Monte Carlo Simulation of Radiation Transport

Agen-689

Advances in Food Engineering

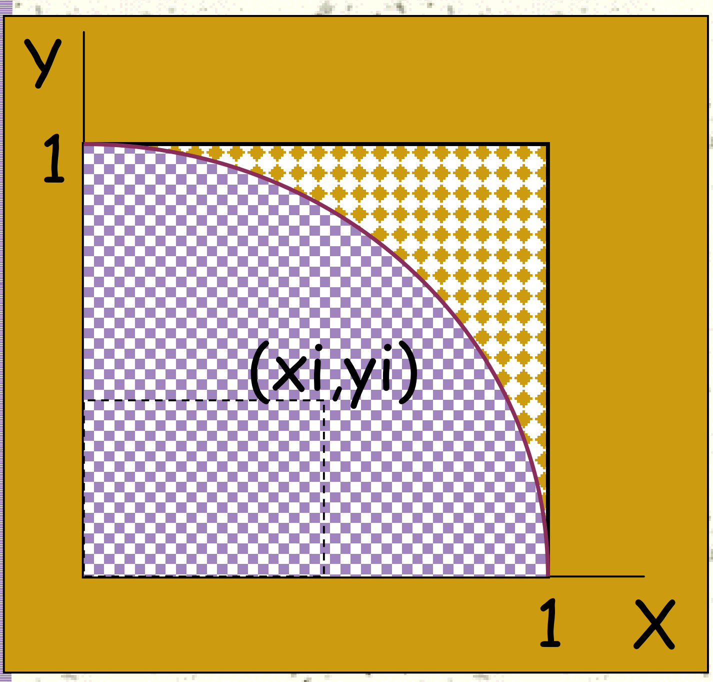
Introduction

- Name Monte Carlo – created in 1940s
- Nuclear scientists working on Los Alamos
- To design a class of numerical methods based on the use of random numbers
- Today widely used to solve complex physical and math problems

The Monte Carlo Method

- A technique of numerical analysis
- Uses random sampling to construct the solution a problem

Find the value of π



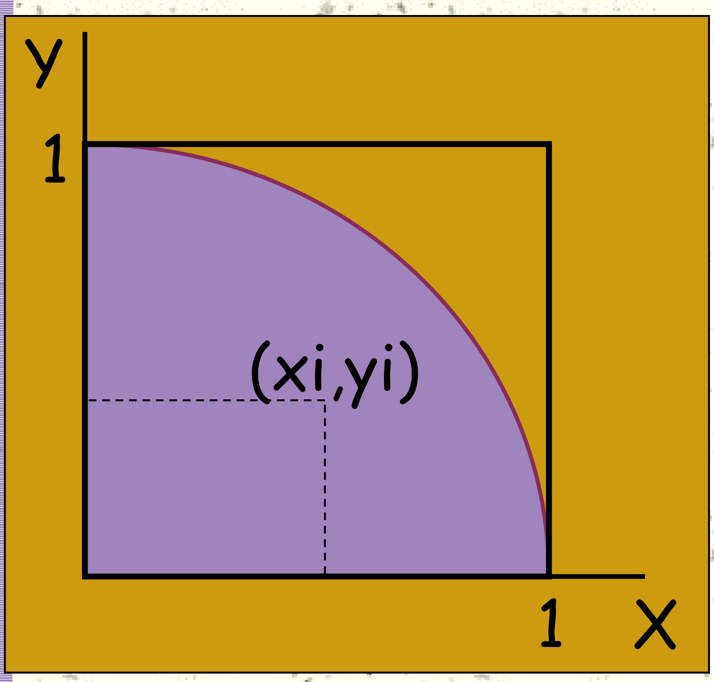
The quadrant of a circle
enclosed by a square having sides of 1

- Using geometry, it is easy to show that:

$$\frac{\#\text{ dots in shaded area}}{\#\text{ dots in square}} = \frac{\frac{1}{4}\pi r^2}{r^2} = \frac{1}{4}\pi$$

$$\pi = 4\,\frac{\#\text{ dots in shaded area}}{\#\text{ dots in square}}$$

Find the value of π



The quadrant of a circle enclosed by a square having sides of 1

- Computer generates sequence of random numbers $0 \leq R < 1$
- Pairs of random numbers (xi,yi) can be selected as values that determined point that lie in the square
- For each point one tests if

