Geant4 11.2.p01

Monte Carlo Methods for Detector Simulation

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based on slides from Makoto Asai (Jefferson Lab)

Outline

- History and applications of Monte Carlo methods
- Monte Carlo basics
- Examples of Monte Carlo particle transport
- Biasing - speeding thing up

History

- Fermi (1930): used random sampling to study neutron moderation
- Ulam and von Neuman (1940s): simulation for weapons development (coined the term "Monte Carlo")
- Metropolis (1948): first Monte Carlo calculations done on a computer (ENIAC)
- Berger (1963): first complete, coupled electron-photon transport code (became known as ETRAN)
- Rapid growth since the 1980s with availability of digital computers

Monte Carlo in HENP

- Detector design
  - test scenarios too complex or expensive to do in lab
  - assists in rapid prototyping
  - no modern detector is built without simulation
- Data analysis
  - simulate experimental results with and without new physics added
  - reduce systematic errors
  - increase confidence in results

Many Other Applications

- Astrophysics
- Molecular modeling
- Semiconductor devices
- Financial markets
- Traffic flow
- Optimization problems
- …

Monte Carlo Basics

Monte Carlo:
Stochastic Method for Numerical Integration

- Generate N random points $\mathbf{x}_i$ in the problem space
- Calculate a "score" $f_i = f(\mathbf{x}_i)$ for the N points
- Then calculate $< f > = \frac{1}{N} \Sigma_{i=1}^{N} f_i$ and $< f^2 > = \frac{1}{N} \Sigma_{i=1}^{N} f_i^2$
- Central limit theorem: for large N, f will approach the true value $\bar{f}$ with an error σ
- Formally:
- $p(< f >) = \frac{exp\left[- \frac{1}{2\sigma^2} (< f > - \bar{f})^2 \right]}{\sigma\sqrt{2\pi}}$, $\sigma^2 = \frac{< f^2 > - < f >^2}{N - 1}$

Probability Density Function (1)

- A variable is random (stochastic) if its value cannot be predicted before observing it
- Suppose x is a single continuous random variable defined over some interval
  - can't predict its value, but $Prob\{x_i \leq X\}$ represents the probability that an observed value x_i will be less than or equal to some specified value X
  - generally, $Prob\{E\}$ represents the probability of event E
- The Probability Density Function (PDF) of a single stochastic variable is a function that is
  - defined on the interval $[a, b]$
  - nonnegative on that interval
  - normalized such that $\int_a^b f(x)dx = 1,\ a, b$ real

Probability Density Function (2)

- $f(x)$ is a density function - it specifies probability per unit x
  - $\rightarrow f(x)$ has units that are the inverse of x
- For a given x, $f(x)$ is not the probability of obtaining x
  - infinitely many values x can assume
  - probability of obtaining a single specific value is zero
- instead $f(x)dx$ is the probability that a random sample x_i will assume a value between x and $x + dx$
  - $\rightarrow$ $f(x) = Prob\{x \leq x_i < x + dx\}$

