Monte Carlo radiation transport codes

How do they work ?

Michel Maire (Lapp/Annecy)

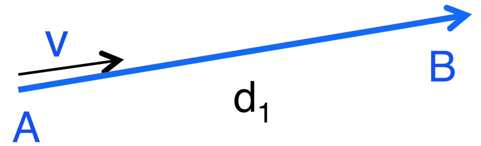
Outline

From simplest case to complete process :

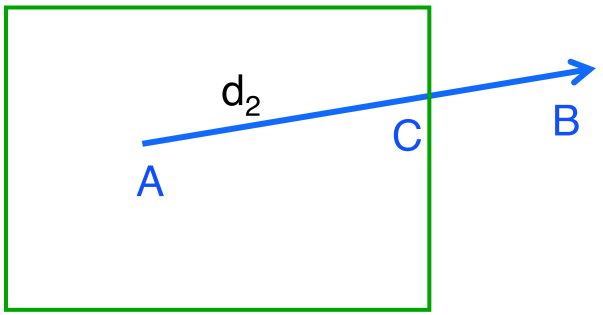
- Decay in flight of an unstable particle
- Photon Compton scattering in matter
- Multiple Coulomb scattering of charged particle ($e^{-/+}$)
- Ionization : energy loss by charged particle

Decay in flight (1)

- An unstable particle have a time of life τ
  initial momentum p (→ velocity v)
  → distance to travel before decay $AB = d_1 = \tau v$
  (non relativist)



- Geometry : the particle is inside a box.
  compute distance to boundary $AC = d_2$

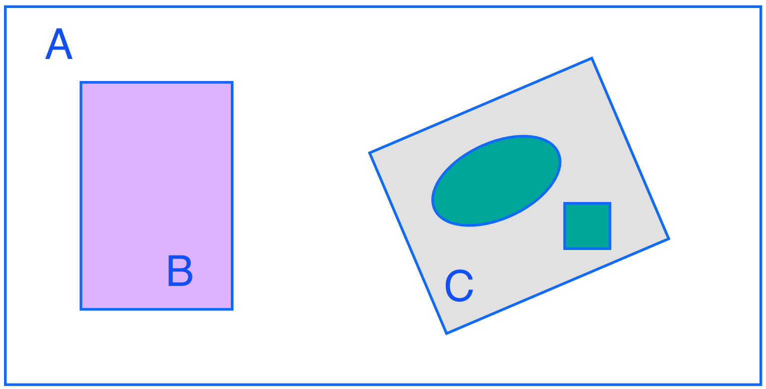


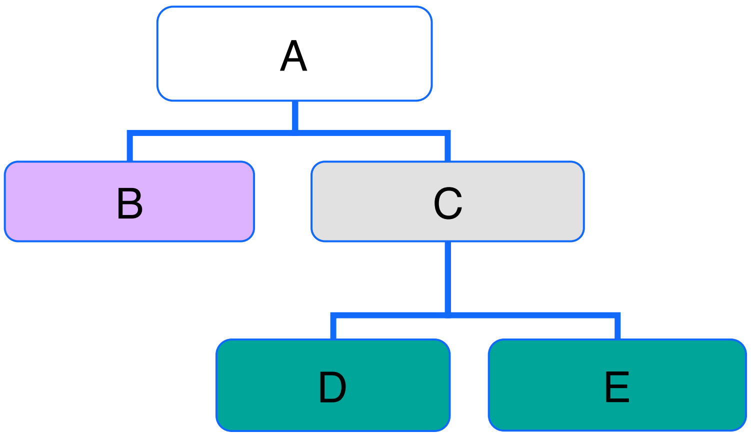
- Transport the particle $s = \min(d_1, d_2)$

- if C < B : do nothing in C,
  but compute the time spent in flight : $\Delta t = AC/v$
  if B < C : decay the particle

Geometry (1)

- The apparatus is described as an assembly of volumes made of homogeneous, amorphous materials
- Volumes can be embedded or assembled with boulean operations

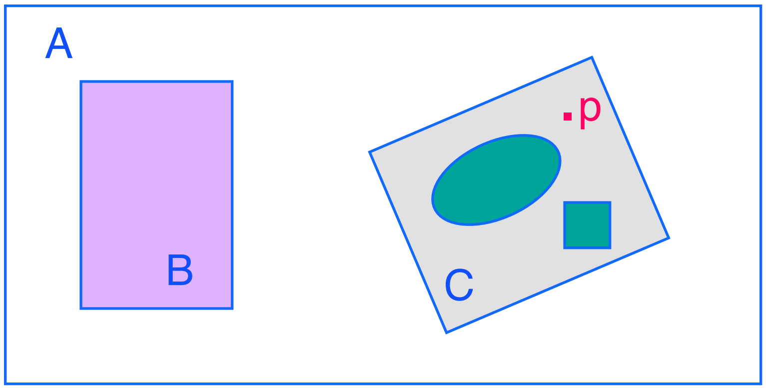


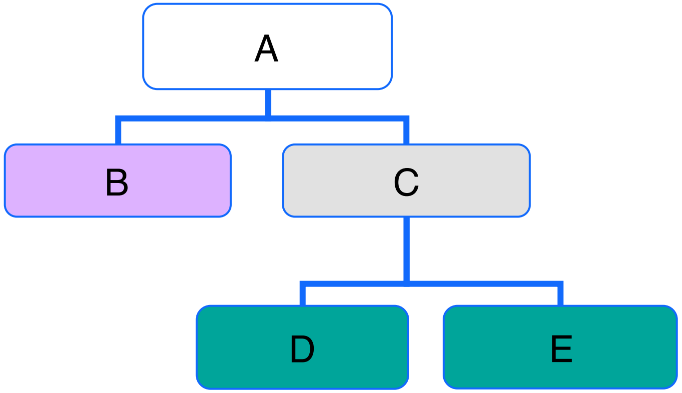


- when travelling inside the apparatus, the particle must know :
  - where I am ? → locate the current volume
  - where I am going ? → compute distance to next boundary