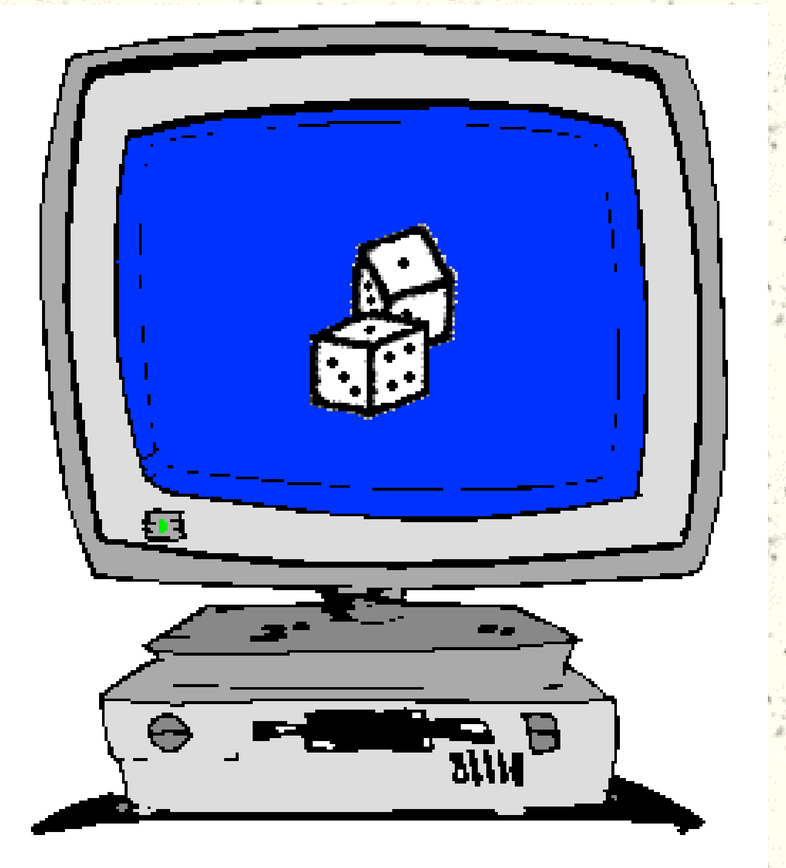
$$x_i^2 + y_i^2 \leq 1$$

- If so, the point lies inside the circle
- After a large number of random trials, π can be determined

Find the value of π

x = (random #)
y = (random #)
dist = sqrt (x^2 +y^2)
If dist $\leq$ 1
Let hits = hits +1

- Do this thousands of times and π will be determined
- See spreadsheet



Radiation transport thru matter

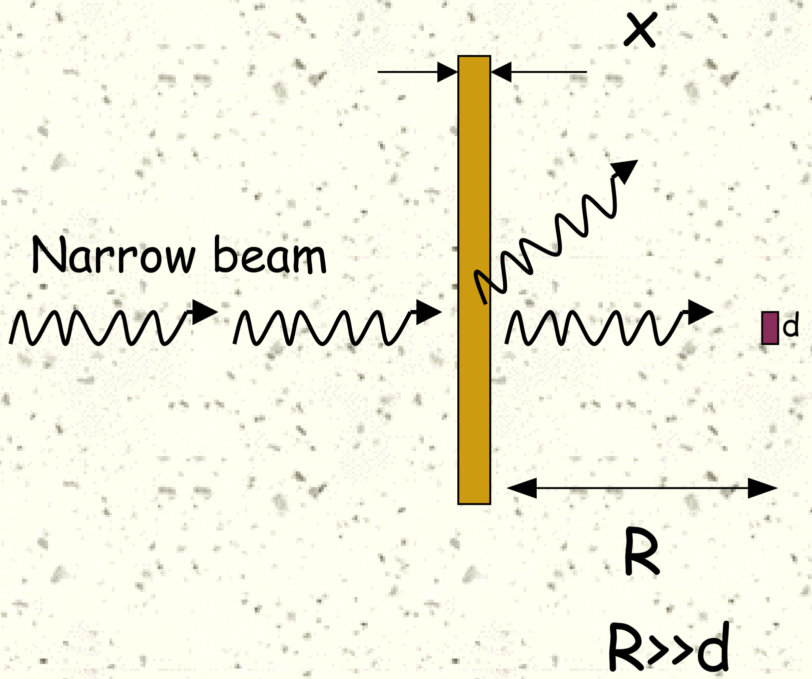
- Governed by attenuation coefficients
- Or cross sections
- Given the interaction probabilities
- The use of linear attenuation coefficient describe the statistical nature of radiation penetration in matter