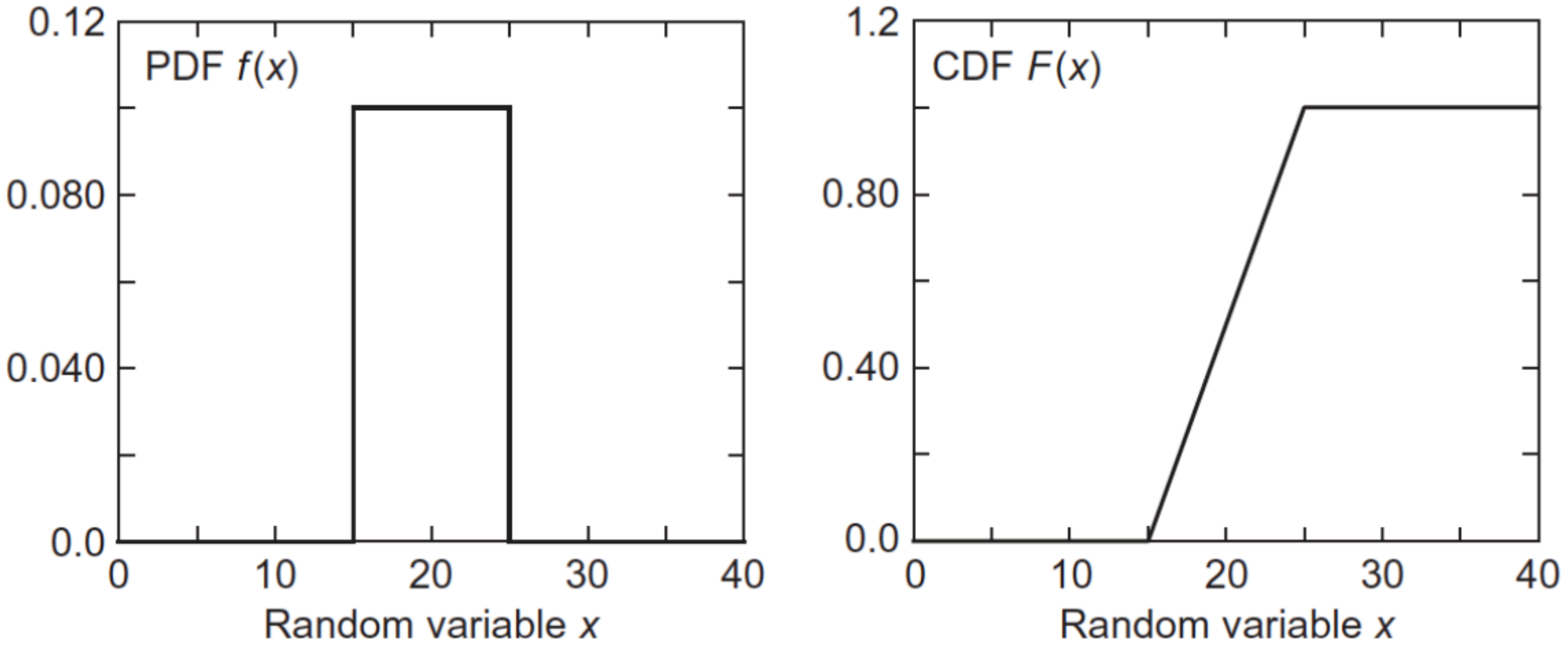
Mean, Variance, Standard Deviation

- Two important features of a PDF $f(x)$ are its mean μ and variance σ^2
- The mean is the expected or average value of x
  - $$\langle x \rangle \equiv E(x) \equiv \mu(x) \equiv \int_a^b x\, f(x)\, dx$$
- The variance describes the spread of the random variable x from the mean:
  - $$\sigma^2 \equiv \langle [x - \langle x \rangle]^2 \rangle = \int_a^b [x - \langle x \rangle]^2 f(x)\, dx = \int_a^b \left[x^2 - 2x\langle x \rangle + \langle x \rangle^2\right] f(x)\, dx$$
    $$= \int_a^b x^2 f(x)\, dx - 2\langle x \rangle \int_a^b x\, f(x)\, dx + \langle x \rangle^2 \int_a^b f(x)\, dx = \langle x^2 \rangle - \langle x \rangle^2$$
  - using $\int_a^b x^2 f(x)\, dx = \langle x^2 \rangle$, $\int_a^b x\, f(x)\, dx = \langle x \rangle$ and $\int_a^b f(x)\, dx = 1$
- The square root of the variance is the standard deviation

Cumulative Distribution Function (CDF)

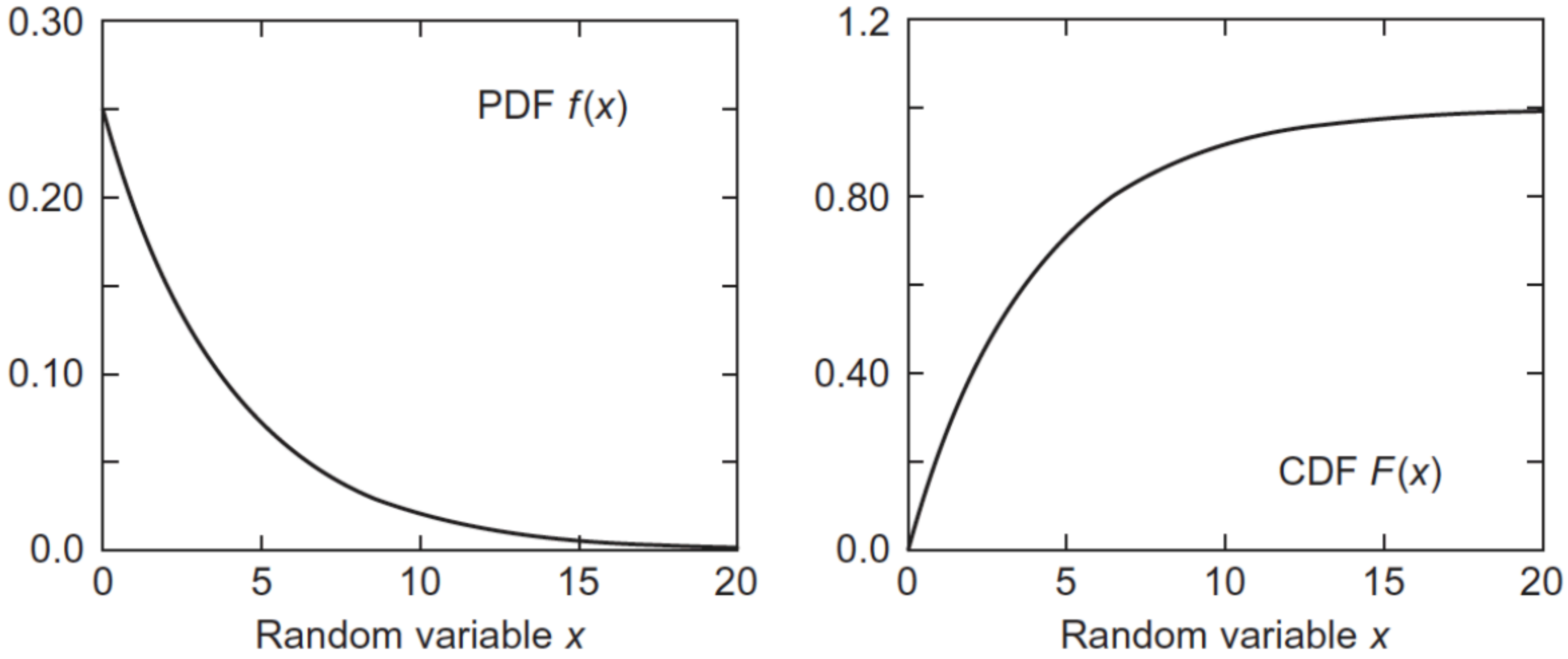
- The CDF is $F(x) = \int_a^x f(x')dx'$, where f is the PDF over the interval $[a, b]$
- and has the properties:
  - $F(a) = 0., F(b) = 1.$
  - monotonically increasing because $f(x)$ is always nonnegative
- CDF is a direct measure of probability. $F(x_i)$ represents the probability that a random sample of x will assume a value between a and x_i , that is $Prob\{a \leq x < x_i\} \ = \ F(x_i)$
- More generally, $Prob\{x_1 \leq x \leq x_2\} \ = \ \int_{x_1}^{x_2} f(x)dx \ = \ F(x_2) - F(x_1)$

