Radiation Transport Calculations by a Monte Carlo Method

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Monte Carlo Method

- A method used to solve a problem with random numbers is called a "Monte Carlo Method".
- A name of "Monte Carlo" was introduced by J. von Neumann and S. M. Ulam.

- Random numbers are key tool for the Monte Carlo method

Random numbers

- Use a dice, a roulette *etc.*– very slow.
- Use a table of random numbers.
  - A table of random numbers has been well examined concerning its statistical characteristics.
  - It is required to store a whole table in computer data storage.
  - It is currently is not very fast to produce random numbers.
- Use physical random numbers like the decay of a radioisotope.
  - It is not easy to digitalize, and has a weakness concerning stability and reproducibility.

Pseudo random Numbers

- Produce random numbers successively from a seed random number, R_0, using a recurrence formula in the form of $R_{n+1}=f(R_n)$
- Pseudo random number residuals by a divider, *m*.
- There are m different integers at most and, therefore, pseudo random numbers have a limited period.
- God pseudo random numbers
  - Fast to create
  - A long sequence
  - Reproducibility
  - Good statistical characteristics
  - It is possible to create pseudo random number between 0 and 1 by dividing by m.

Another Type of Random Number Generator

- RANECU random number generator
  - F. James, “A review of pseudorandom number generators”, *Comp. Phys Comm* **60** (1990) 329-344.
  - Periodicity --- 10^{18}
  - Can be easily controlled by 2 seeds (iseed1 and iseed2)
  - Use as the random number generator of egs5
- Marasaglia-Zaman random number generator
  - G. Masaglia and A. Zaman, “A New Class of Random Number Generator”, *Annals of Applied Probability* 1(1991)462-480.
  - Long periodicity –2^{144} ~10^{43}.
  - Portable to all 32-bit machines

Pseudo Random Number

- Linear congruence methods proposed by D. H. Lehmer is most widely used. $R_{n+1}=mod(aR_n+b,m)$
- *a, b* and *m* are positive integer and *m* is the length of the integer value allowed in the compiler.

Name	a	b	m
RANDU	65539	0	2^{31}
SLAC RAN1	69069	0	2^{31}
SLAC RAN6	663608491	0	2^{31}

Production of pseudo random numbers using pocket calculator

- Produce 10 random numbers for R_0=3, a=5, b=0 and m=16.
- Confirm that the same random sequence appears from some point.
- What is a sequence in this case ?
- Check for a different R_0.

n	R_n	R_n*5	R_{n+1}=mod(R_n*a,m)
0	R_0=3	15	R_1=15-INT(15/16)*16=15
1			
2			
3			

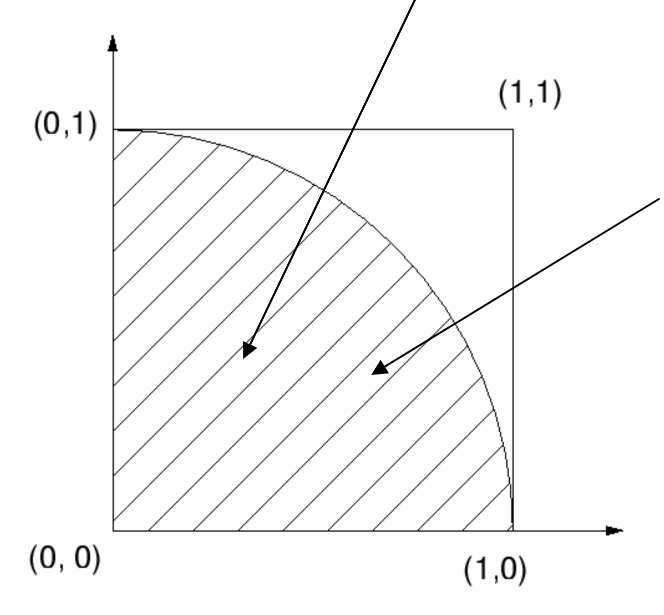
mod(R_n*a,m)= R_n*a-INT(R_n*a/m)

INT(15/16)=0

Calculation π using random numbers

- Select 2 random numbers from an arbitrary place in Table 2 (created using SLAC RAN6) in order
- Count the number of pair which satisfy

$$R = \sqrt{\xi^2 + \eta^2} \leq 1.0$$



AREA= π /4

π= 4 x (probability within this area)

Discrete probability process

- If a probability variable (x) takes on discrete value (x_i) with probabilities (p_i) such that

$$F(x_n) = \sum_{i=1}^{n} p_i = 1,$$

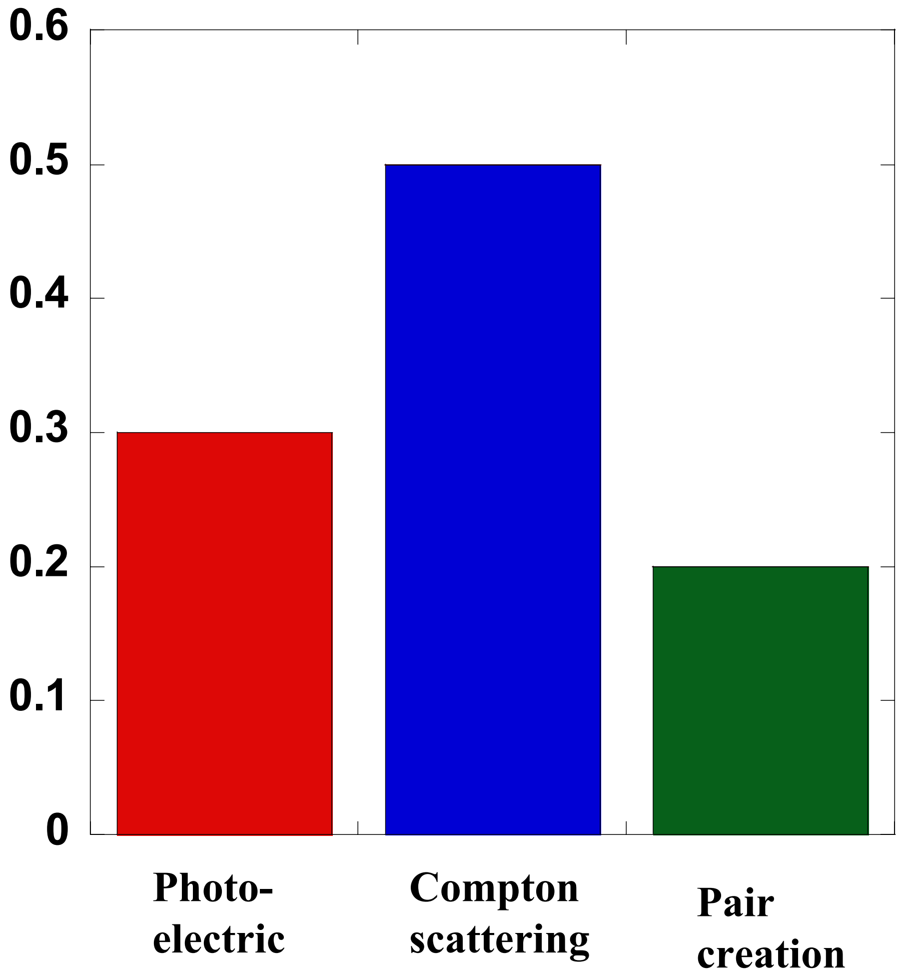
Cumulative probability function (PDF)