Consider photons, for example

- The probability that a normally incident photon will reach the depth x in a material without interact is

$$P(x) = e^{-\mu x}$$

$$N(x) = N_o e^{-\mu x}$$



In general

- The probability that the first interaction of an incident photon will take place at a depth between x and $x + dx$ is:

$$P_1(x)dx = P(x)\mu dx$$

The probability that it will reach the depth x — $P(x)$

The probability that it will interact in dx — μdx

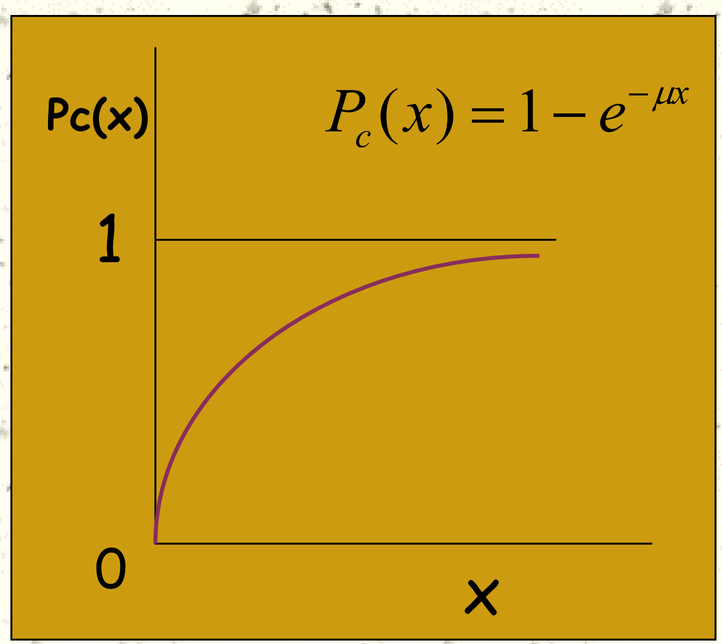
The cumulative probability

- That a normally incident photon will interact before reaching a depth *x*:

$$P_c(x) = \int_0^x P_1(x)dx = \mu \int_0^x e^{-\mu x}dx = 1 - e^{\mu x}$$

- The relative number that have interact is equal to 1 minus the relative number that have not

The cumulative probability



- that a given incident photon has its first interaction before reaching a depth x
- The linear attenuation coefficient is μ

Radiation transport simulation

- From the knowledge of the numerical value of μ, we can also simulate radiation transport on a computer by using Monte Carlo procedures

Monte Carlo simulation of radiation transport

- The history (track) of a particle is viewed as a random sequence of 'free flights'
- The flights end with an interaction event
- In the event the particle changes its direction of movement, loses energy, and can produces secondary particles

Monte Carlo simulation of radiation transport

- To simulate the random histories an interaction model – a set of differential cross sections (DCS) – is needed
- The DSCs determine the probability distribution functions (PDF) of the random variables
  - Free path between successive interaction events
  - Kind of interaction
  - Energy loss and angular deflection

Monte Carlo simulation of radiation transport

- Yields the same information as the solution of the Boltzmann transport equation
- With the same interaction model
- But easier to implement

Monte Carlo simulation of radiation transport

- The main drawback of this method lies on its random nature
- All the results are affected by statistical uncertainties
- But, can easily be solved by increasing the sampled population and computer time and variance-reduction techniques

Simulation of radiation transport

- Considering
  - Particle with energy E moving in a medium
  - Homogeneous 'random scattering' media