Example 1: Flat PDF

- PDF is a rectangle: $f(x) = \frac{1}{b-a}$, 0 elsewhere , CDF: $F(x) = \int_a^x \frac{1}{b-a} dx' = \frac{x-a}{b-a}$
- 

Example 2: Exponential PDF

- PDF: $f(x) = \alpha e^{-\alpha x}$, CDF: $F(x) = \int_0^x \alpha e^{-\alpha x'} dx' = 1 - e^{-\alpha x}$



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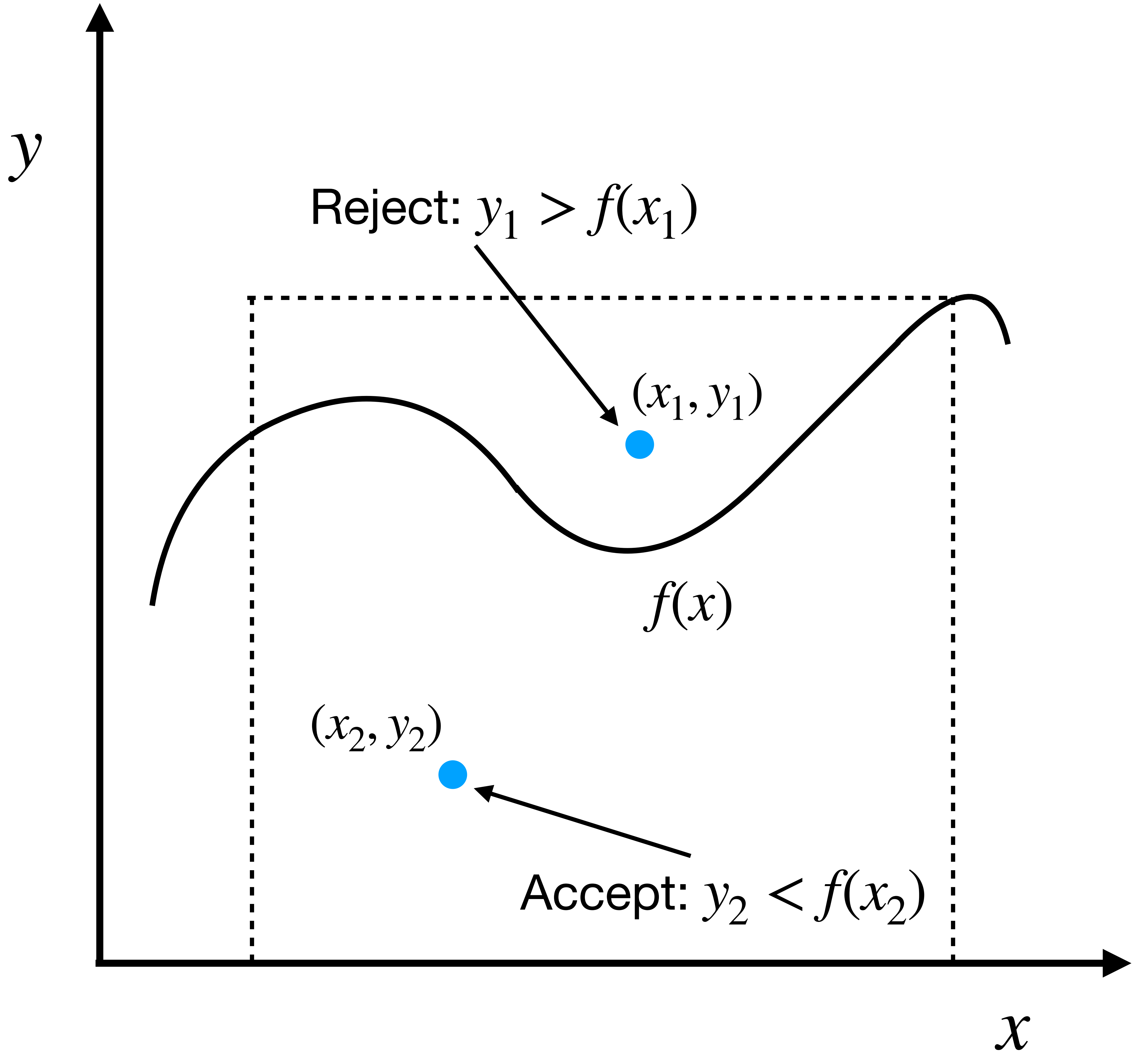
Example 3: Arbitrary PDF

- A function may not have a closed-form integral, or the integral may not be invertable
- Select (x_i, y_i) randomly from range and domain of function f
- When $y_i > f(x_i)$, point lies above curve, x_i is rejected; when $y_i \leq f(x_i)$, x_i is accepted
- Fraction of accepted points is equal to area below curve -> accept/reject method
- For efficiency, choose bounding curve carefully