- $x = x_i$ if

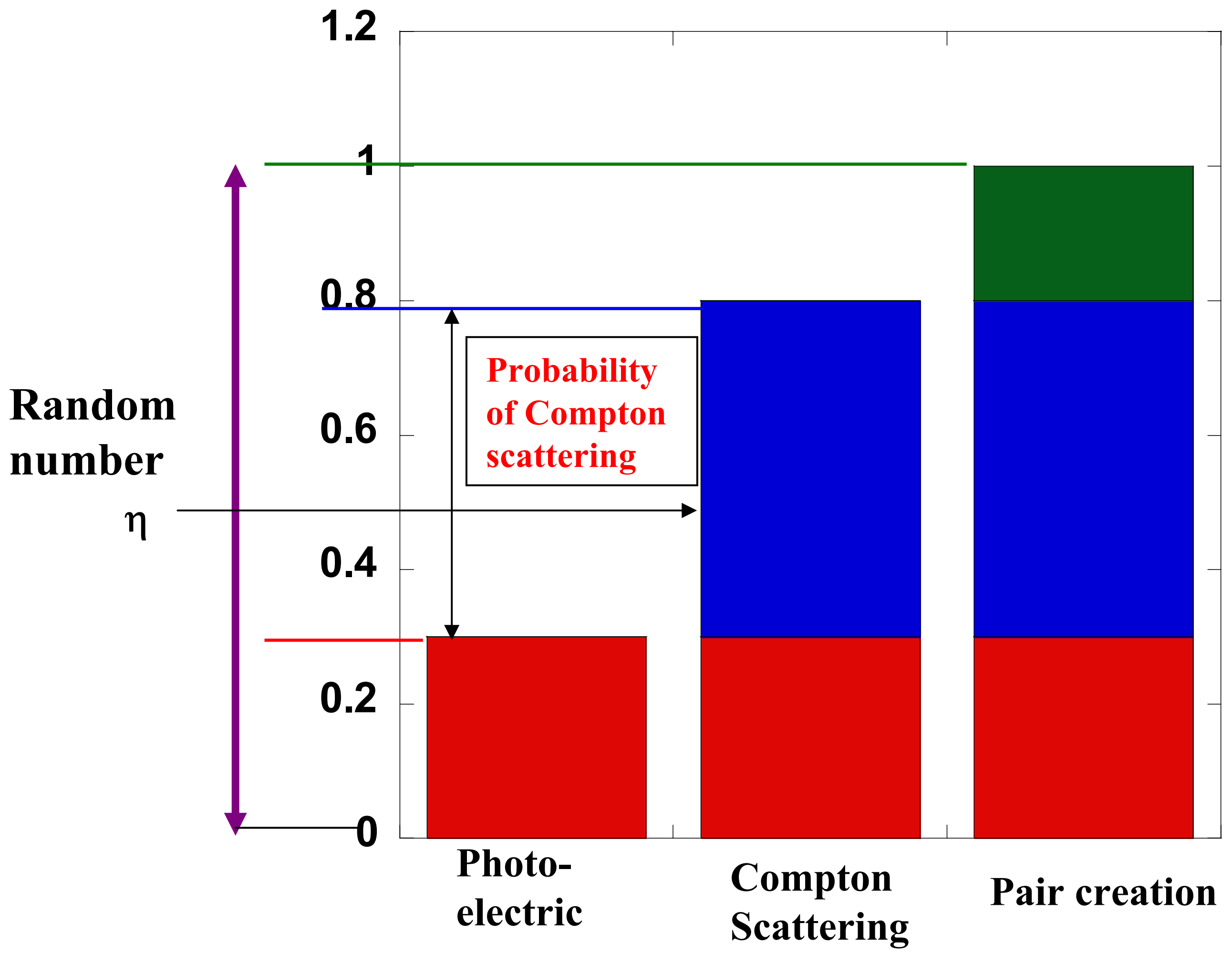
$$F(x_i) = \sum_{j=1}^{i} p_j \leq \eta < F(x_{i+1}) = \sum_{j=1}^{i+1} p_j$$

Discrete type sampling(1)

Example) Sample reaction when photoelectric is 30%, Compton scattering 50% and pair production 20%.



Discrete type sampling (2)



Cumulative probability function (pdf)

Example – determination of photon reaction

- The probability of the photoelectric effect, Compton scattering and pair creation at a photon interaction are P_{photo}, P_{Compt} and P_{pair}, respectively.
- $P_{photo} + P_{Compt} + P_{pair} = 1$
- $\eta \leq P_{photo}$, photoelectric
- $P_{photo} \leq \eta < P_{photo} + P_{Compt}$, Compton scattering
- $P_{photo} + P_{Compt} \leq \eta$, pair creation

Sampling method (direct sampling)

- A probability distribution function (PDF:*f(x)*) is defined over the range [*a,b*].

$$(\int_a^b f(x)dx = 1)$$

- Its cumulative probability function (CDF:*F(x)*)