Simulation of radiation transport

- Each interaction:
  - Particle may lose energy W
  - And/or change its direction of movement
    - Angular deflection determined by the scattering angle θ
    - And the azimuthal and ϕ

Simulation of radiation transport

- Assuming that the particle can interact by 2 mechanisms A & B:
  - The scattering model is specified by the molecular DCSs:

$$\frac{d^2\sigma_A}{dW d\Omega}(E;W;\theta) \text{ and } \frac{d^2\sigma_B}{dW d\Omega}(E;W;\theta)$$

Total CSs and PDFs

- The total cross sections per molecule:

$$\sigma_{\mathrm{A,B}}(E) = \int_0^E dW \int_0^\pi 2\pi \sin\theta d\theta \quad \frac{d^2\sigma_{A,B}}{dWd\Omega}(E;W;\theta)$$

- The PDFs of W and θ:

$$p_{A,B}(E;W;\theta) = \frac{2\pi \sin\theta}{\sigma_{A,B}(E)dWd\theta} \quad \frac{d^2\sigma_{A,B}}{dWd\Omega}(E;W;\theta)$$

The PDF

- Gives the (normalized) probability that in scattering event of type *A*:
  - The particle loses energy in the interval (W, W+dW)
  - Is deflected into directions with polar angle in the interval (θ, θ+dθ)

The azimuthal scattering angle

- In each collision it is uniformly distributed in the interval $(0, 2\pi)$

$$p(\phi) = \frac{1}{2\pi}$$

Generation of random tracks

- Each particle starts off at a given position and energy
- The state of the particle after an interaction is defined by:
  - Its position coordinates **r** = (x, y,z)
  - Energy E
  - Direction of flight, the component of vector <u>**d**</u> = (u, v, w)

Generation of random tracks

- Each simulated track is caracterized by a series of states:
  - $\mathbf{r}_n$ (position of the nth scattered event)
  - E_n (energy after the event)
  - $\underline{\mathbf{d}}_n$ (direction of movement after the event)

Generation of random tracks

- The random variables that are sampled from the corresponding PDFs are:
  - The length *s* of the free path to the next collision
  - The scattering mechanism
  - The change in direction
  - The energy loss in the collision

The length of free path, s

- Is distributed according to the PDF:

$$p(s) = \lambda^{-1} \exp(s / \lambda)$$

- Random variables of s are generated by using the sampling equation:

$$s = \lambda - \ln \xi$$

- The following interaction occurs at the position $\mathbf{r}_{n+1} = \mathbf{r}_n + s\underline{\mathbf{d}}_n$

ξ stands for random number uniformly distributed in the interval (0,1)

The type of interaction (A,B) and else

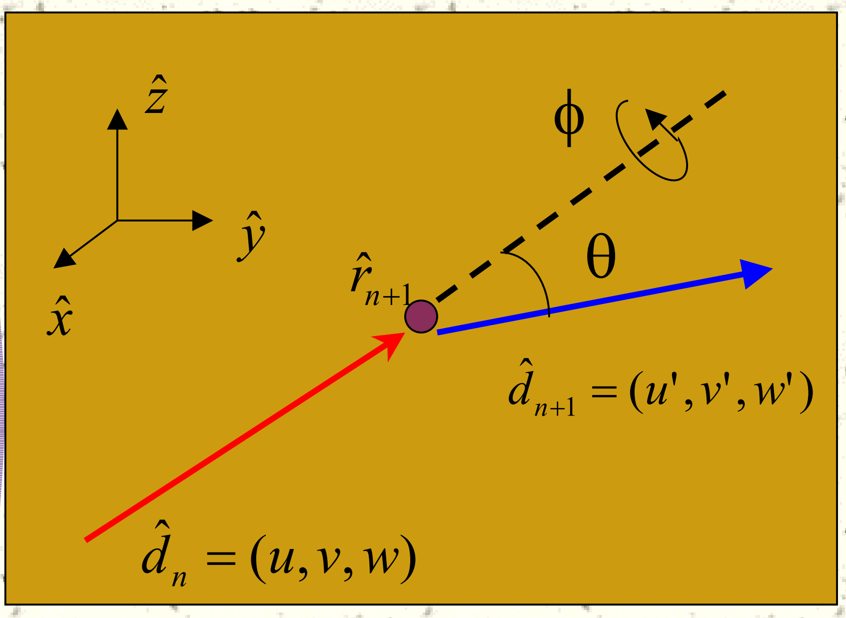
- Is selected from point probabilities:

$$p_A = \frac{\sigma_A}{\sigma} \text{ and } p_A = \frac{\sigma_B}{\sigma}$$

- The energy loss W and θ are sampled from the distribution $p_{A,B}(E;W,\theta)$
- The azimuthal angle is generated as:

$$\phi = 2\pi\xi$$

Angular deflections in single-scattering events



- After sampling the values of W, θ and ϕ,
- The energy is reduced
- The direction after the interaction $\mathbf{d}_{n+1}$ is obtained by performing a rotation of $\mathbf{d}_n$

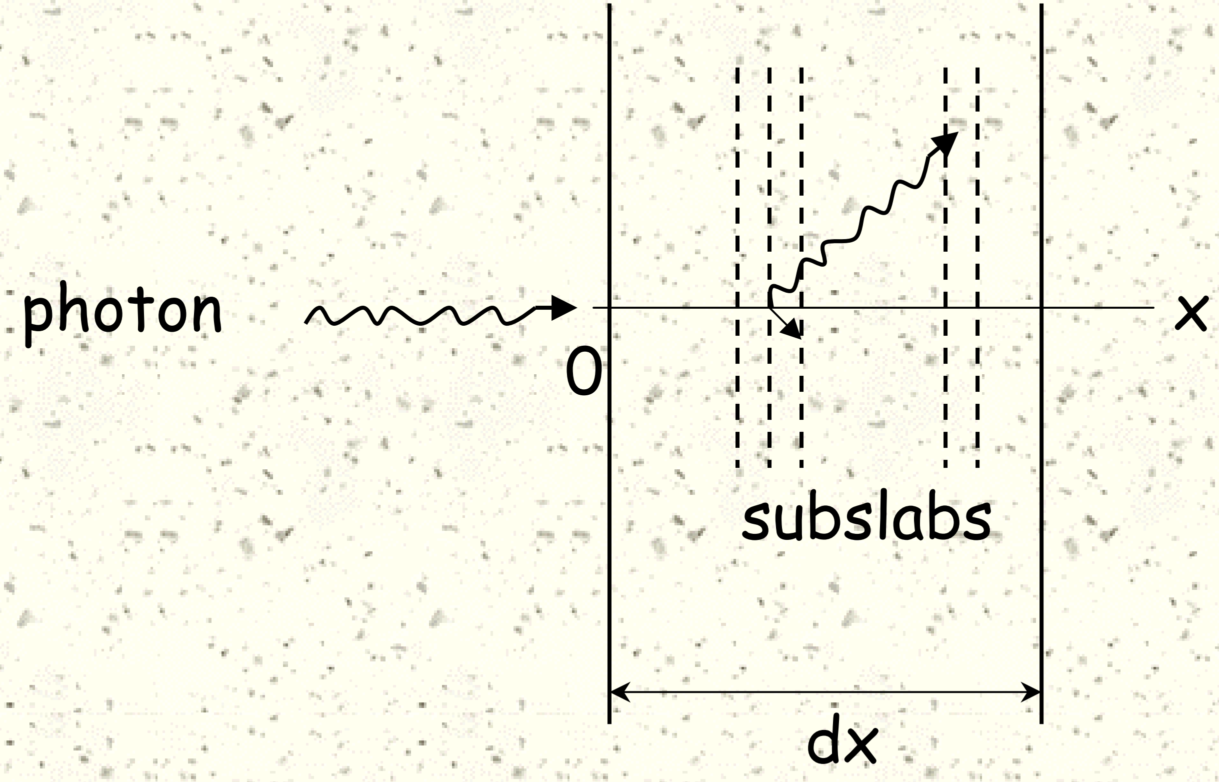
The track simulation

- The steps are repeated
- The track is finished when
  - It leaves the material
  - Or the E become smaller than a given Eabs (the energy is absorbed in the medium)

Example of Monte Carlo

- Consider a 100-keV photon normally incident on a fresh produce slab having a thickness of 3 cm. The linear attenuation coefficient μ_i by element for 100-keV photons in produce are given in Table. Develop a Monte Carlo procedure to calculate the energy deposited at different depths in the slab as a result of 100-keV incident photons. Use the 'random' number to compute the photon history.