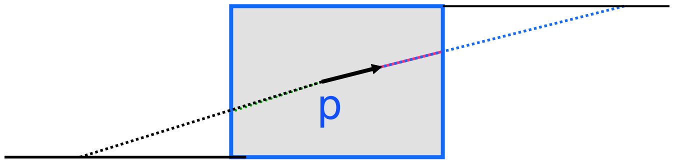
Geometry (2)

- remember : a computer program in blind …





- where I am ? → locate the current volume
- where I am going ? → compute distance to next boundary



example : a point P in a box

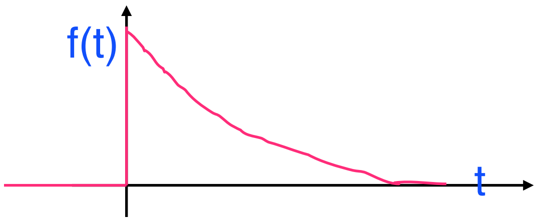
→ compute intersections with 6 planes

Decay in flight (2)

- The time of life, t, is a random variable with probability density function :

$$f(t) = \frac{1}{\tau}\exp\left(-\frac{t}{\tau}\right) \quad t \geq 0$$

τ is the mean life of the particle



- It can been demonstrated in a general way that the cumulative distribution function is itself a random variable with uniform probability on [0,1]

$$r = F(t) = \int_{-\infty}^{t} f(u)du$$

therefore : 1- choose r uniformly random on [0,1]

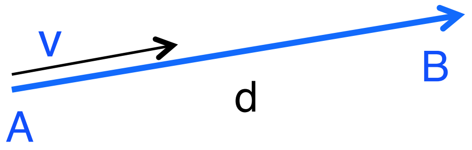
2 - compute $t = F^{-1}(r)$

- For the exponential law, this gives : $t = -\tau \ln(1- r) = -\tau \ln(r')$

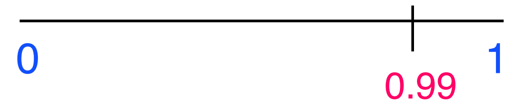
Decay in flight (3)

- When the particle travel on a distance d, one must update the elapsed time of life :

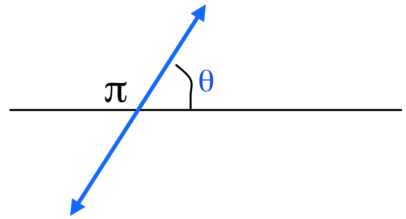
$$t \leftarrow (t - d/v)$$



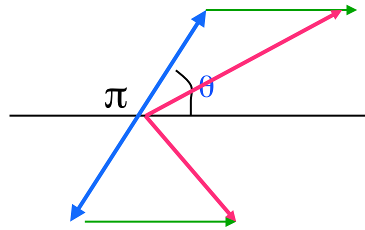
- When t = 0, one must trigger the decay of the of the particle
  - for instance $\pi^0 \rightarrow \gamma\,\gamma$ (~ 99%)
    $\rightarrow \gamma$ e+ e- (~1%)



- Select a channel according the branching ratio
  $\rightarrow$ choose r uniformly on [0,1]



- Generate the final state
  - in the rest fram of the π^0 : $d\Omega = \sin\theta\, d\theta\, d\phi$
  - apply Lorentz transform



Decay in flight : comments

- the generation of the whole process needs at least 4 random numbers

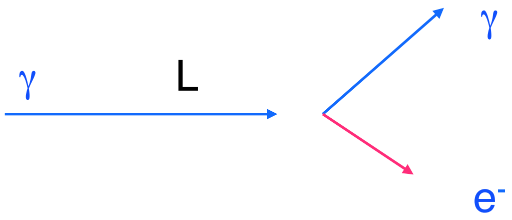
- the decay is the simplest but general scheme of the so called analogue Monte Carlo transport simulation

- comparison with geometry and particle transport : what is really needed is step length, not directly time of life

Compton scattering (1)

$\gamma + e^- \rightarrow \gamma + e^-$

The distance before interaction, L, is a random variable



cross section per atom : $\sigma(E,z)$

nb of atoms per volume : $n_{at} = \dfrac{\rho N}{A}$

cross section per volume : $\eta(E,\rho) = n_{at}\sigma$ (η is in 1/cm)

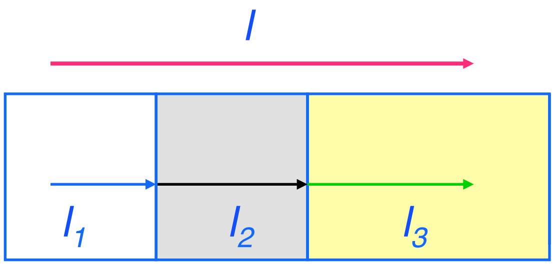
- $\eta(E,\rho)$ is the probability of Compton interaction per cm
- $\lambda(E,\rho) = \eta^{-1}$ is the mean free path associated to the process (Compton)

The probability distribution of L : $f(l) = \eta \exp(-\eta l) = \dfrac{1}{\lambda}\exp\left(-\dfrac{l}{\lambda}\right)$

→ Sample $l = -\lambda \ln(r)$ with r uniform in [0,1]

Compton scattering (2)

- $\lambda(E,\rho)$, and l, are dependent of the material
- one define the number of mean free path :



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

• n_λ is independent of the material and is a random variable with distribution : $f(n_\lambda) = \exp(-n_\lambda)$

- sample n_λ at origin of the track : $n_\lambda = -\ln(r)$
- update elapsed n_λ along the track : $n_\lambda \leftarrow (n_\lambda - dl_i / l_i)$
- generate Compton scattering when $n_\lambda = 0$

Compton scattering (3)

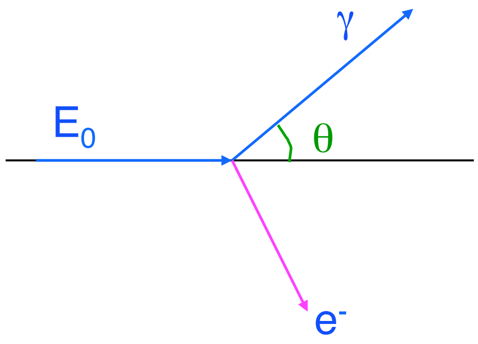
- Let define :

energy of the scattered photon : $\varepsilon = \frac{E}{E_0}$

kinetic energy of scattered e$^-$: $t = \frac{T}{E_0} = 1 - \varepsilon$

angle of scattered photon : $\sin^2\left(\frac{\theta}{2}\right) = \frac{mc^2}{2E_0}\left[\frac{1}{\varepsilon} - 1\right]$