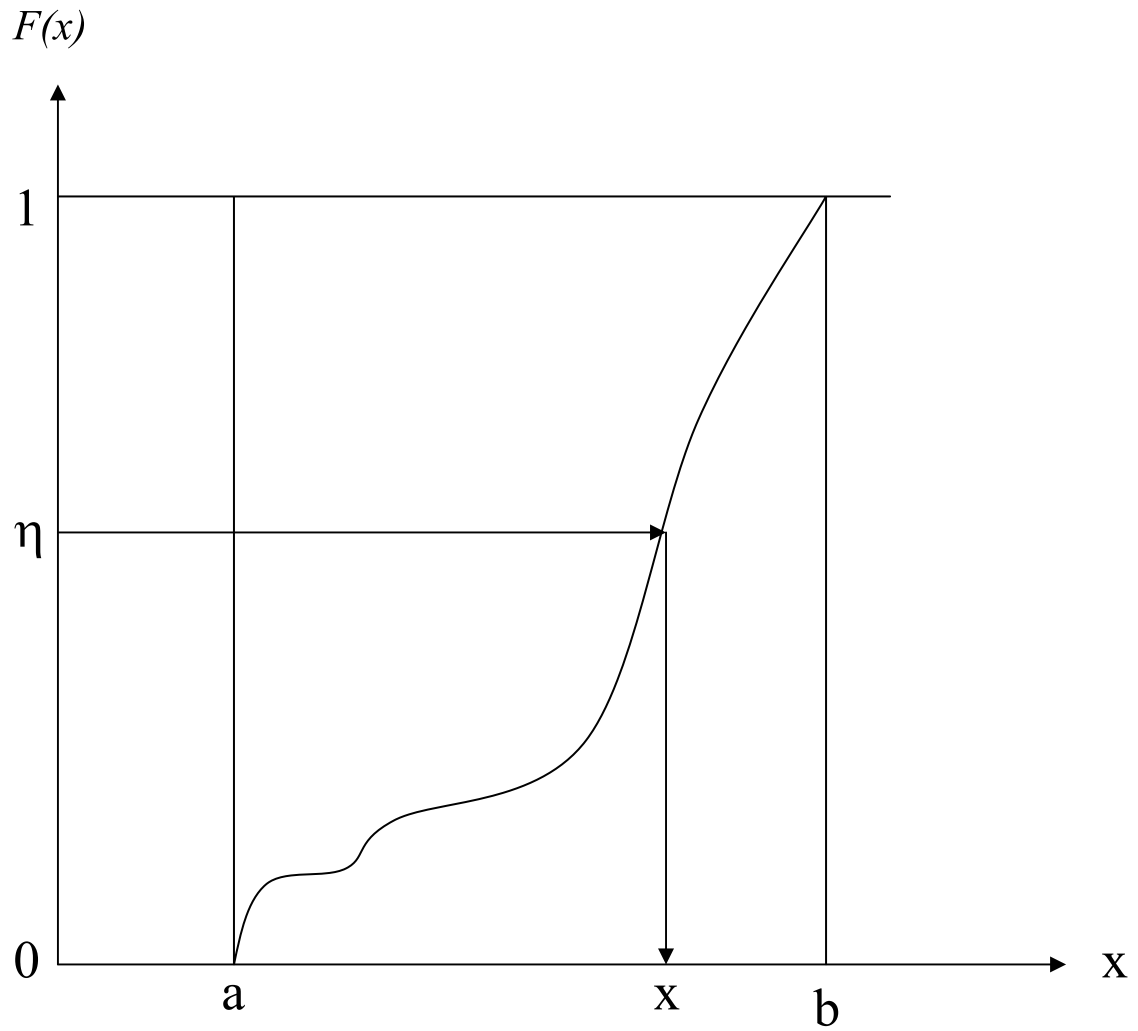
$$F(x) = \int_a^x f(x_i)dx_i$$

- By its definition, we can map F(x) onto a range of random variable, η, where $0 \le \eta \le 1$.

  Having mapped the random number onto F(x), we may invert the equation to give

$$x = F^{-1}(\eta)$$

The way to determine *x* by solving the above equation is called a "direct method".


F(x)
1
η
0
a
x
b
x

Example-determination of flight distance

- If the interaction probability of a particle per unit distance is Σ_t, the probability that a first interaction occurs between l and $l+dl$ is

$$p(l)dl = e^{-\Sigma_t l}\Sigma_t dl$$

$$\eta = P(l) = \int_0^l p(l_1)dl_1 = 1 - e^{-\Sigma_t l}$$

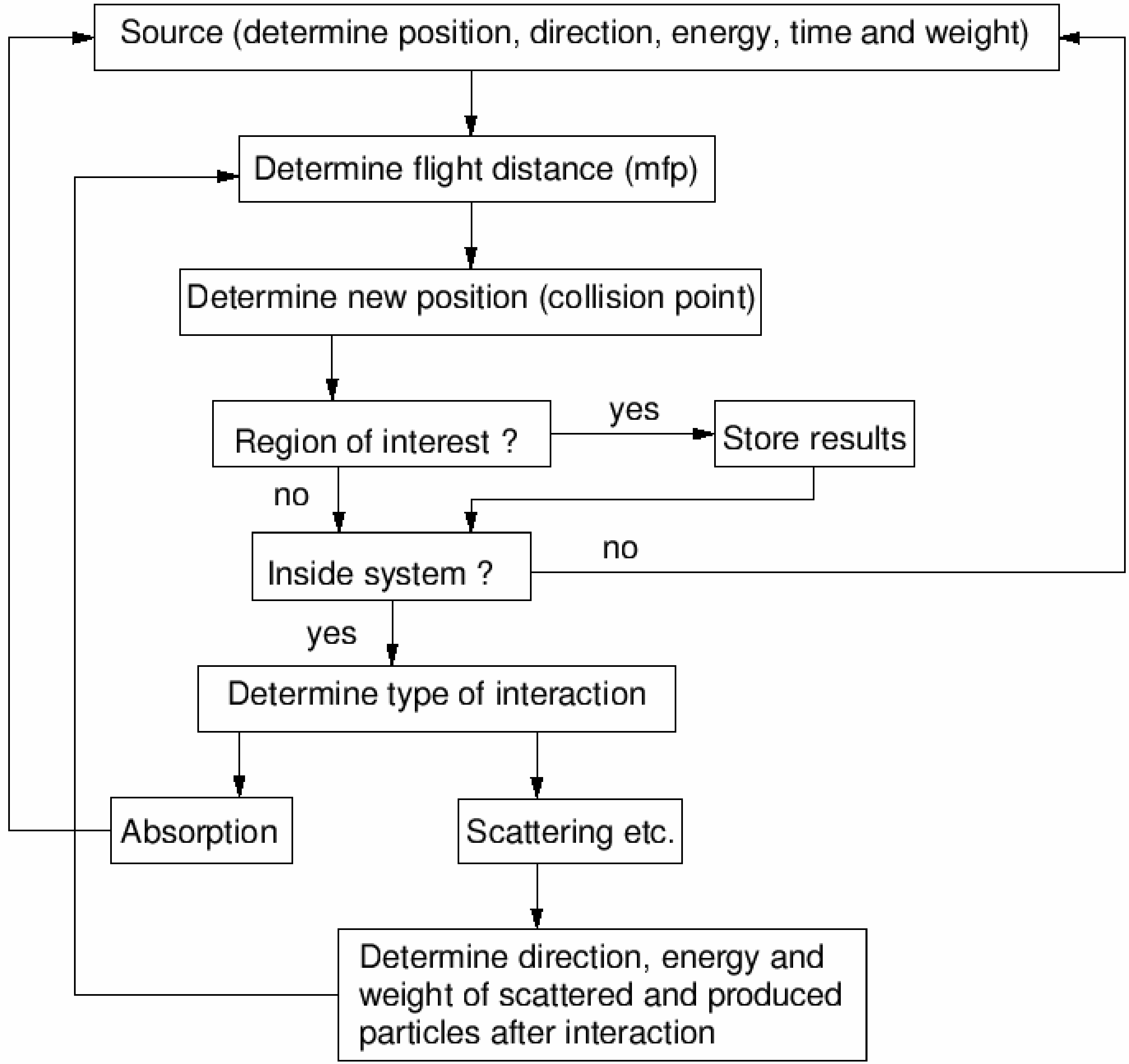
$$l = -\frac{1}{\Sigma_t}\ln(1-\eta) = -\lambda \ln(1-\eta)$$

l : flight distance

λ: mean free path

$1-\eta$ is equivalent to η

$$\boxed{l = -\lambda \ln(\eta)}$$



Source (determine position, direction, energy, time and weight)
Determine flight distance (mfp)
Determine new position (collision point)
Region of interest ?
yes
Store results
no
Inside system ?
no
yes
Determine type of interaction
Absorption
Scattering etc.
Determine direction, energy and weight of scattered and produced particles after interaction

