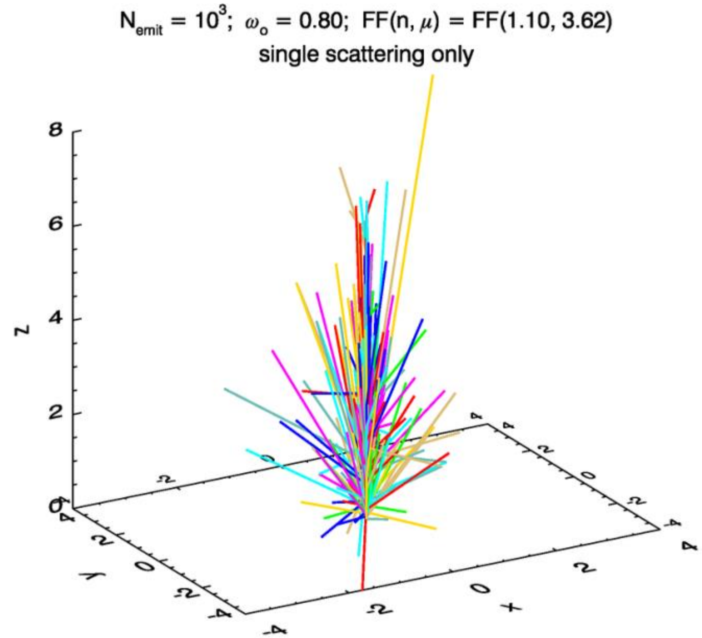
Rather that lose some rays to absorption, consider each ray to be a bundle of many parallel rays starting with power w = 1 Watt. At each interaction, multiply the current weight w by ω_o to account for loss of some of the original power to absorption. This increases the number of rays that contribute to the answer (although some may still miss the target).



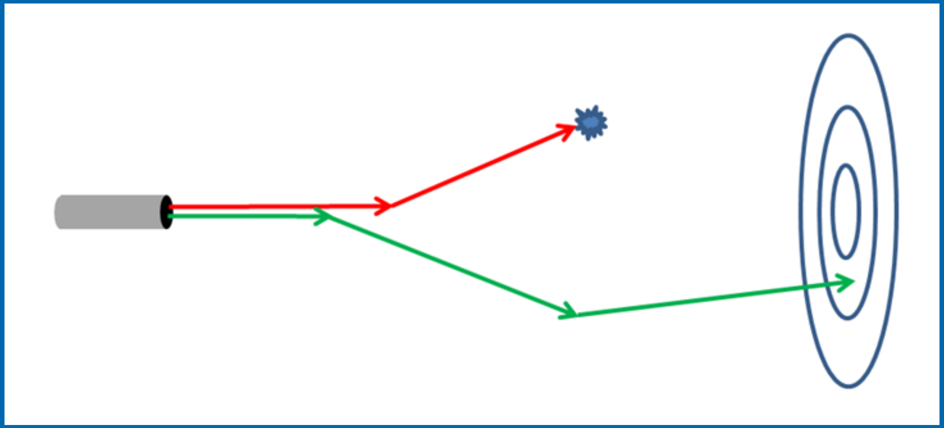
Usually kill the ray when w < 10^{-8}, for example, if it hasn't hit the target.