$\rightarrow$ then $\varepsilon \in [\varepsilon_0, 1]$ with $\varepsilon_0 = \frac{mc^2}{mc^2 + 2E_0}$



- the differential cross section is :

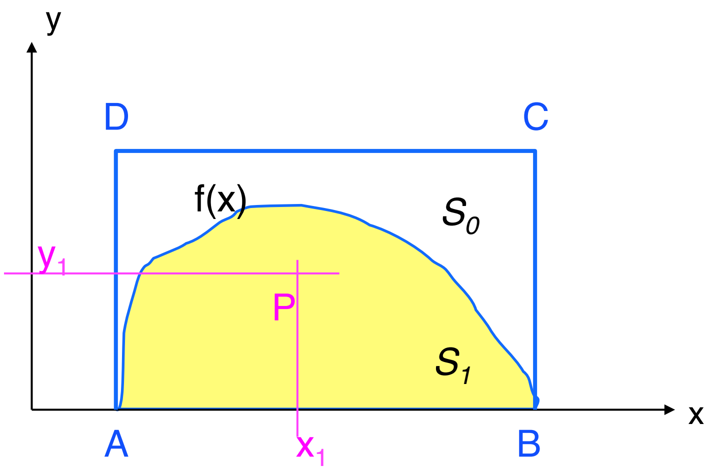
$$\frac{d\sigma}{d\varepsilon} = \frac{K}{E_0^2}\left[\frac{1}{\varepsilon} + \varepsilon\right]\left[1 - \frac{\varepsilon \sin^2(\theta/2)}{1+\varepsilon^2}\right] = \frac{K}{E_0^2} d(\varepsilon) w(\varepsilon)$$

- sample ε with the ‘acceptation-rejection’ method

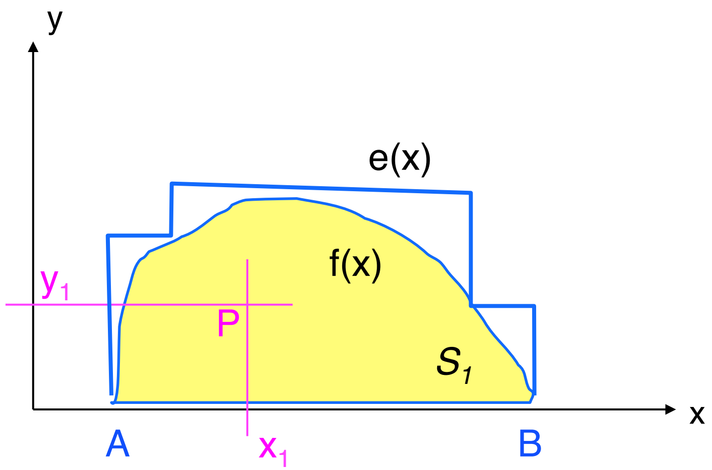
→ *remark : the generation of the whole Compton scattering process needs at least 5 random numbers*

MC : acceptation-rejection method (1)

- let f(x) a probability distribution.
  S_1 the surface under f
- assume we can enclose f(x) in a box ABCD, of surface S_0
- choose a point $P(x_1,y_1)$ uniformly random within S_0
- accept P only if P belong to S_1



→ x will be sample according to the probability distribution f



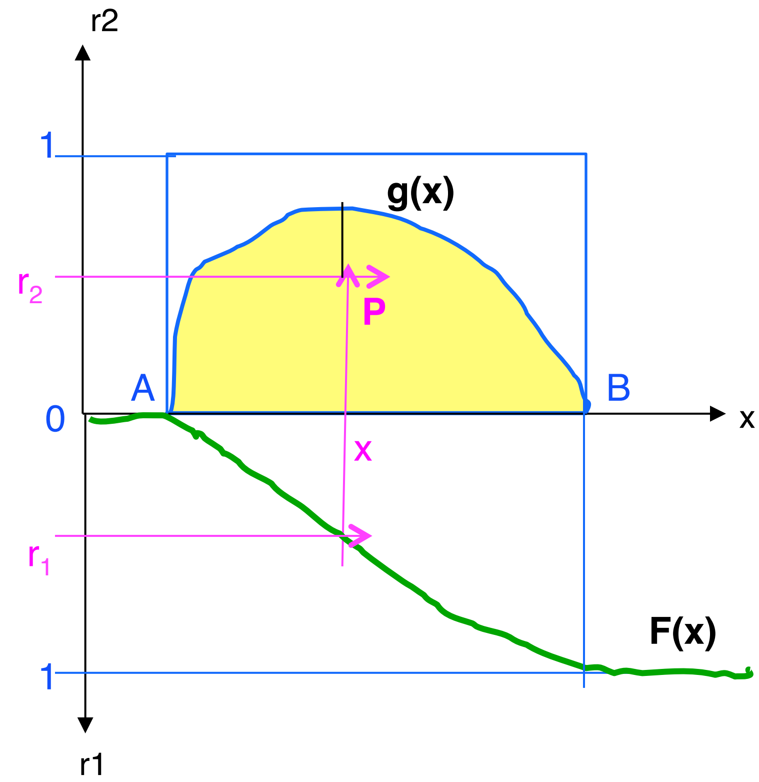
- the envelope can be a distribution function e(x) simple enough to be sampled with inversion technique
- In this case x in sampled with e(x) and rejected with f(x)

MC : acceptation-rejection method (2)

- assume that we can factorize : P(x) = K f(x) g(x)
  - f(x) : probability distribution simple enough to be inverted
  - g(x) : 'weight' function with values in [0,1]
  - K > 0 : constant to assure proper normalization of f(x) and g(x)

→ step 1 : choose x from f(x) by inversion method

→ step 2 : accept-reject x with g(x)