Red:in User Code

Black:egs5

Infinite geometry

Photon

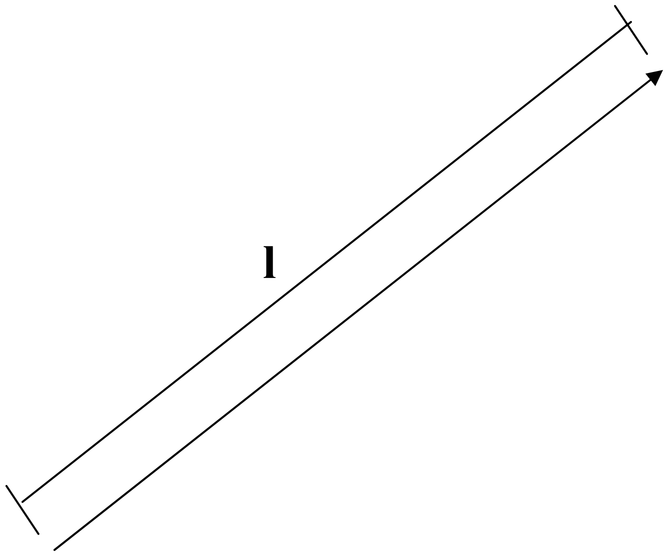
Initial Condition：Energy、Position、Direction