Examples of Monte Carlo Particle Transport

Decay in Flight (1)

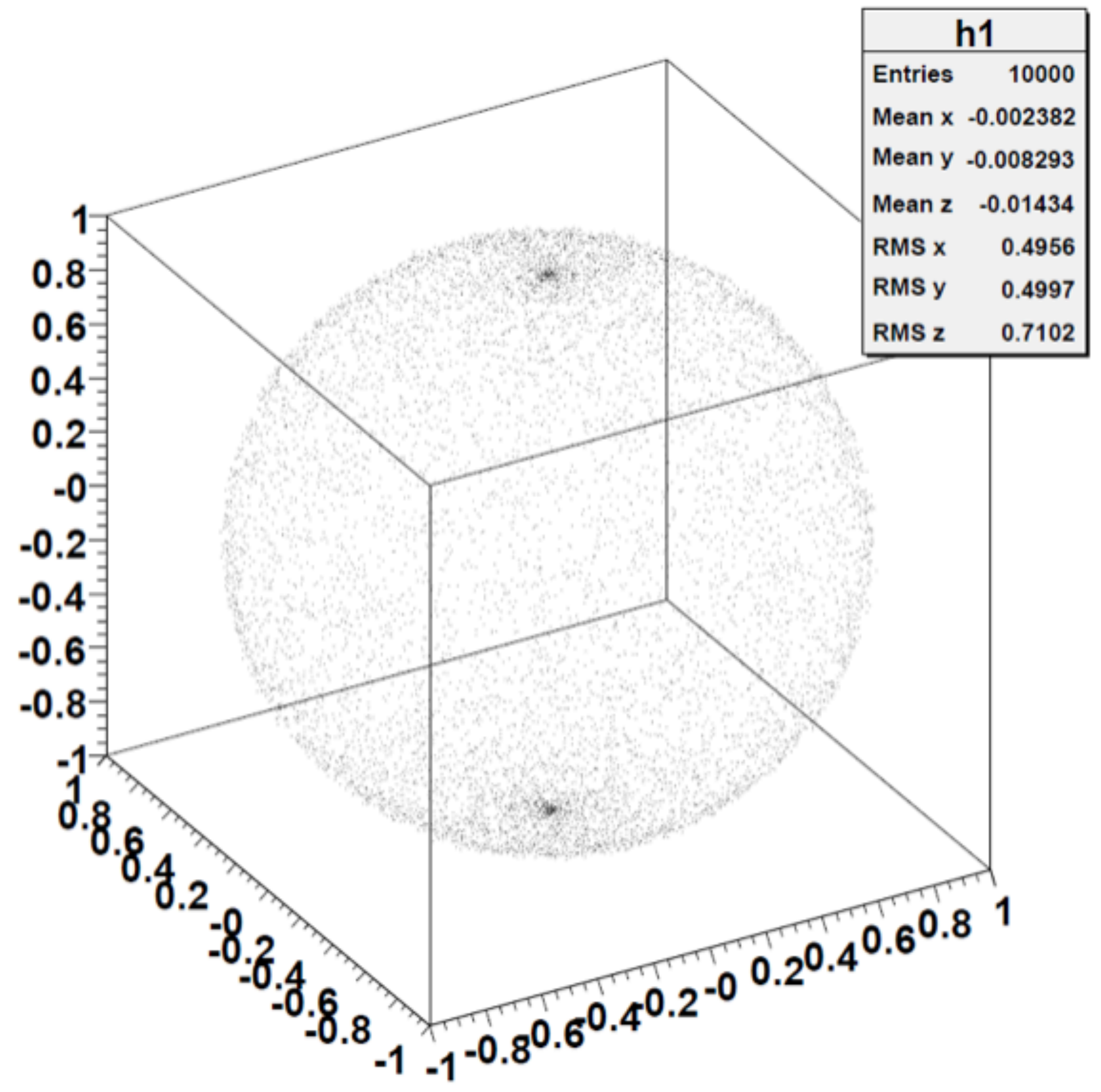
- An unstable particle with mean life τ has momentum p (velocity v)
  - travels distance $d = vt$ before decaying
- Decay time t is a random value with probability density function
  - $f(t) \ = \frac{1}{\tau} exp\left(-\frac{t}{\tau}\right)\ , t \geq 0$
- The probability that the particle decays at time t is the CDF, which is itself a random variable with uniform probability on $[0,1]$
  - $r = F(t) = \int_0^t f(u)du \ = \ 1 - exp\left(-\frac{t}{\tau}\right)$
- Because r is uniformly distributed on $[0,1]$ the value of t can be sampled using the inverse of the CDF
  - $t = F^{-1}(r) = -\tau \ ln(1-r)\ , \ \ 0 \leq r < 1$