Visualizing Ray Paths

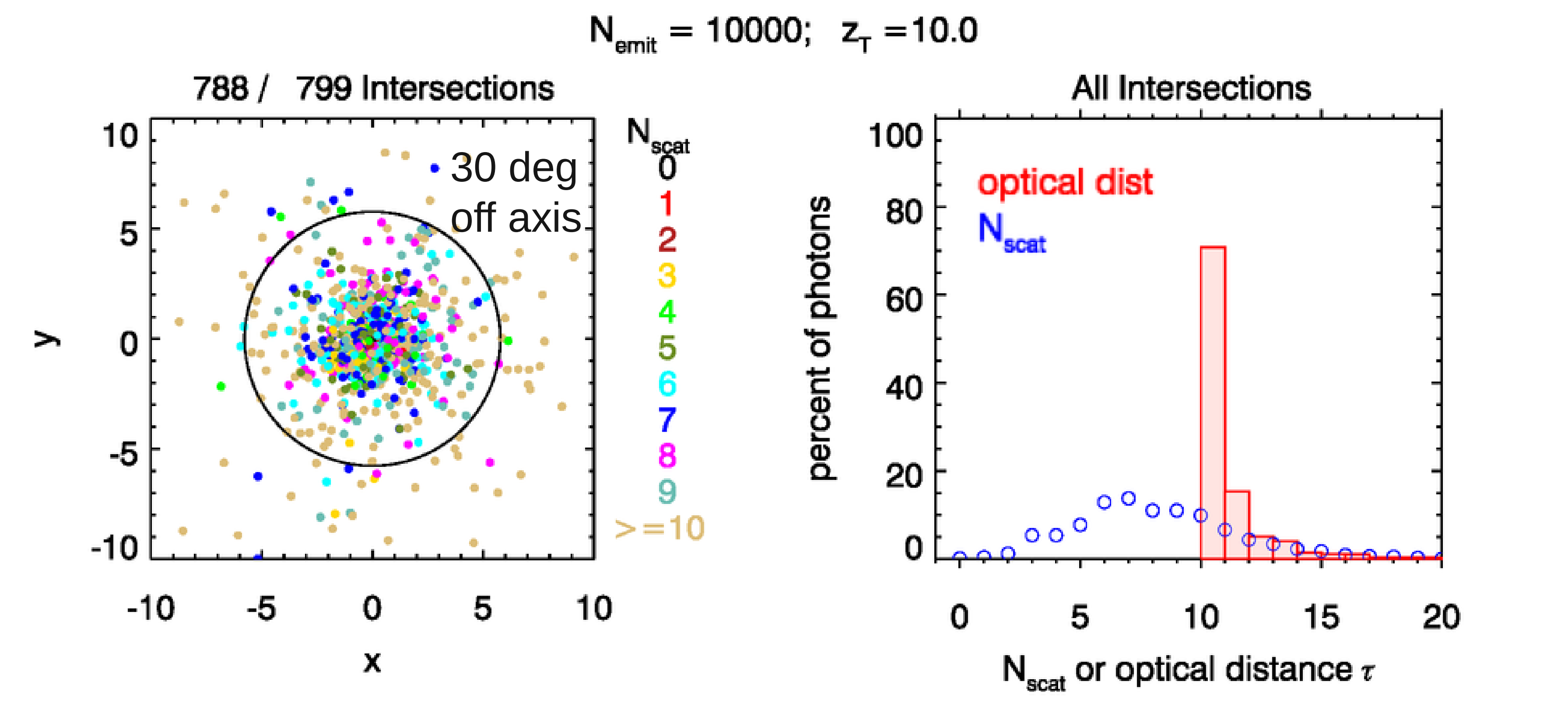




Visualizing Ray Paths

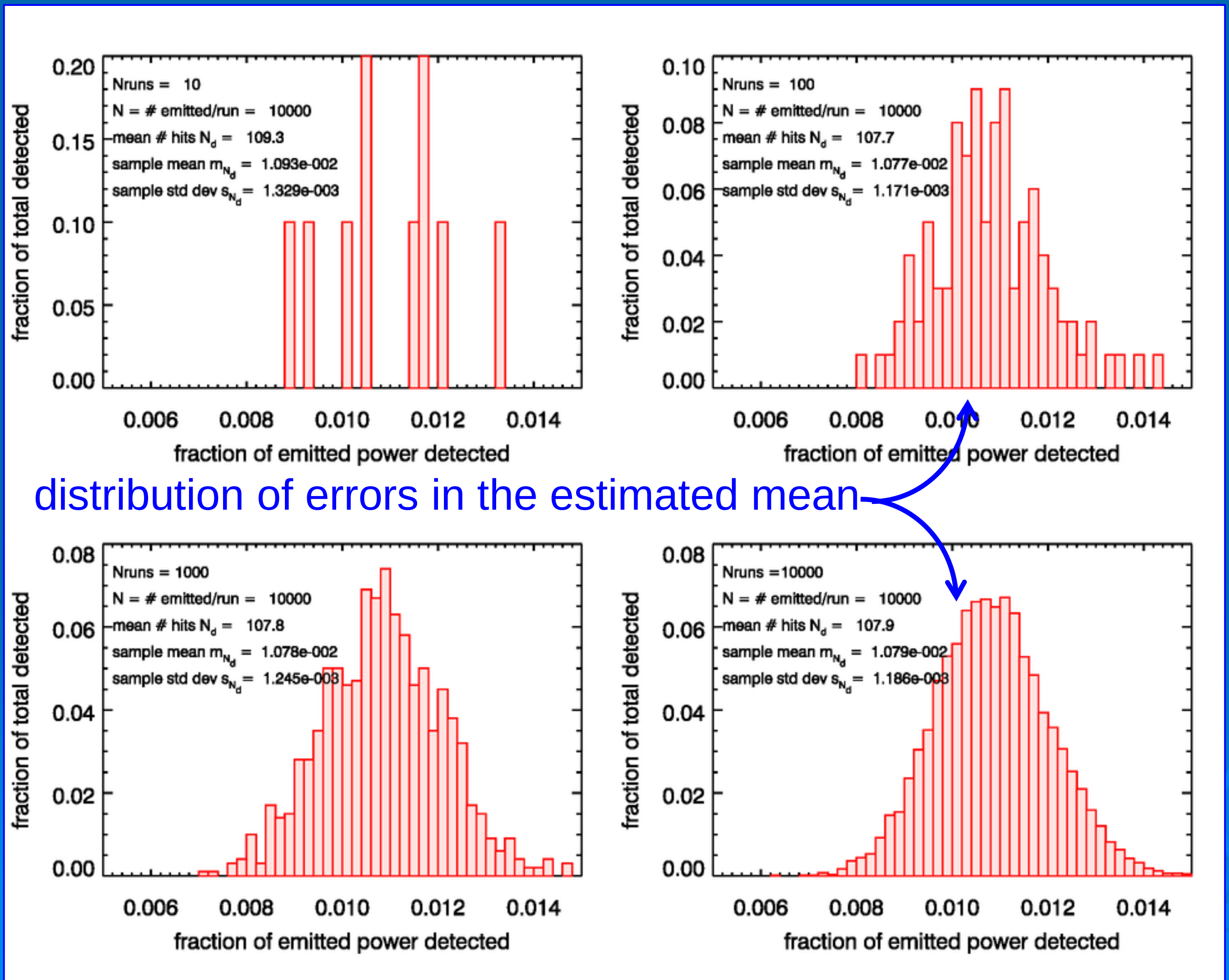


Monte Carlo simulation gives understanding at the individual ray level, which can't be obtained from radiance (e.g., from HydroLight)