$E_0, X_0, Y_0, Z_0, U_0, V_0, W_0$

Determine Interaction Point

$$l=-\ln(\delta)/\mu$$

$$x=x_0+u_0l,\ y=y_0+v_0l.\ z=z_0+w_0l$$



Initial Condition：Energy、Position、Direction

$$e_0,\ x_0,\ y_0,\ z_0,\ u_0,\ v_0,\ w_0$$

Determine Interaction Type

Photoelectric：a, Compton scattering:b,

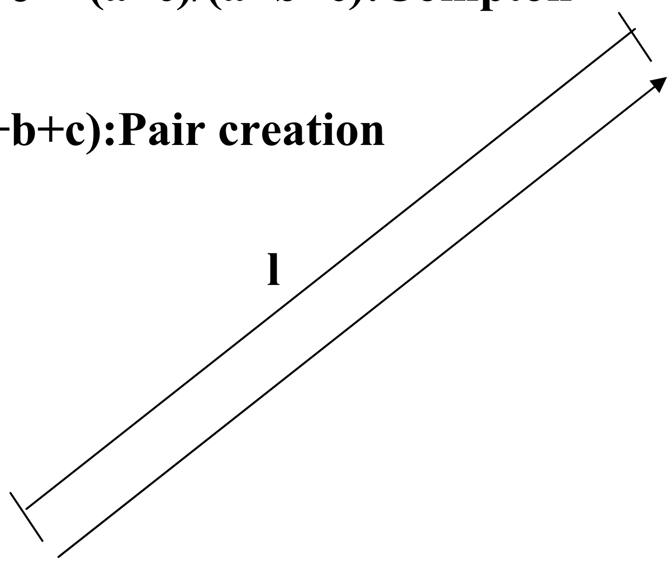
Pair creation：c

$\delta <= a/(a+b+c)$:Photoelectric

$a/(a+b+c) < \delta <= (a+c)/(a+b+c)$:Compton scattering

$\delta > (a+c)/(a+b+c)$:Pair creation

$x = x_0 + u_0 l$, $y = y_0 + v_0 l$. $z = z_0 + w_0 l$

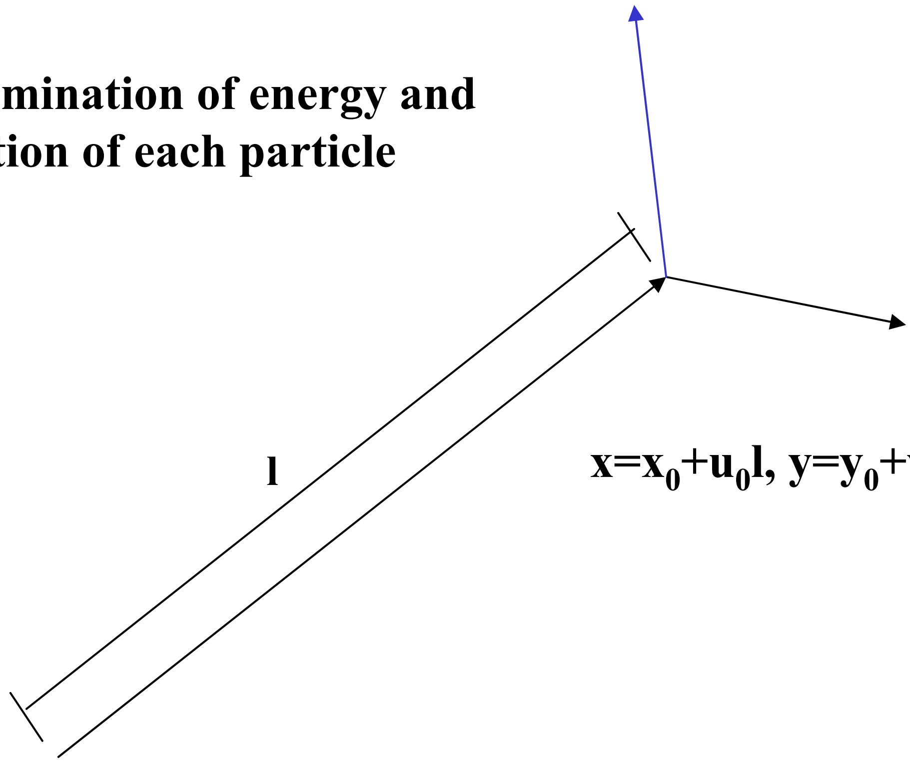


Initial Condition：Energy、Position、Direction

e_0, x_0, y_0, z_0, u_0, v_0, w_0

Follows produced particle

Determination of energy and direction of each particle



$$x=x_0+u_0 l,\ y=y_0+v_0 l.\ z=z_0+w_0 l$$

Initial Condition：Energy、Position、Direction

$e_0,\ x_0,\ y_0,\ z_0,\ u_0,\ v_0,\ w_0$

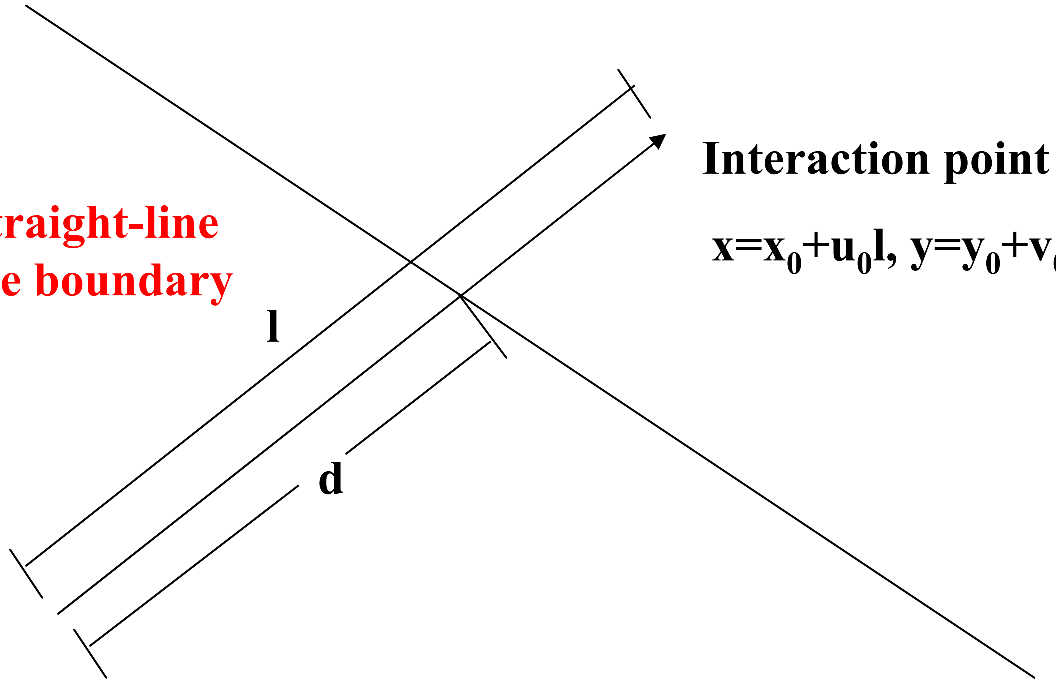
d>l：Move to Interaction point

d<=l：Move a distance d

Same material：Distance to Interaction point=l-d

Different material：Determine Interaction point

Region boundary



Interaction point：

$x=x_0+u_0l$, $y=y_0+v_0l$. $z=z_0+w_0l$

Calculate a straight-line distance to the boundary

(HOWFAR)

Initial Condition：Energy、Position、Direction

e_0, x_0, y_0, z_0, u_0, v_0, w_0

Store Information (AUSGAB)