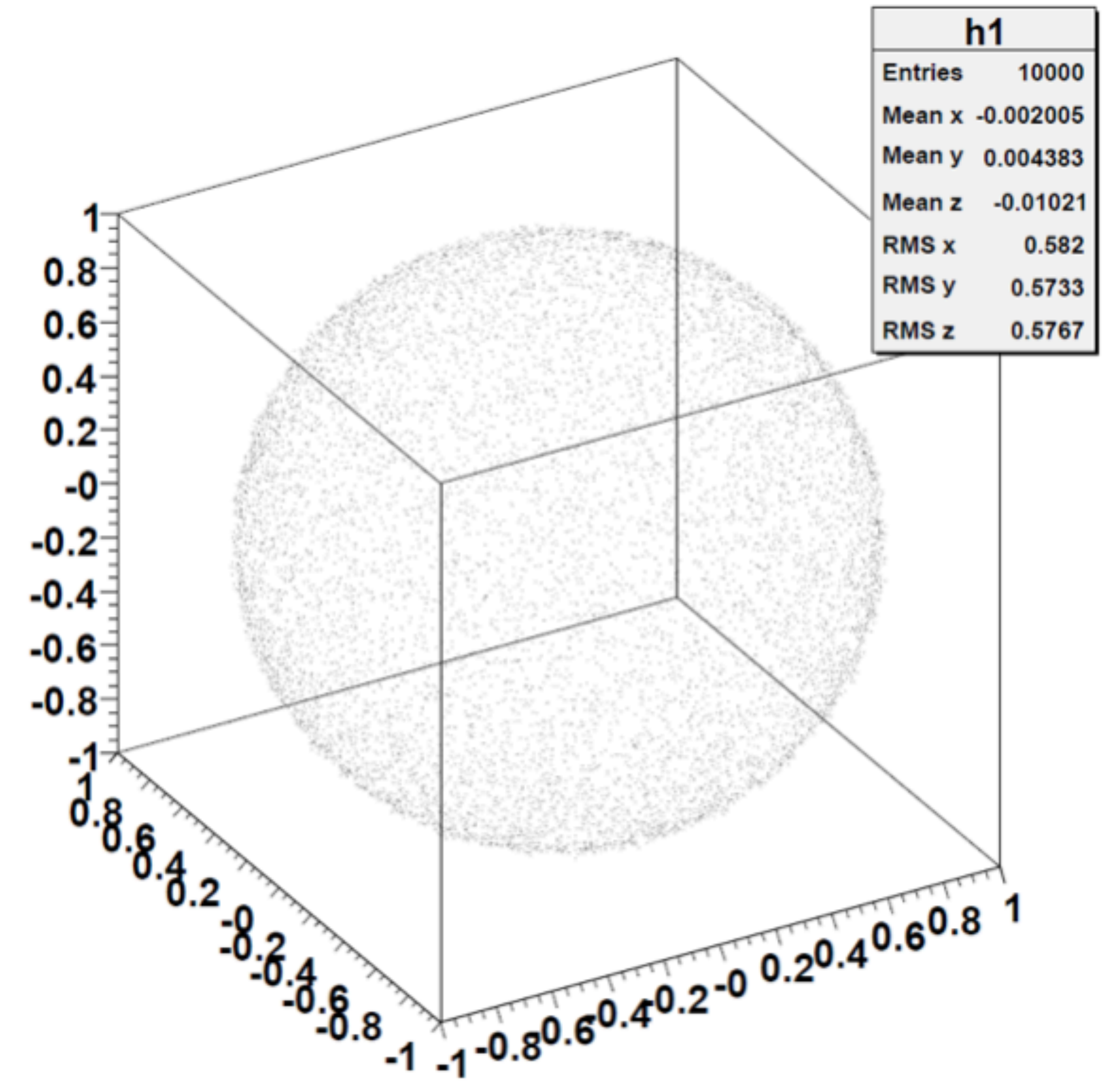
Decay in Flight (2)

- Final state of decay can be randomly sampled, too
  - shoot a random number, compare to table of branching ratios
  - π^+ for example:
    - $\pi^+ \rightarrow \mu^+ \nu_\mu \quad (99.9877\ \%)$
    - $\pi^+ \rightarrow \mu^+ \nu_\mu \gamma \quad (2.00 \times 10^{-4}\ \%)$
    - $\pi^+ \rightarrow e^+ \nu_e \quad (1.23 \times 10^{-4}\ \%)$
    - $\pi^+ \rightarrow e^+ \nu_e \gamma \quad (7.39 \times 10^{-7}\ \%)$
    - …
- In rest frame of parent particle, rotate decay products in $\theta\ [0, \pi]$ and $\phi\ [0, 2\pi]$
- Then Lorentz-boost the decay products
- At least 4 random numbers needed to simulate decay in flight

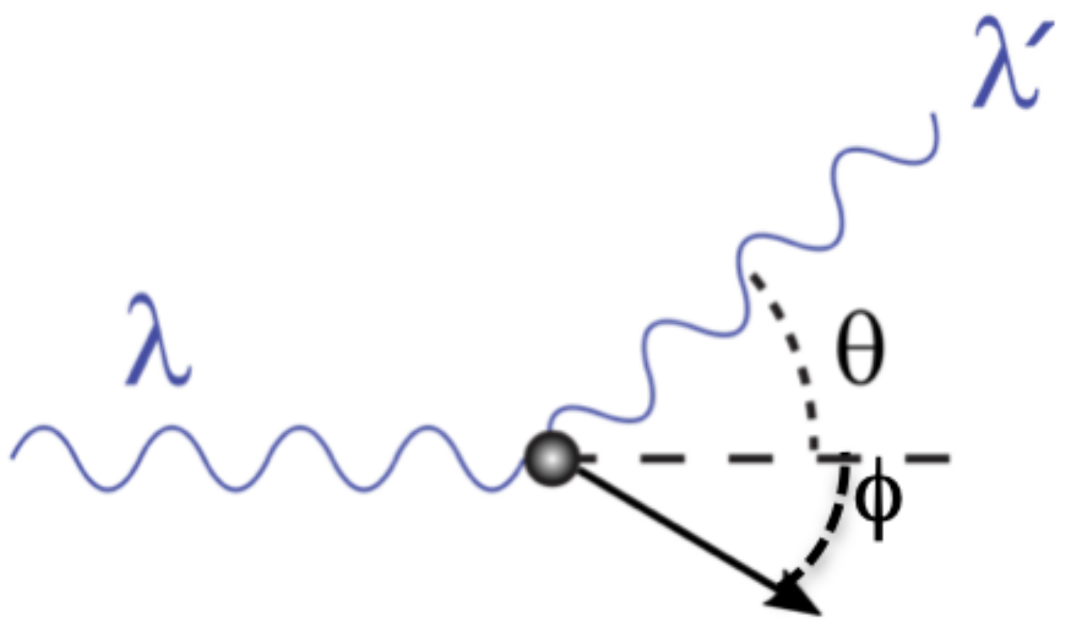
Decay in Flight (3)