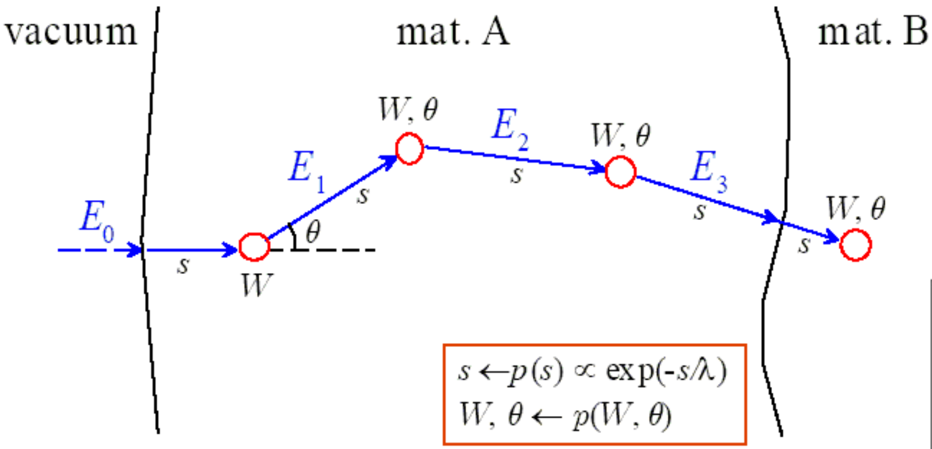


• even : P(x) = K1 f1(x) g1(x) + K2 f2(x) g2(x) + …

→ step 0 : choose term i with probability Ki

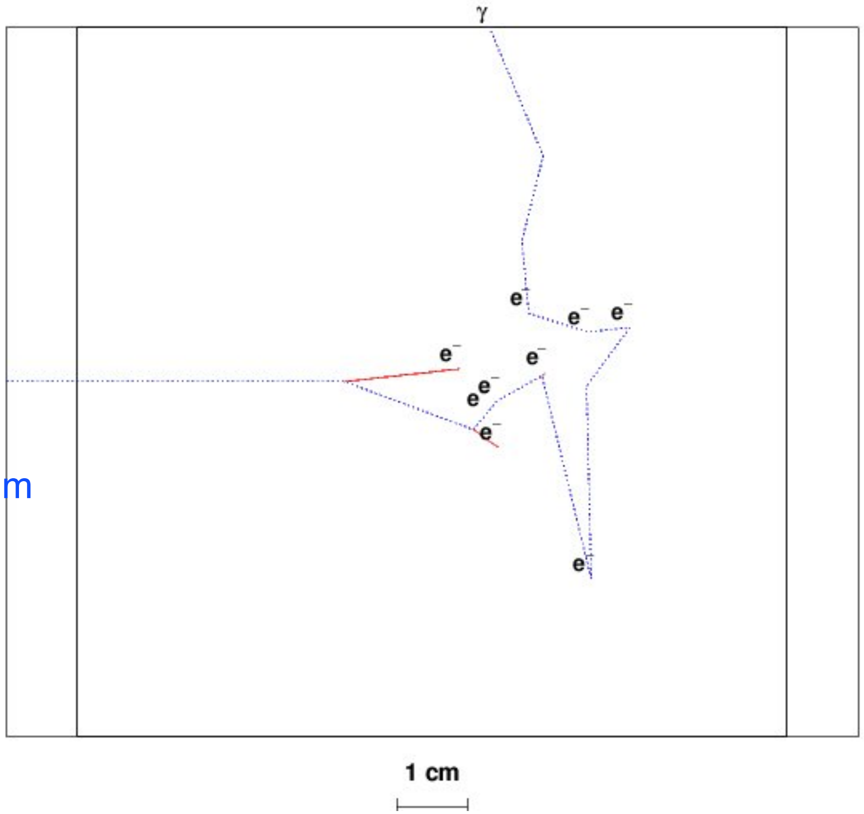
Detailed (analogue) simulation

- All interaction events are simulated in chronological succession:



- The method is nominally exact (for energies higher than ~ 1 keV)
- Feasible only for **photons** and **low-energy electrons and positrons**
- High-energy electrons and positrons are more difficult...

CERN 27/06/2006

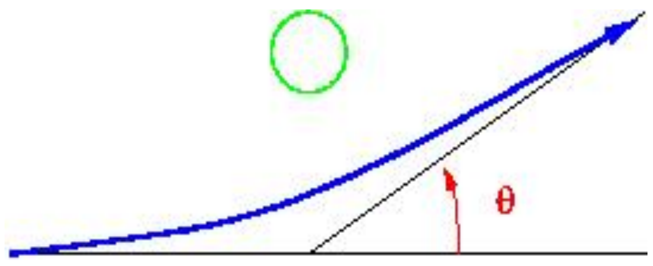


γ 10 MeV in Aluminium

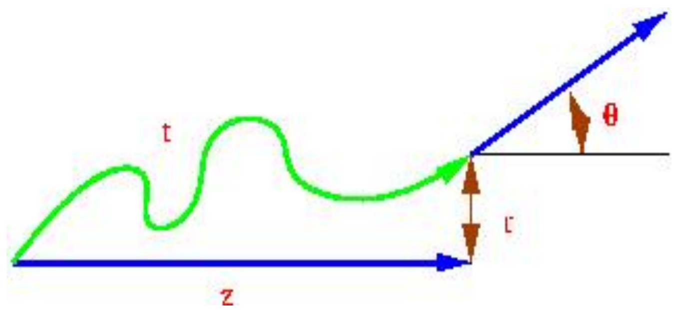
Simulation of charged particles ($e^{-/+}$)

- Deflection of charged particles in the Coulomb field of nuclei.
  - small deviation; pratically no energy loss
- In finite thickness, particles suffer many repeated elastic Coulomb scattering
  - $> 10^6$ interactions / mm
- The cumulative effect is a net deflection from the original particle direction
- Individual elastic collisions are grouped together to form 1 multiple scattering

→ condensed history technique (class 1 algorithms)