Particle moves：Energy deposition

Track length

Boundary crossing

Photoelectric：Energy deposition

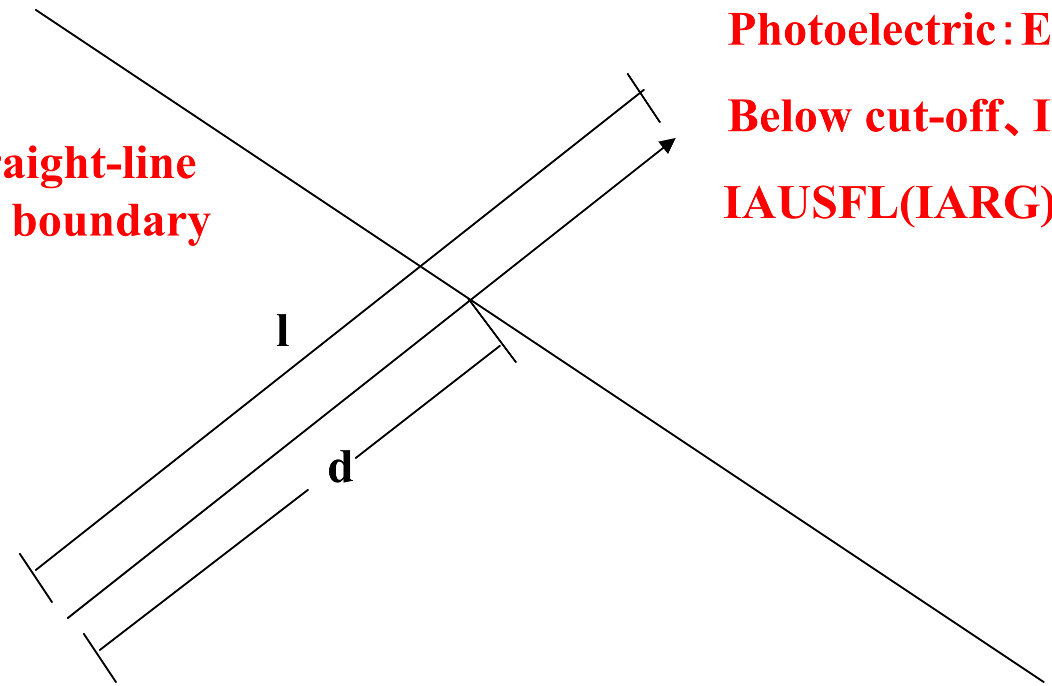
Below cut-off、IDISC=1

IAUSFL(IARG)=1:optional

Region boundary

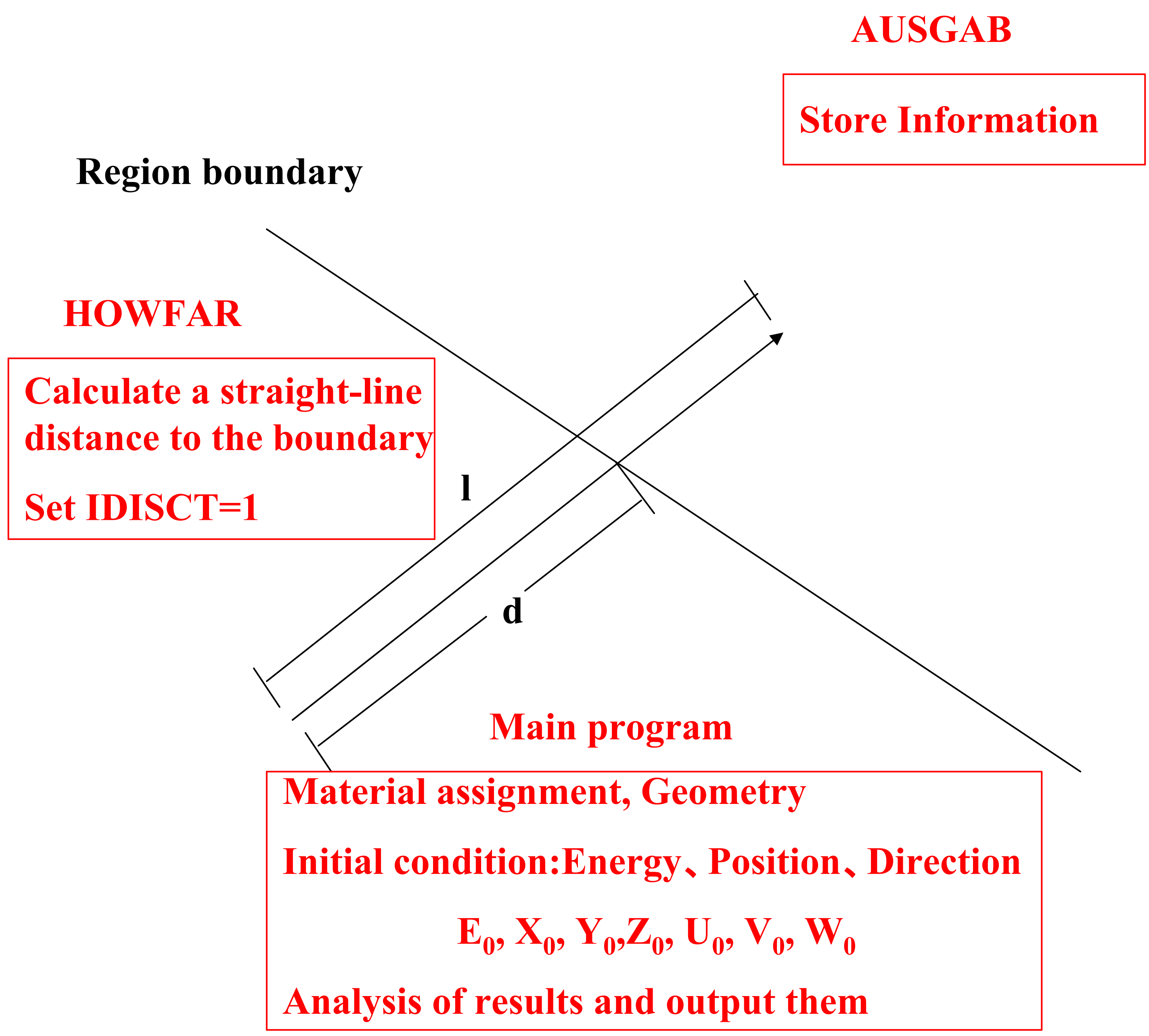
Calculate a straight-line distance to the boundary

(HOWFAR)



Initial Condition：Energy、Position、Direction

e_0, x_0, y_0, z_0, u_0, v_0, w_0



AUSGAB
Store Information
Region boundary
HOWFAR
Calculate a straight-line distance to the boundary
Set IDISCT=1
l
d
Main program
Material assignment, Geometry
Initial condition:Energy、Position、Direction
E_0, X_0, Y_0,Z_0, U_0, V_0, W_0
Analysis of results and output them

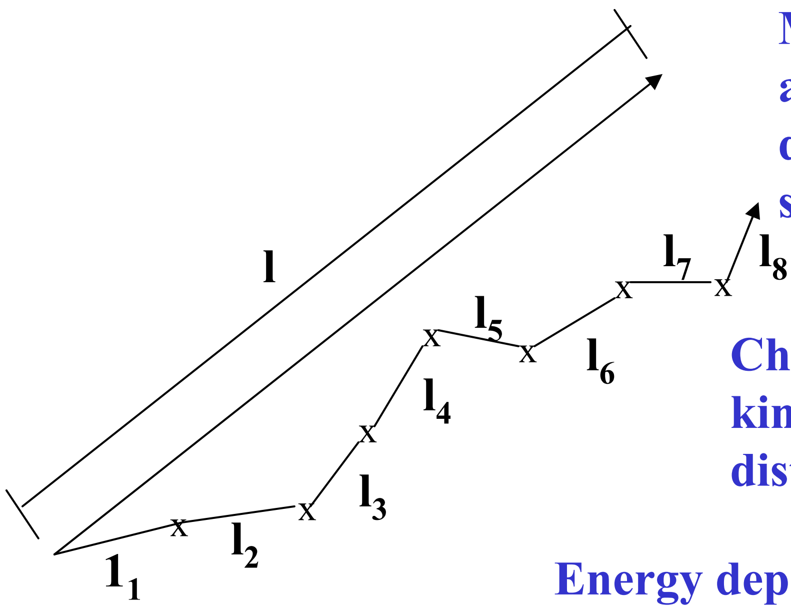
It is difficult to treat an elastic scattering of electrons (or positrons) like photons due to its large number.

Determine Interaction Point

$l=-\ln(\delta)/\Sigma$

Condensed History Technique

Divide flight path to many small steps and apply "Multiple Scattering Model" to obtain true track length and change of direction and displacement due to many elastic scattering



Charged particle lose a part of its kinetic energy when it moves some distance via ionization or excitation

Energy deposition at each step

True track length x Stopping power (dE/dx)