- Throw directions (θ, ϕ) uniformly in the solid angle
  - $d\Omega \;= dsin\theta \; d\theta \; d\phi \;=\; d(cos\theta) \; d\phi$
- Wrong:
  - $\theta \;=\; \pi r_1, \;\; \phi \;=\; 2\pi r_2$
  - $0 \le r_1, r_2 < 1$
- Right:
  - $\theta \;=\; cos^{-1}(2r_1 - 1), \;\; \phi \;=\; 2\pi r_2$
  - $0 \le r_1, r_2 < 1$





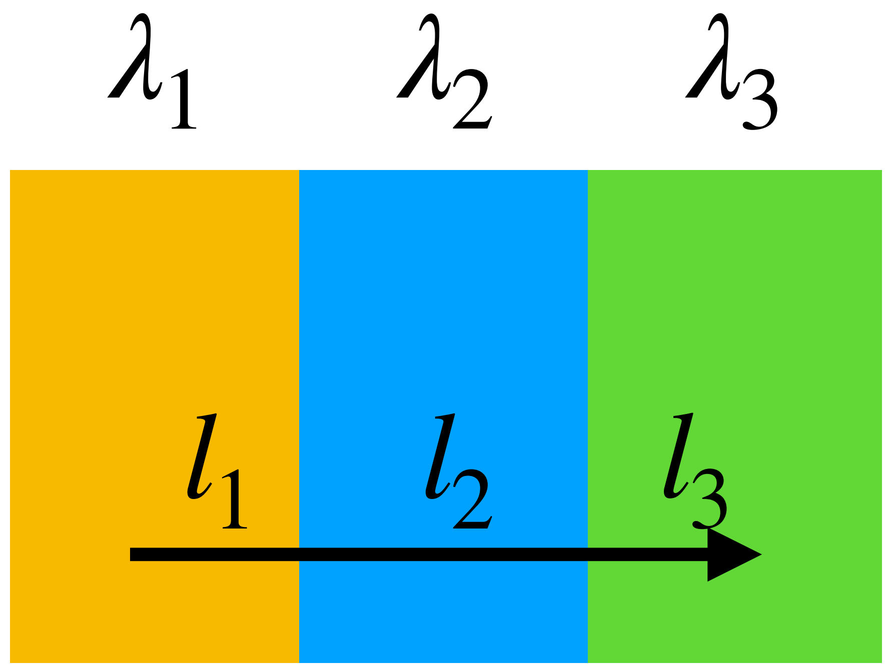
Compton Scattering (1)



- $\gamma e^- \rightarrow \gamma e^-$
- Distance l traveled before Compton scattering is a random value
- Cross section per volume: $\eta(E, \rho) = n\sigma$
    - cross section per atom: $\sigma(E, z)$
    - number of atoms per volume: $n = \rho N_A / A$ (ρ = density, N_A = Avogadro's number, A = atomic mass)
- η is the probability of Compton scattering per unit length
- $\lambda(E, \rho) = \dfrac{1}{\eta}$ is the mean free path associated with the Compton scattering process
- The PDF: $f(l) = \eta\, exp(-\eta l) = \dfrac{1}{\lambda} exp\left(-\dfrac{l}{\lambda}\right)$
- With random number r uniformly distributed on $[0,1]$, sample the distance: $l = -\lambda\, ln(1 - r)$

Compton Scattering (2)

- Ratio $\frac{l}{\lambda}$ (distance traveled to mean free path) is independent of material



- $n_\lambda = \frac{l_1}{\lambda_1} + \frac{l_2}{\lambda_2} + \frac{l_3}{\lambda_3} = \int_0^{end} \frac{dl}{\lambda(l)}$

- n_λ is material-independent and a random value with PDF $f(n_\lambda) = exp(-n_\lambda)$
  - sample n_λ at the particle's origin: $n_\lambda = -ln(1-r)\ ,\ \ 0 \le r < 1$
  - update elapsed n_λ along the path of the particle: $n_\lambda = n_\lambda - \frac{l_i}{\lambda_i}$