Statistical Noise

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



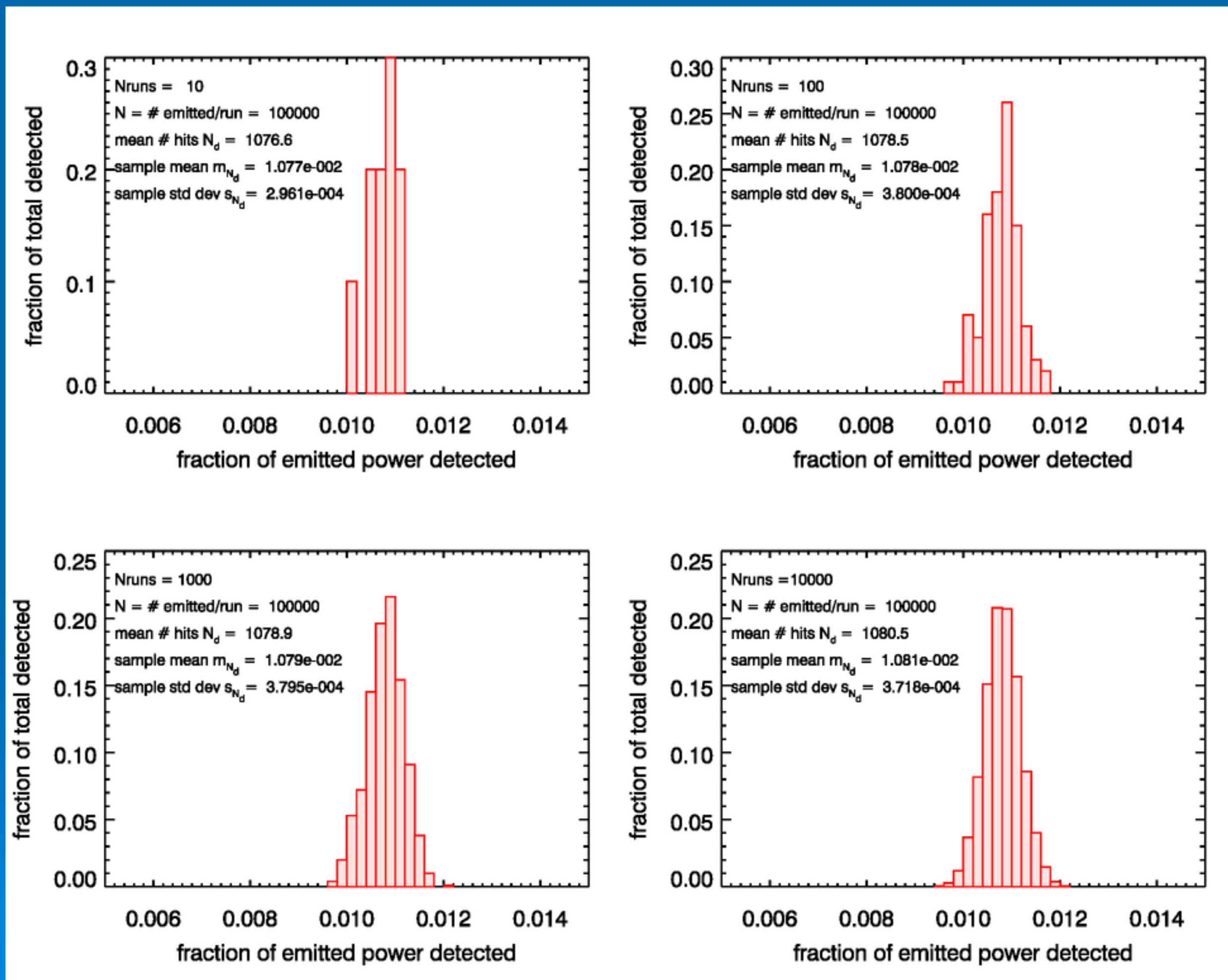
Repeated runs (different sequences of random numbers) with the same number of rays per run.

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

The Central Limit Theorem in action

Statistical Noise

Is the spread of the estimates (coefficient of variance) too large?
Trace more rays...



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

The variance in the computed values is ~1/N, N = number of rays *detected*

$$\sigma \propto \frac{1}{\sqrt{N}}$$

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

Variance Reduction

You now know enough to do the Monte Carlo lab.

However, before writing your own MC code to do extensive simulations, read about other ways to get more rays 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 (“backward ray tracing”, “importance sampling,”, “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 rays 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 Ray

Variance Reduction: Backward Monte Carlo

Emit rays from the *detector* with weight *w* = 1 and the angular distribution of the detector response, and trace to the source. Then weight the "detected" rays at the source to apply the correct source weight. Only ray paths conecting the true source (e.g., the sky) and the true detector are then traced.