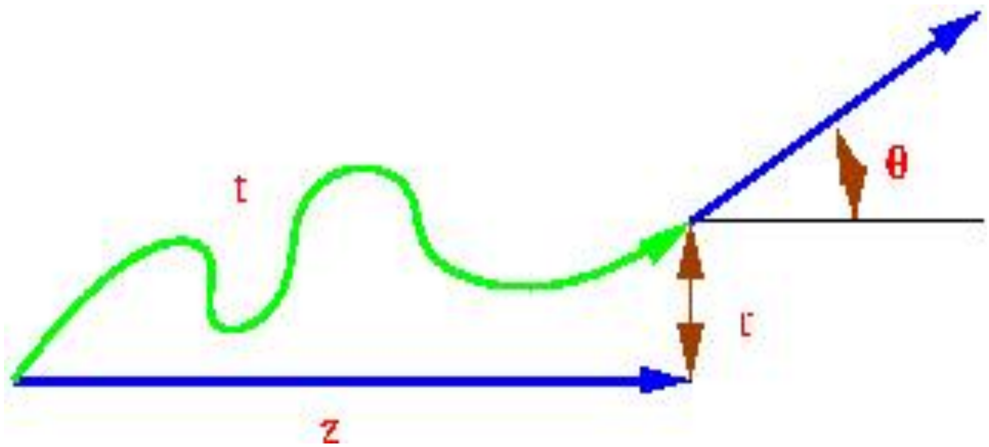


single atomic deviation



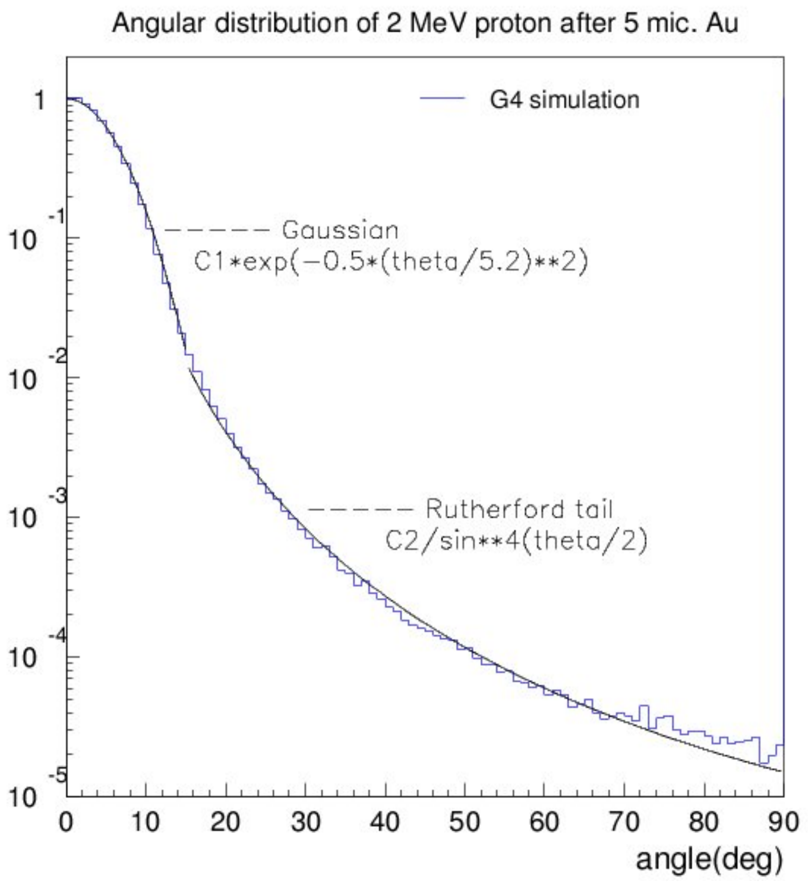
macroscopic view

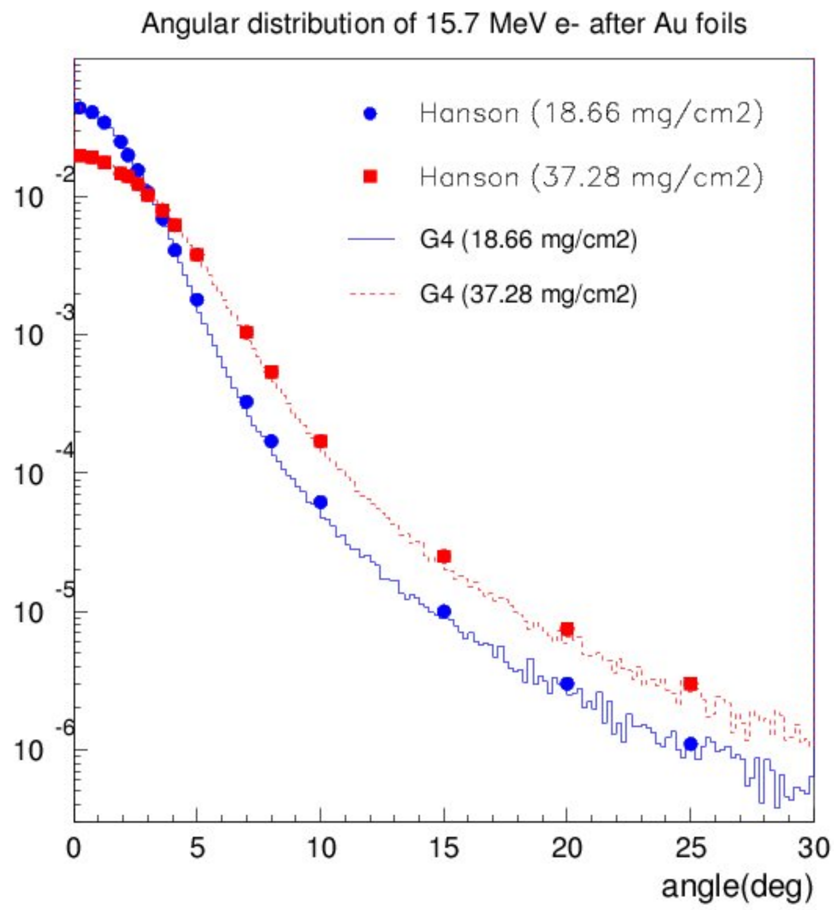
Multiple Coulomb scattering (1)