- Compton scattering happens when $n_\lambda = 0$

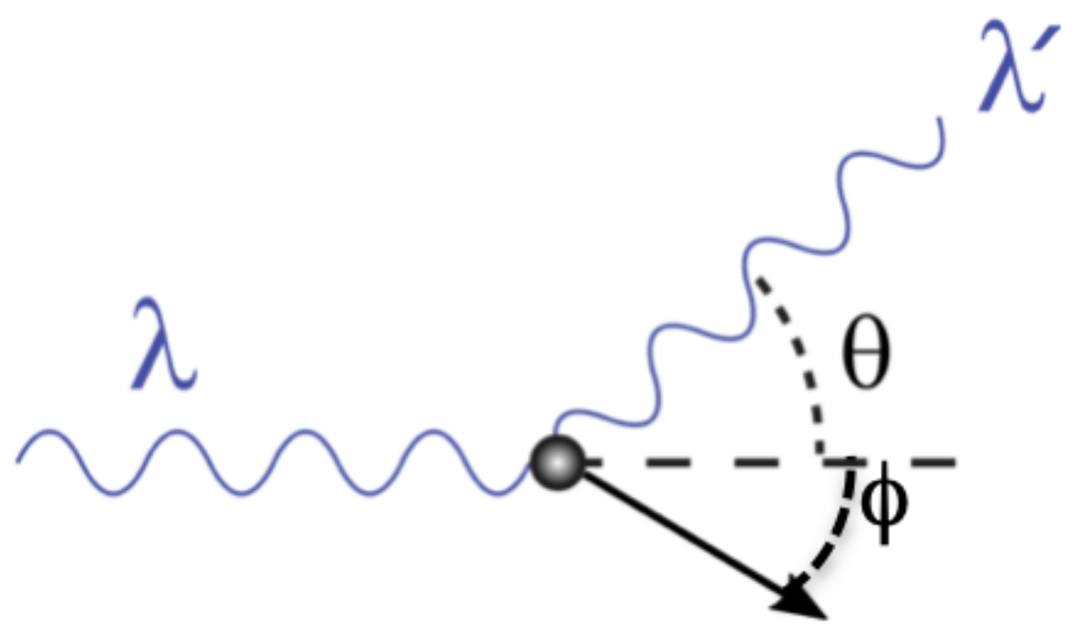
Compton Scattering (3)

- The relation between photon deflection (θ) and energy loss for Compton scattering is determined by 4-momentum conservation between photon and recoil electron

$$h\nu = \frac{h\nu_0}{1 + \left(\frac{h\nu_0}{m_e c^2}\right)(1 - \cos\theta)},$$

$$E = h\nu_0 - h\nu = m_e c^2 \frac{2(h\nu_0)^2 \cos^2\phi}{(h\nu_0 + m_e c^2)^2 - (h\nu_0)^2 \cos^2\phi},$$

$$\tan\phi = \frac{1}{1 + \left(\frac{h\nu_0}{m_e c^2}\right)} \cot\frac{\theta}{2},$$



- For unpolarized photons, the angular distribution is given by the Klein-Nishina formula

$$\begin{aligned} \frac{d\sigma_c^{KN}}{d\Omega}(\theta) &= r_0^2 \frac{1+\cos^2\theta}{2} \frac{1}{[1+h\nu(1-\cos\theta)]^2} \left\{1 + \frac{h\nu^2(1-\cos\theta)^2}{(1+\cos^2\theta)[1+h\nu(1-\cos\theta)]}\right\} \\ &= \frac{1}{2} r_0^2 \left(\frac{k}{k_0}\right)^2 \left(\frac{k}{k_0} + \frac{k_0}{k} - \sin^2\theta\right) \qquad (cm^2 sr^{-1} electron^{-1}), \end{aligned}$$

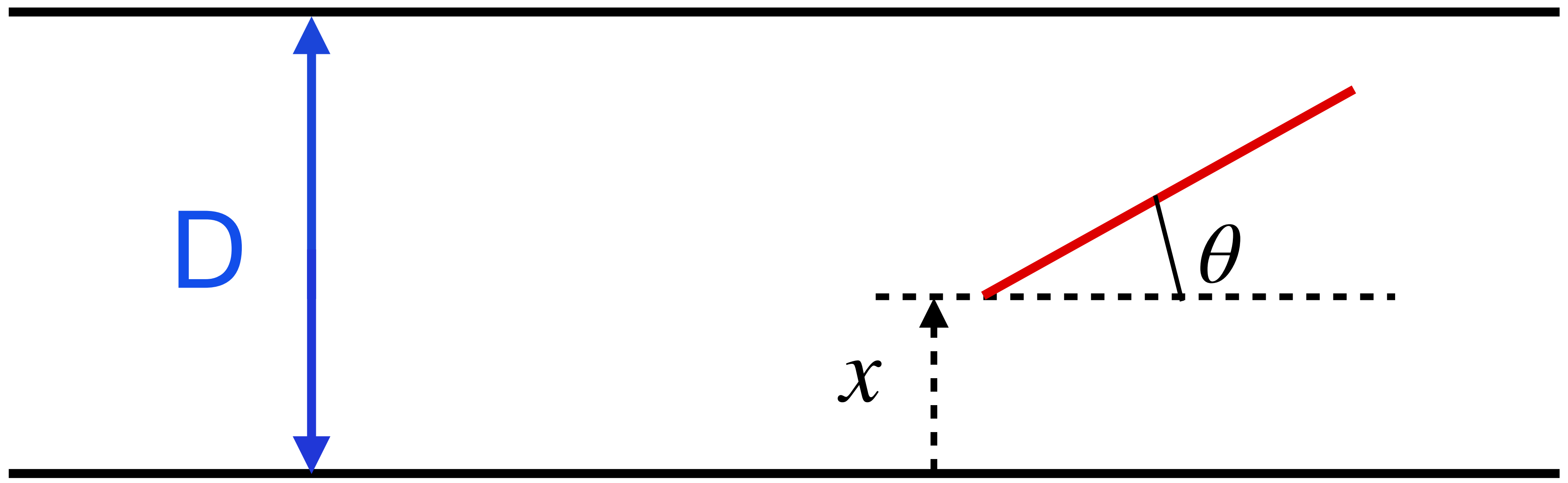
$$k_0 = \frac{h\nu_0}{m_e c^2}, \qquad k = \frac{h\nu}{m_e c^2}$$