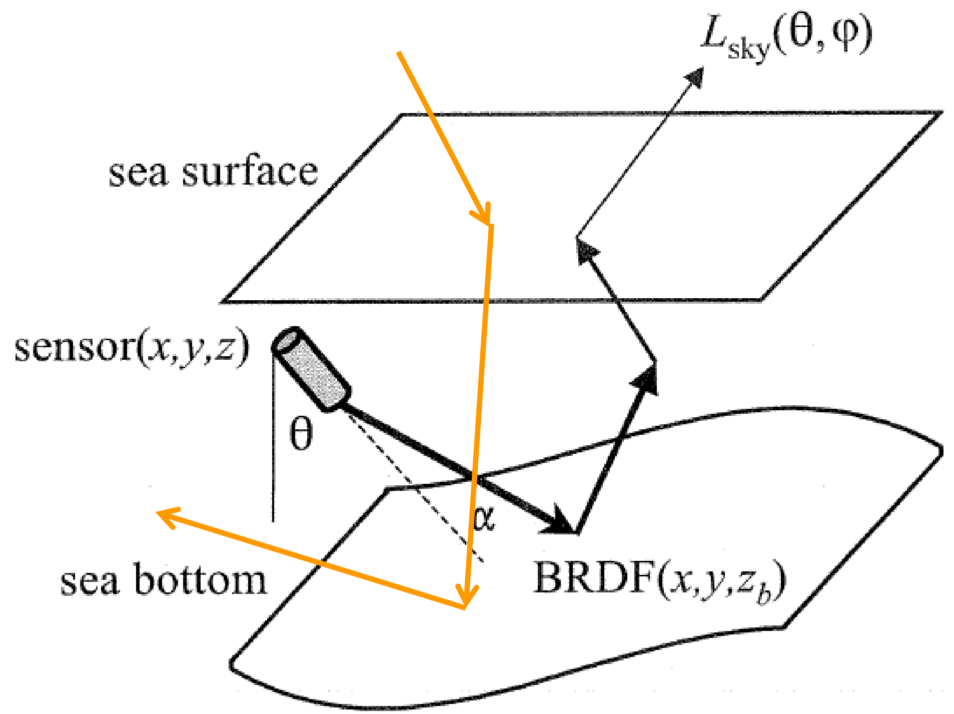


Fig. 1. Illustration of backward Monte Carlo ray tracing. The photon packets are traced from the sensor to the sky, rather than from the sky to the sensor.

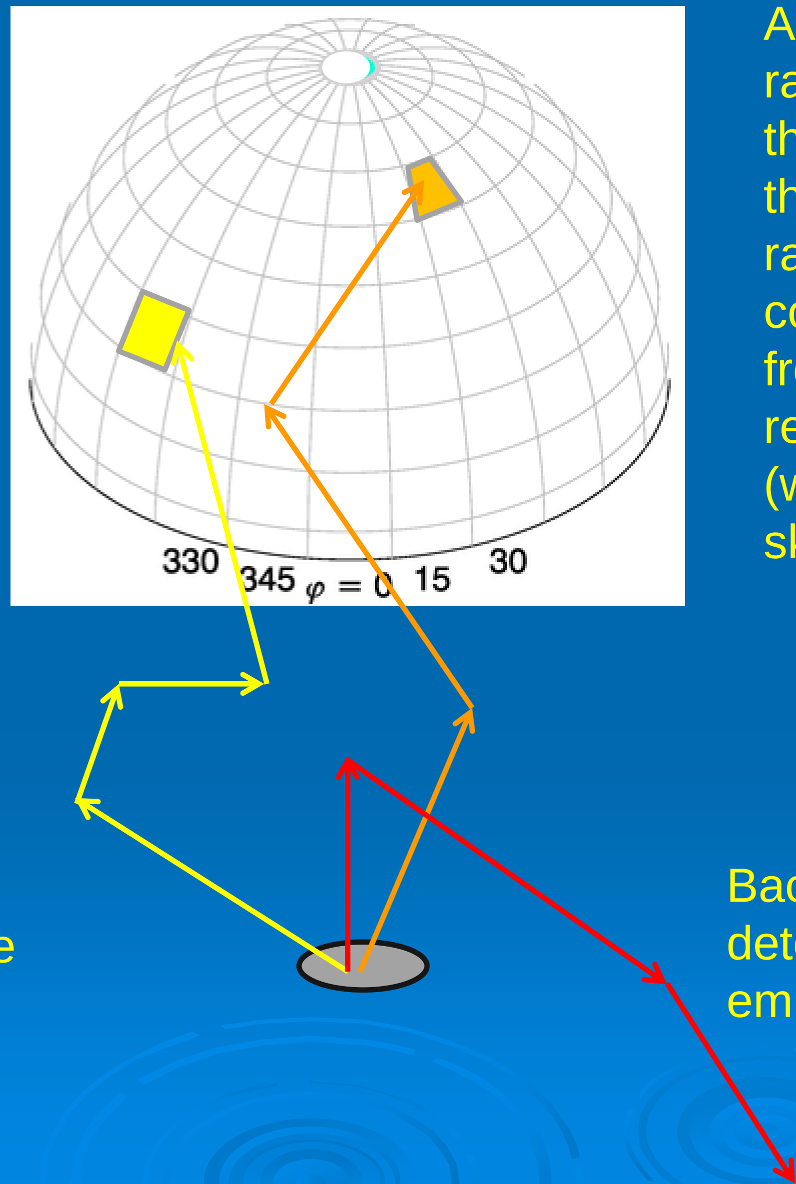
The Principle of Electromagnetic Reciprocity says that a ray will trace the same path going in either direction (If I can see you, you can see me.)