- longitudinal displacement : z *(or geometrical path length)*
- lateral displacement : r, Φ
- true (or corrected) path length : t
- angular deflection : θ, ϕ

Multiple Coulomb scattering (2)

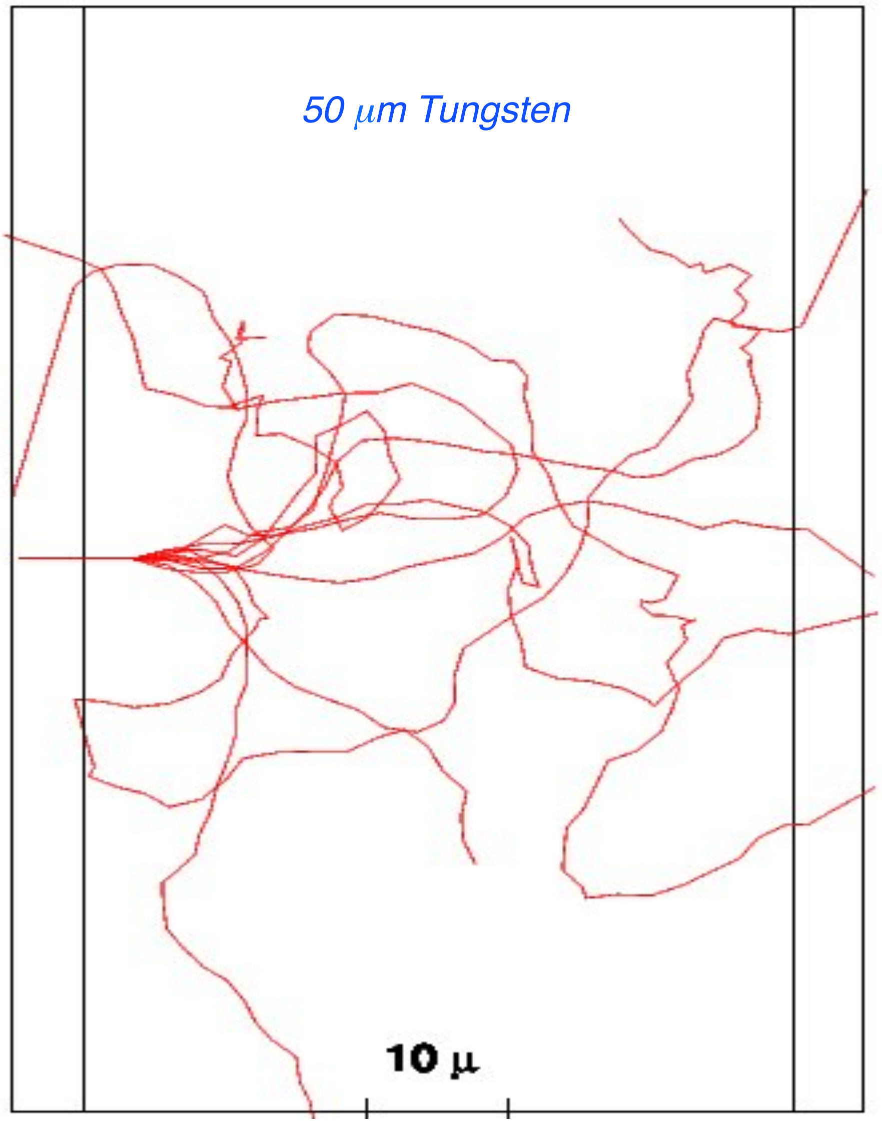


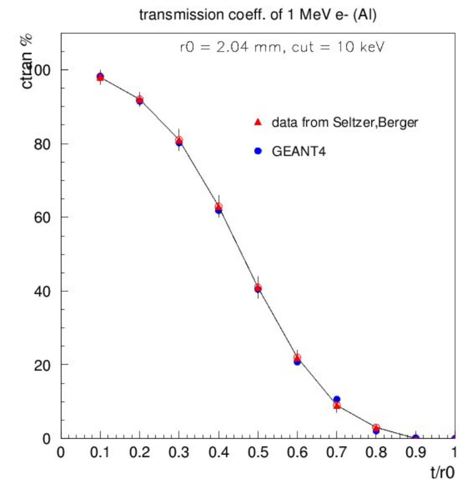


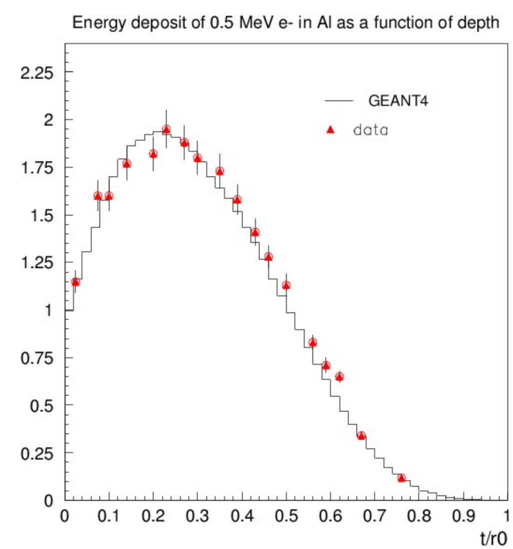
Multiple Coulomb scattering (3)

10 e⁻

600 keV

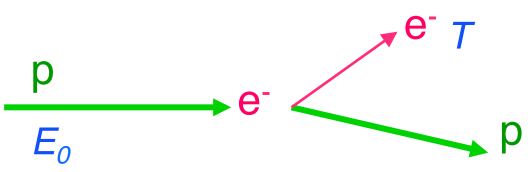


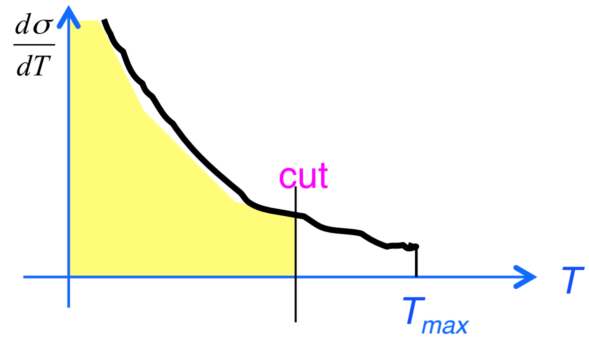




Ionization (1)