Geometric arrangement



Data use to simulate photons transport

Element	μ_i [cm^{-1}]	μ_i/μ	Cumulative μ_i/μ
H	0.2944	0.391	0.391
O	0.1551	0.206	0.597
C	0.1514	0.201	0.798
N	0.1529	0.202	1
TOTAL	0.7538	1	

Random Numbers

i	R_i
1	0.87810
2	0.68671
3	0.03621
4	0.10389
5	0.97268

Example

- First select the first photon collision, based on the attenuation coef. for the photons of specific energy in the produce
- This is accomplished by setting the cumulative probability of interaction equal to the first R1:

$$P_c(x) = 1 - e^{-\mu x} = R_1$$

- With 0 $\leq$ R1 $\leq$ 1.
- Solving for x (the location of the first collision)

$$x = -\frac{1}{\mu}\ln(1 - R_1)$$

Example

- So, from previous tables:

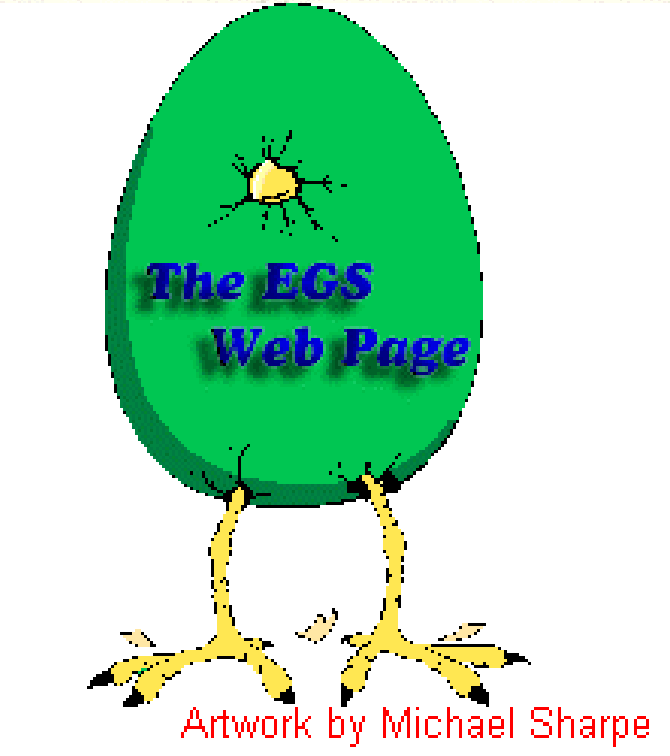
$$x = -\frac{1}{0.7538}\ln(1 - 0.87810) = 2.79cm$$

Computer Simulators

- EGS
- MCNP
- PENELOPE

EGS - Electron Gamma Shower

- The Code was developed at Stanford University - Department of Nuclear Physics
- A general purpose package for the Monte Carlo simulation of the coupled transport of electrons and photons in an arbitrary geometry for particles with energies from a few keV up to several TeV.
- Some have referred to the EGS code as the *de facto* gold standard for clinical radiation dosimetry



MCNP – Monte Carlo N-Particle

- Developed by Los Alamos National Lab
- A code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport, including the capability to calculate eigenvalues for critical systems.
- The code treats an arbitrary three-dimensional configuration of materials in geometric cells bounded by first- and second-degree elliptical tori.

MCNP

- Pointwise cross-section data are used.
- For photons
  - incoherent and coherent scattering,
  - fluorescent emission after photoelectric absorption,
  - absorption in pair production,
  - bremsstrahlung.
- A continuous-slowing-down model is used for electron transport that includes positrons, x-rays, and bremsstrahlung.
- Code include
  - Powerful general source, criticality source, and surface source;
  - Geometry and output tally plotters;
  - A collection of variance reduction techniques;
  - A tally structure;
  - Extensive collection of cross-section data.