- Use accept-reject method to sample the distribution

Boosting the Simulation

Buffon's Needle

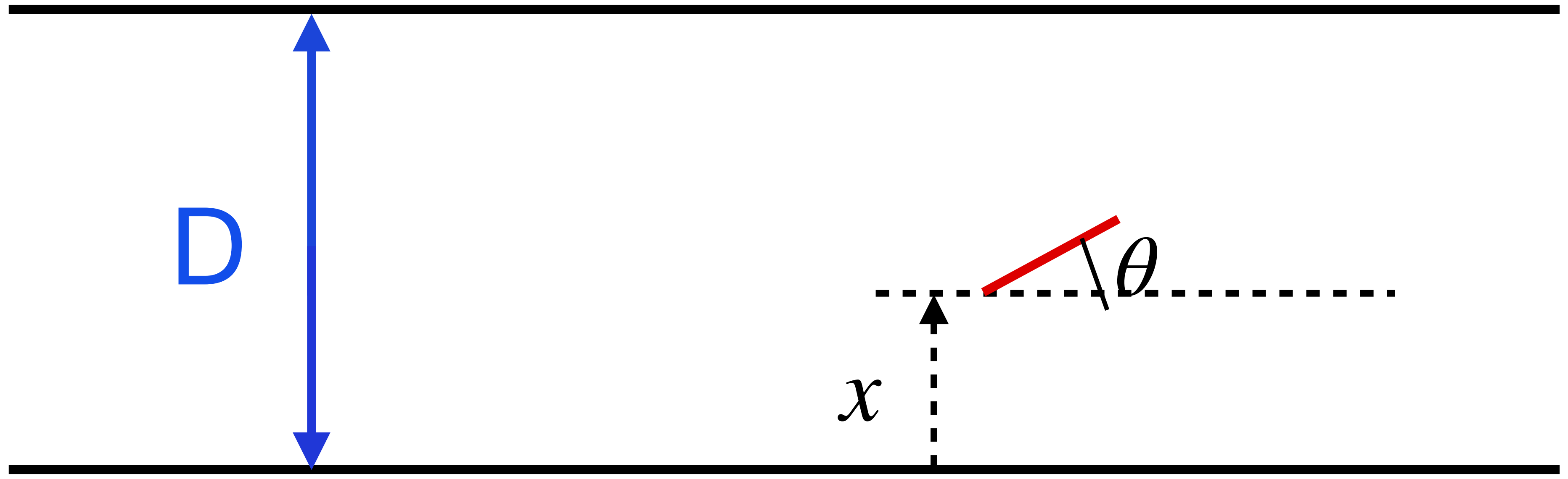
- Calculate π by dropping a needle on a lined sheet of paper and determine the probability that the needle crosses one of the lines
- Probability is directly related to the value of π



- Needle of length L will cross line if $x \leq L\ sin\theta$. Assuming $L \leq D$, the probability of a line crossing is
  - $P_{cross} = \int_0^\pi \frac{d\theta}{\pi} P_{cross}(\theta) = \int_0^\pi \frac{d\theta}{\pi} \frac{L\ sin\theta}{D} = \frac{2L}{\pi D}$
- Dropping a needle N times and counting N_c , the number of crossings, gives P_{cross} and thus π

Boosting Buffon's Needle

- If the length of the needle is much smaller than the spacing of the lines, the estimate of π will take a long time
  - $\pi \sim (2L/D) * (N/N_c)$, x sampled uniformly over $[0, D]$



- Speed things up by sampling x over the interval $[0, L]$ instead
  - probability that $0 \leq x < L$ is $\dfrac{L}{D/2}$
  - each successful count should be multiplied by a weight $\dfrac{2L}{D}$
  - then, $\pi \sim (2L/D) * \dfrac{N}{N_c(2L/D)}$

Biasing (Variance Reduction)

- In boosting Buffon's needle, we biased the simulation
    - by sampling over a subset of the original interval that was of more interest
    - applying a weight to successful events to correct for bias
    - significantly speeding up the simulation
- Called variance reduction because the variance of the result for a given simulation effort is reduced (precision increased)
- Very useful for sampling events which are rare due to physics or geometry
- Can make otherwise impossible Monte Carlo problems solvable
- Care is required - use of variance reduction techniques requires skill and experience
- See talk on biasing and fast simulation for some of these techniques

Summary

- Detector simulation an essential part of nuclear and high energy physics
    - Monte Carlo methods widely used outside HENP, too
- Stochastic methods used where deterministic methods don't apply
    - Central limit theorem: get close to the answer with large enough statistics
- Many methods to sample functions of random variables
    - integrate PDF to get CDF, invert CDF to get sampling formula
    - complicated PDF -> use accept/reject method
- Simulating physical processes involves throwing lots of independent random numbers
    - sample number of mean free paths, momentum, angular distributions, …
    - increase confidence in results
- Biasing can really speed things up
    - care is required