A charged particle hits a quasi-free electron (δ-ray)





$$\frac{d\sigma(E_0,T)}{dT}$$: cross section for the ejection of an e^- of energy T

mean energy of a 'soft' e^- : $\left\langle T_{soft}(E_0)\right\rangle_{cut} = \frac{1}{\sigma_{tot}}\int_0^{cut}\frac{d\sigma(E_0,T)}{dT}T\,dT$

mean energy lost by the projectile due to sub cutoff e^- : $\left(\frac{dE}{dx}\right)_{cut} = n_{at}\sigma_{tot}\left\langle T_{soft}\right\rangle_{cut}$

cross section for creation of an e^- with T > cut : $\sigma(E_0,cut) = \int_{cut}^{T_{max}}\frac{d\sigma(E_0,T)}{dT}dT$

Ionization (2)

mean energy lost by the projectile due to sub cutoff e$^-$: $\left(\frac{\mathrm{dE}}{\mathrm{dx}}\right)_{cut} = n_{at}\sigma_{tot}\left\langle T_{soft}\right\rangle_{cut}$

→accounted in the condensed history of the incident particle

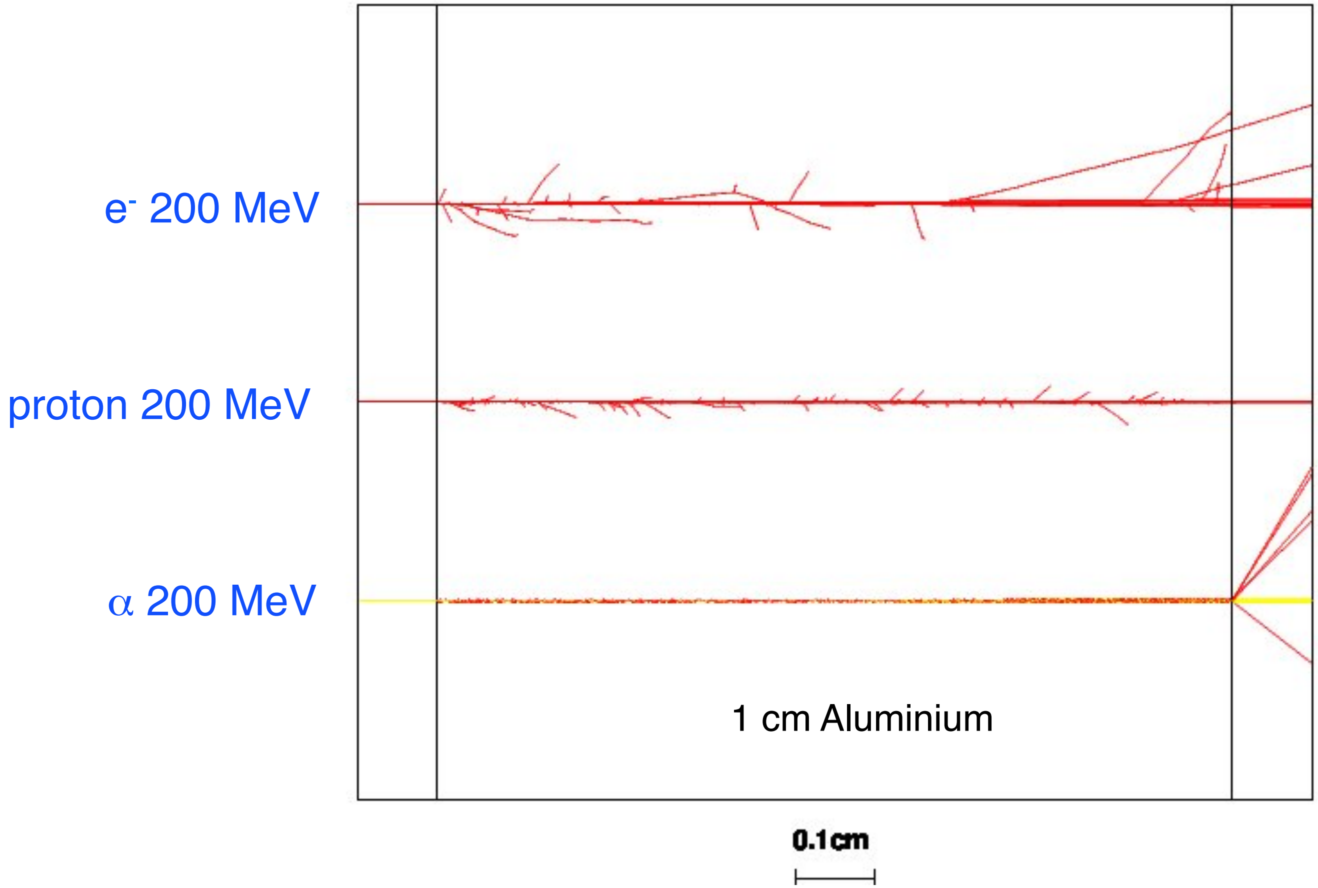
dE/dx is called (restricted) stopping power or linear energy transfered

cross section for creation of an e$^-$ with T > cut : $\sigma(E_0, cut) = \int_{cut}^{T_{\max}} \frac{d\sigma(E_0,T)}{dT} dT$

→ explicit creation of an e$^-$: analogue simulation

Ionization (3)