PENELOPE

AEN NEA Agence pour l'énergie nucléaire
Nuclear Energy Agency

- PENetration & Energy Loss of Positrons & Electrons
- A code system for Monte Carlo simulation of electron and photon transport
- Developed by the Nuclear Energy Agency of the Organization for Economic Co-operation and Development

PENELOPE

- It performs Monte Carlo simulation of coupled electron-photon transport in arbitrary materials and complex quadric geometries.
- Uses a mixed procedure for the simulation of electron and positron interactions (elastic scattering, inelastic scattering and bremsstrahlung emission)
- Photon interactions (Rayleigh scattering, Compton scattering, photoelectric effect and electron-positron pair production) and positron annihilation are simulated in a detailed way.

Simulation of Compton events

- Assuming scattering by free electrons at rest

$$\frac{d^2\sigma_A}{dW d\Omega} = \frac{r^2}{2}\left(\frac{Ec}{E}\right)^2\left(\frac{Ec}{E} + \frac{E}{Ec} - \sin^2\theta\right)F(p_z)S'(E,\theta)$$

- The PDF of cos θ and E′

$$P(\cos\theta, E') = \left(\frac{Ec}{E}\right)^2\left(\frac{Ec}{E} + \frac{E}{Ec} - \sin^2\theta\right)F(p_z)S'(E,\theta)$$

Simulation of Compton events

- Integration of PDF over E':

$$P(\cos\theta) = \left(\frac{Ec}{E}\right)^2 \left(\frac{Ec}{E} + \frac{E}{Ec} - \sin^2\theta\right) S(E,\theta)$$

Simulation of Compton events

- The PDF of the cos θ is:

$$P_\tau(\tau) = P_\theta(\cos\theta)\frac{d(\cos\theta)}{d\tau} =$$

$$P_\tau(\tau) = \left(\frac{1}{\tau^2} + \frac{\kappa^2 - 2\kappa - 2}{\tau} + (2\kappa + 1) + \kappa^2\tau\right)S(E,\theta)$$

$$P_\tau(\tau) = [a_1 P_1(\tau) + a_2 P_2(\tau)]T\cos\theta$$

$$a_1 = \ln(1+2\kappa), \quad a_2 = \frac{2\kappa(1+\kappa)}{(1+2\kappa)^2}$$

$$P_1(\tau) = \frac{1}{\ln(1+2\kappa)}\frac{1}{\tau}; P_1(\tau) = \frac{(1+2\kappa)^2}{2\kappa(1+\kappa)}\tau$$

Simulation of Compton events

- Random values for cos θ from the PDF can be generated as:

$$\tau \equiv \frac{Ec}{E} = \frac{1}{1+\kappa(1-\cos\theta)}$$

$$\kappa = E / mc^2$$

$$\tau_{\min} = \frac{1}{1+2\kappa};\ \tau_{\max} = 1$$

The algorithm to sample cosθ

- Sample a value of the integer *i* (=1,2):

$$\pi(1) = \frac{a_1}{a_1 + a_2}; \; \pi(2) = \frac{a_2}{a_1 + a_2}$$ **(point probabilities)**

- Sample τ using:

$$\tau = \begin{cases} \tau_{\min}^{\xi} & \text{if } i = 1 \\ \left[\tau_{\min}^{\xi} + \xi(1 - \tau_{\min}^{2})\right]^{1/2} & \text{if } i = 2 \end{cases}$$

The algorithm to sample cosθ

- Determine cos θ using:

$$\cos\theta = 1 - \frac{1-\tau}{\kappa\tau}$$

- Generate a new random number ξ
- If ξ>T(cosθ), go to step 1
- Deliver cosθ

The algorithm to sample cosθ

- $\phi = 2\pi\xi$
- $E_e = E - E_c$
- $\phi_e = \phi + \pi$
- $\cos\theta_e$ is:

$$\cos\theta_e = \frac{E + mc^2}{E}\left(\frac{E\text{-}Ec}{2mc^2 + E - Ec}\right)^{1/2}$$

- $\lambda = 1/(n\sigma)$
- $s = -\lambda * \xi$

Simulating

- Using the algorithm described before we can generate the random walk of a photon incident in a wall
- Spreadsheet example