Electron and positron

Initial Condition：Energy、Position、Direction

$e_0, x_0, y_0, z_0, u_0, v_0, w_0$

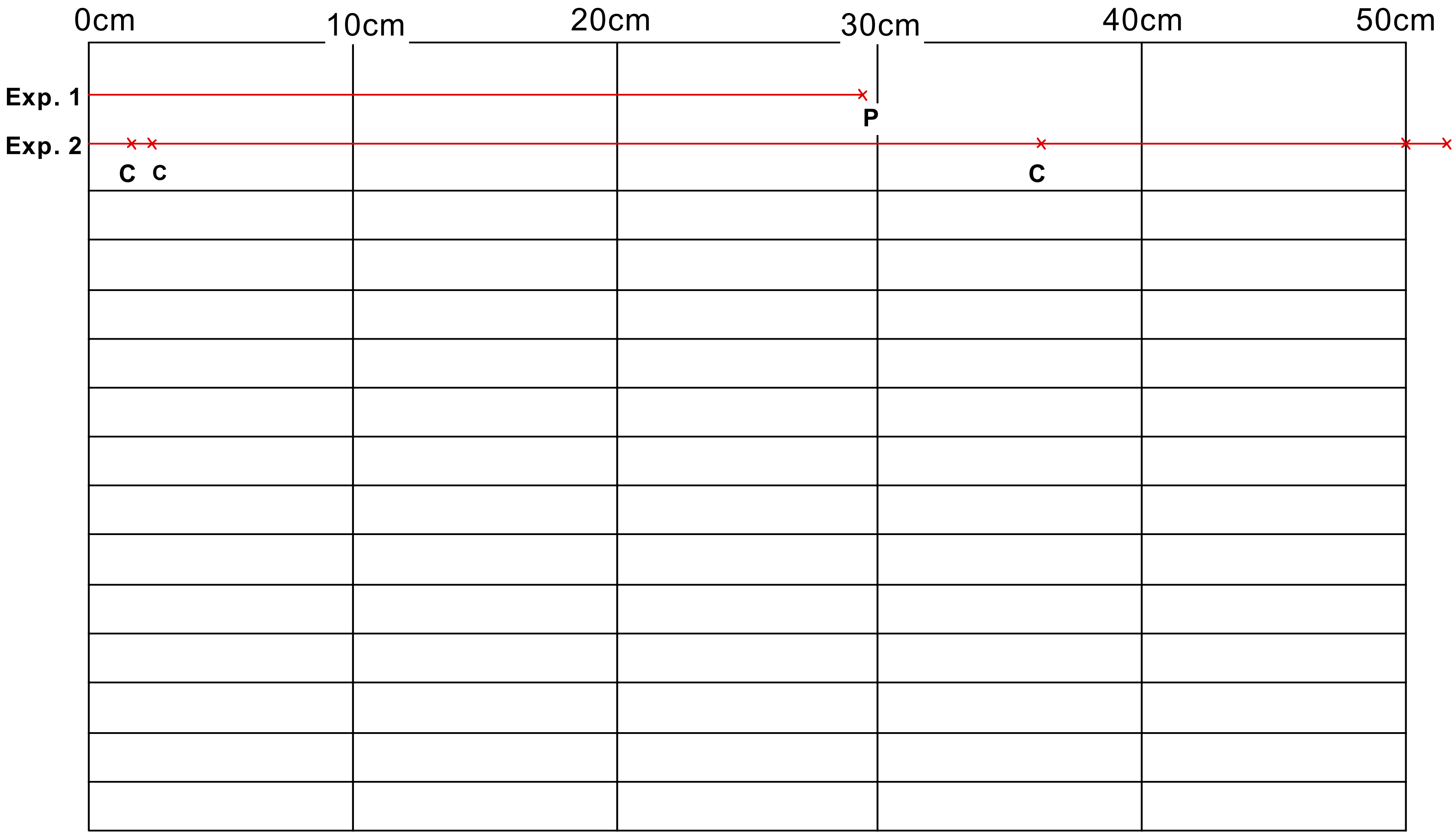
Photon transport using a pocket calculator (Fig.1)

- Suppose that material A having thickness of 50 cm exist as shown Fig. 1
  - 0.5 MeV photons enter this system from the left end,
  - the mean free path is 20 cm,
  - the ratio of the photoelectric effect and Compton scattering is 1:1 and,
  - a scattered photon does not change its energy or direction.
- Exp.1
  - First random number 0.2336 – λ=-20.0ln(0.2336)=29.08
  - 29.08(cm)<50.0(cm)
  - Next random number is 0.20830 (<0.5).– photoelectric effect
- Exp. 2
  - Next random number is 0.90602 -- λ=-20.0ln(0.90602)=1.974
  - 1.974(cm)<50.0(cm)
  - Next random number is 0.71624 (>0.5).– Compton scattering
  - Next random number is 0.99585 -- λ=-20.0ln(0.99585)=0.0832
  - 0.0832(cm)<50.0-1.974(cm)

Single layer

No.	d(cm)	Random number	l(cm)	d>l	d≤l	Random number	Photo.	Compt.
Exp.1	50.0	0.2336	29.08	*		0.20830	*	
Exp.2	50.0	0.90602	1.974	*		0.71624		*
	48.03	0.99585	0.0832	*		0.60020		*
	47.95	0.18307	33.958	*		0.86838		*
	13.99	0.35139	20.92		*			

Fig. 1 Trajectories for a single layer



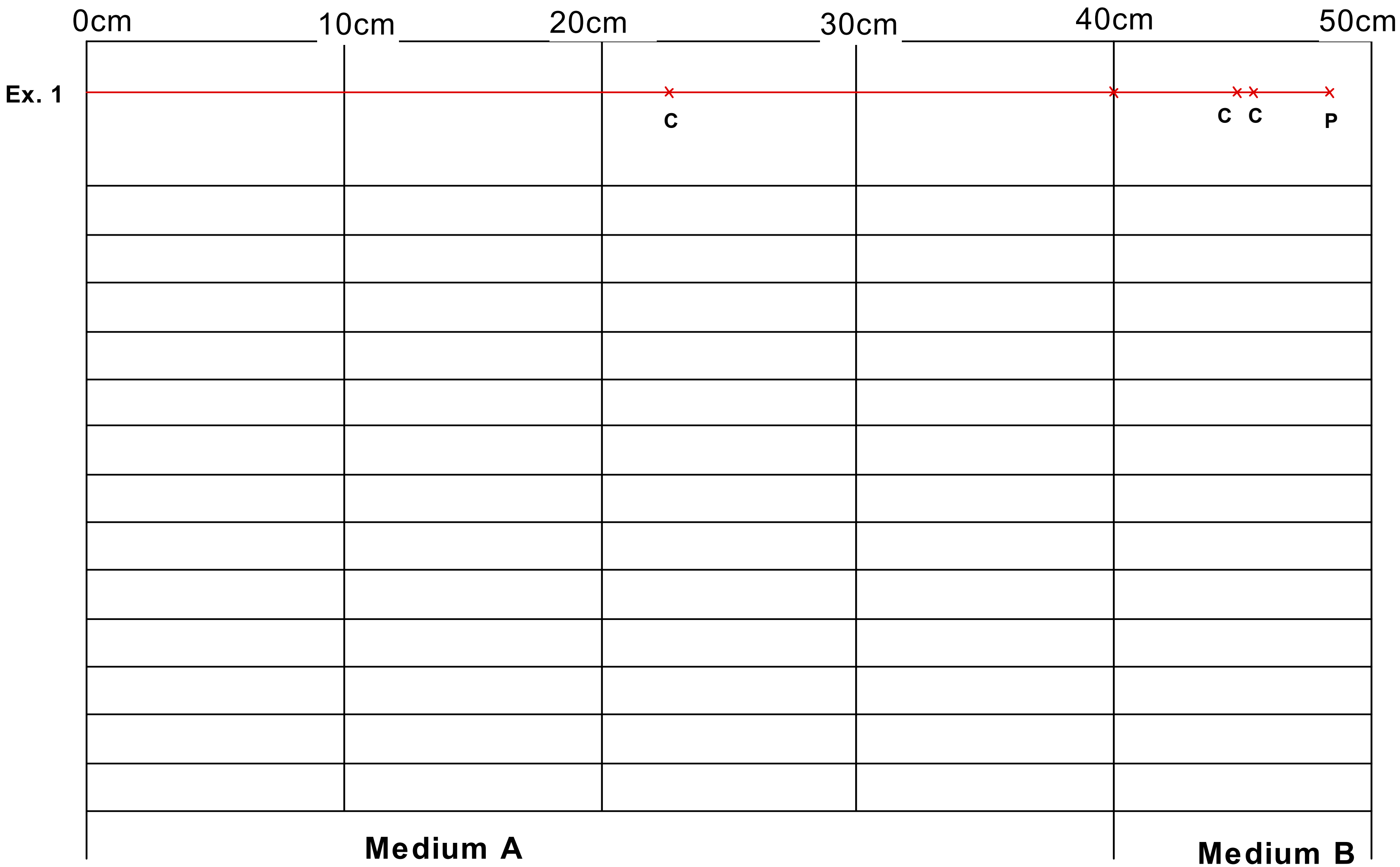
Photon transport using a pocket calculator (Fig.2)