‘hard’ inelasic collisions → δ-rays emission

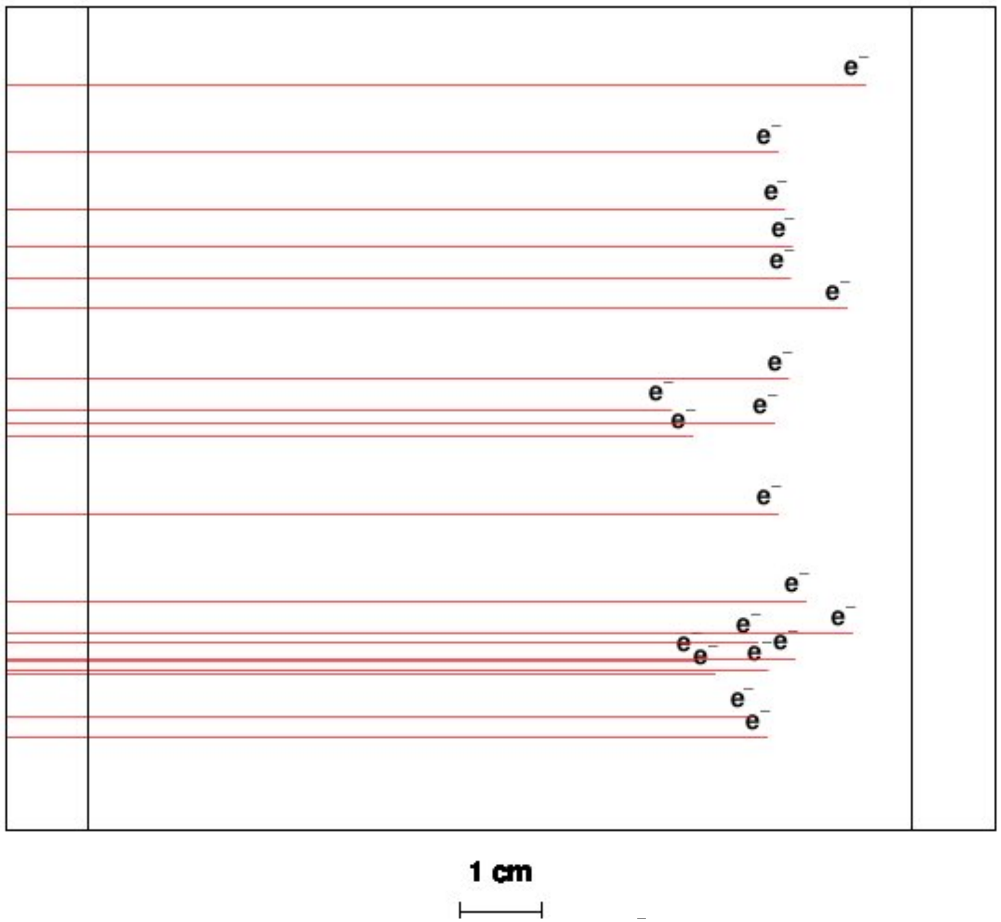


Ionization (4)

straggling : ΔE = [ΔE] + fluctuations

e- 16 MeV in water

(muls off)



Condensed history algorithms

group many charged particles track segments into one single 'condensed' step

grouped collisions

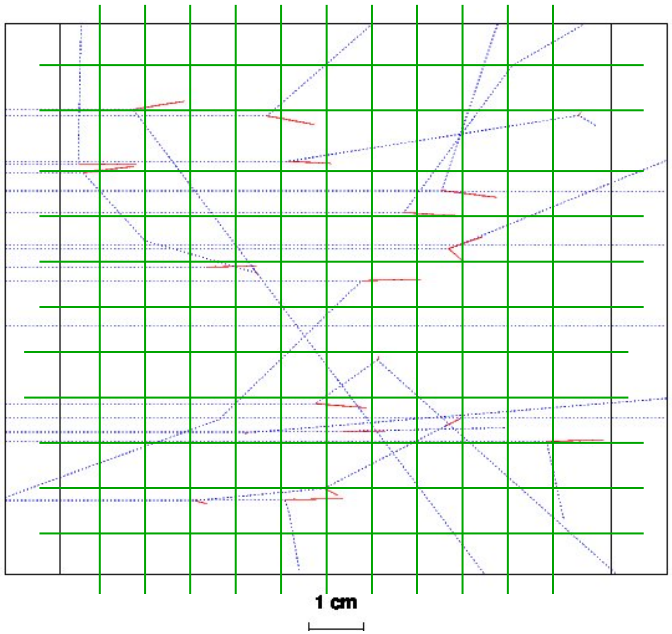
- elastic scattering on nucleus
  - multiple Coulomb scattering
- soft inelastic collisions
  - collision stopping power (restricted)
- soft bremsstrahlung emission
  - radiative stopping power (restricted)

discrete collisions

- 'hard' δ-ray production
  - energy > cut
- 'hard' bremstrahlung emission
  - energy > cut
- positron annihilation

Principle of Monte Carlo dose computation

- Simulate a large number of particle histories until all primary and secondary particles are absorbed or have left the calculation grid
- Calculate and store the amount of absorbed energy of each particle in each region (voxel)
- The statistical accuracy of the dose is determined by the number of particle histories



$$\text{mean value : } \langle D \rangle = \frac{1}{N} \sum_{i=1}^{N} D_i$$

$$\text{root mean square (rms) : } \sigma = \sqrt{\langle D^2 \rangle - \langle D \rangle^2}$$

$$\text{precision on mean : } \Delta D = \frac{\sigma}{\sqrt{N}}$$

A non exhaustive list of MC codes (1)

- ETRAN (Berger, Seltzer; NIST 1978)
- EGS4 (Nelson, Hirayama, Rogers; SLAC 1985)

  www.slac.stanford.edu/egs
- EGS5 (Hirayama et al; KEK-SLAC 2005)

  rcwww.kek.jp/research/egs/egs5.html
- EGSnrc (Kawrakow and Rogers; NRCC 2000)

  www.irs.inms.nrc.ca/inms/irs/irs.html
- Penelope (Salvat et al; U. Barcelona 1999)

  www.nea.fr/lists/penelope.html

A non exhaustive list of MC codes (2)

- Fluka (Ferrari et al; CERN-INFN 2005)
  www.fluka.org
- Geant3 (Brun et al; CERN 1986)
  www.cern.ch
- Geant4 (Apostolakis et al; CERN++ 1999)
  geant4.web.cern.ch/geant4
- MARS (James and Mokhov; FNAL)
  www-ap.fnal.gov/MARS
- MCNPX/MCNP5 (LANL 1990)
  mcnpx.lanl.gov