Mobley and Sundman, L&O, 2003

Variance Reduction: Backward Monte Carlo

Each sky quad records the fraction of power emitted from the detector that reaches the quad.

After ray tracing (with rays from the detector to the sky) is complete, then apply a sky radiance model to compute the total power from the sky that would reach the E_d detector (with the rays going from sky to detector)

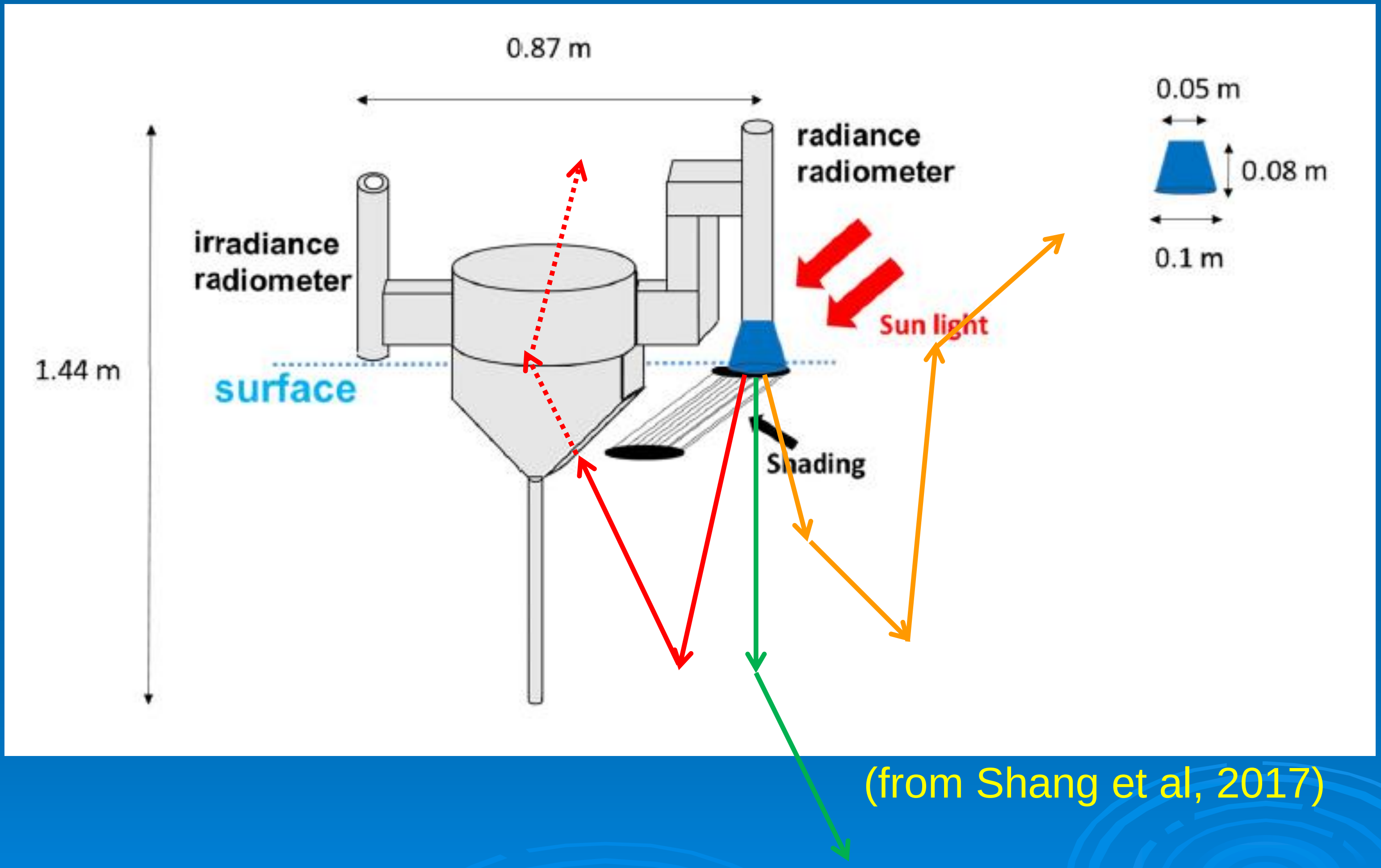


Forward MC: an E_d detector has a cosine response

Backward MC: an E_d detector has a cosine emission pattern

Example: Backward Monte Carlo

Developing a shadow correction for the Lee method.

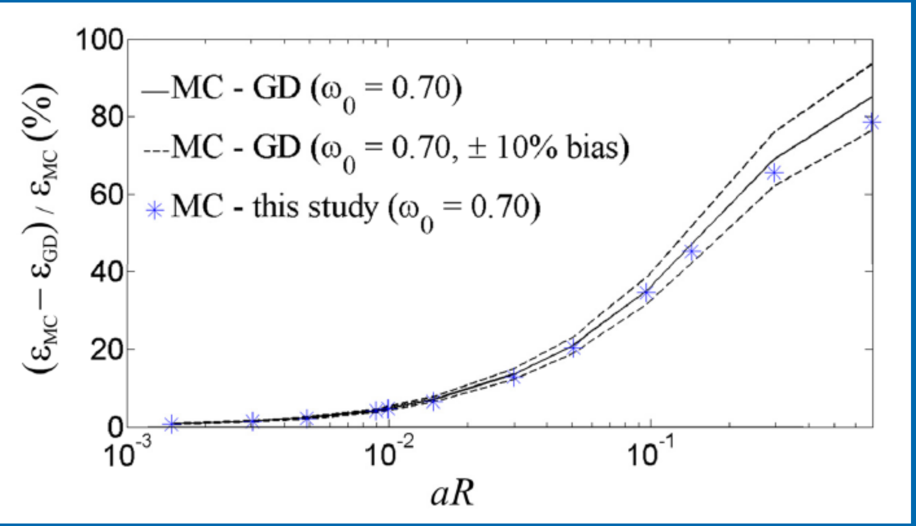


(from Shang et al, 2017)

Example: Backward Monte Carlo

First they compared their BMC code with HydroLight, for no instrument present (1 D geometry); agreement 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 function 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 ray-level and the energy-level formulations of radiative transfer theory.

- **They are relatively simple to program.** The resulting computer code can be simple (compared to other techniques), and the tracing of rays is well suited to parallel processing.

Monte Carlo Weaknesses

- **They can be computationally very inefficient.** Monte Carlo simulation is inherently a "brute force" technique. If care is not taken, much of the computational time can be expended tracing rays 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 rays penetrating the ocean decreases exponentially with the optical depth. Likewise, the simulation of a small source and a 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 rays, each of which is independent of the others.

Following Marco Polo Along the Silk Road in Western China

Tang tri-color horse and camel
Shaanxi Provincial Museum, Xi’an; Tang 618–907)

Bronze wine jug, Western Zhou Dynasty (1000-900 BC), Shaanxi Provincial Museum, Xi’an

Tomb bricks, Gobi Desert near Jiayuguan, Gansu Province. Wei-Jin era (200-400 AD)

Gold ibex (?) and Teapot, Shaanxi Provincial Museum, Xi’an

Mogau Grottos near Dunhuang (c 400 – 1500 AD)

http://www.xrez.com/blog/mogao-caves-vr/

https://www.askideas.com/30-most-beautiful-paintings-inside-the-mogao-caves-in-dunhuang-china/

The Flying Horse of Gansu, Han (25-200 CE)
Gansu Provincial Museum, Lanzhou