- Suppose that material B (10cm) exits behind material A (40cm) as shown in Fig. 2.
  - 0.5 MeV photons enter this system from the left end,
  - the mean free path and the ratio of the photoelectric effect and Compton scattering in medium A are same as the previous case,
  - the mean free path of medium B is 3cm,
  - ratio of the photoelectric effect and Compton scattering of medium B is 3:1 and,
  - a scattered photon does not change its energy or direction.
- Exp.1
  - First random number 0.32891 – λ=-20.0ln(0.32891)=22.3
  - 22.3(cm)<40.0(cm)
  - Next random number is 0.6116 (>0.5).– Compton scattering
  - Next random number is 0.2336 --λ=-20.0ln(0.2336)=27.093
  - 27.093(cm)>40.0-22.3(cm)
  - Move to boundary (40.0cm)
  - Next random number is 0.28083 --λ=-3.0ln(0.28083)=4.706
  - 4.706(cm)<10.0(cm)

	Medium A							
No.	d(cm)	Random number	l(cm)	d>l	d≤l	Random number	Photo.	Compt
Exp.1	40.0	0.32891	22.3	*		0.616		*
	17.76	0.2336	27.093		*			

	Medium B							
	d(cm)	Random number	l(cm)	d>l	d≤l	Random number	Photo.	Compt
	10.0	0.28083	4.706	*		0.906		*
	5.293	0.7162	1.001	*		0.99585		*
	4.292	0.6002	2.761	*		0.18307	*	

Fig. 2 Trajectories in double layers.



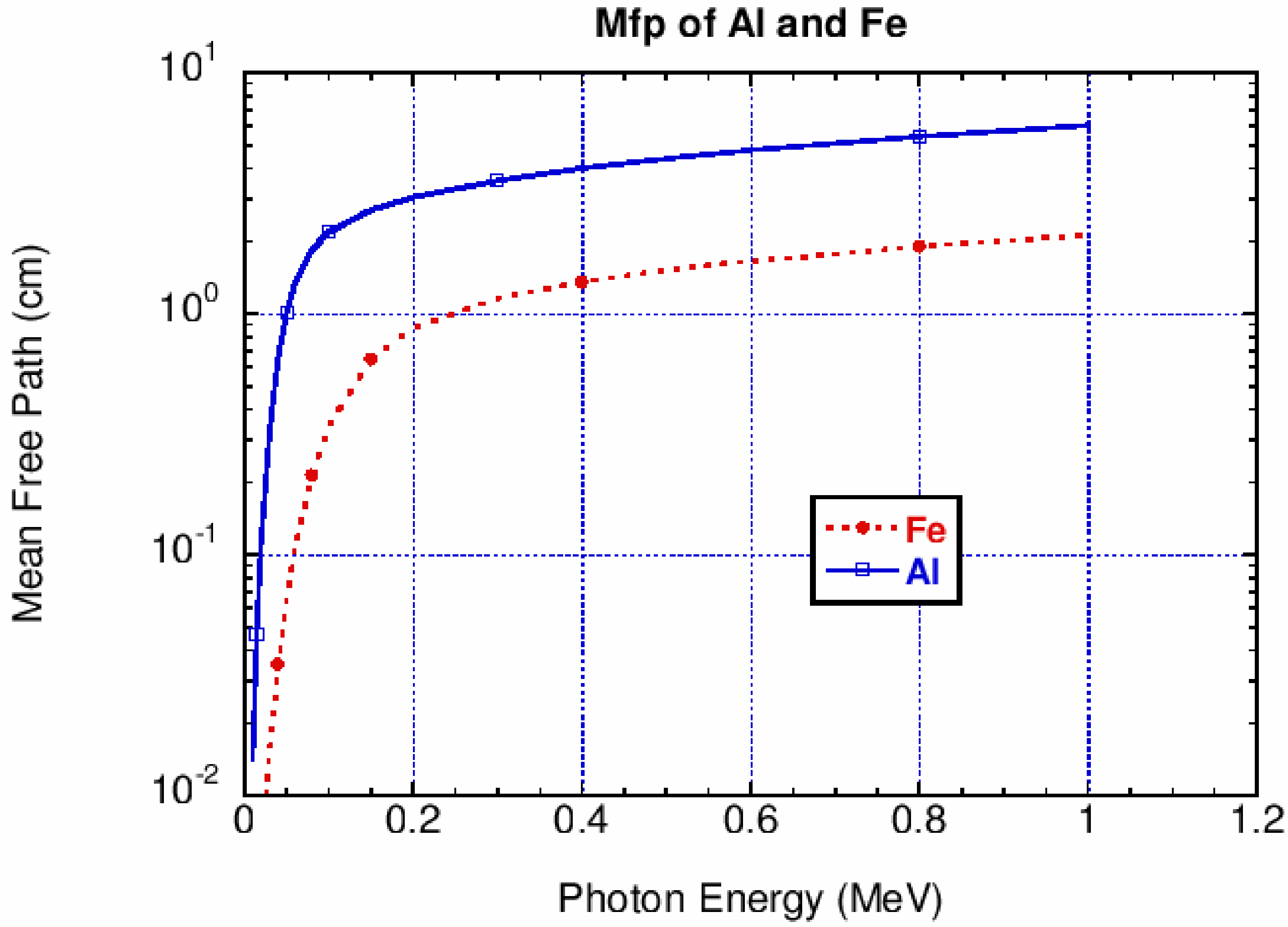
Complex, but more realistic, example of photon transport

- Consider 10cm aluminum plate shown in Fig.3. Suppose that
- 0.5 MeV photon enters this system from left end.
- Photon is scattered with equal probability for each 45° at Compton scattering for all photon energies.
- The photon energy after scattering is calculated by

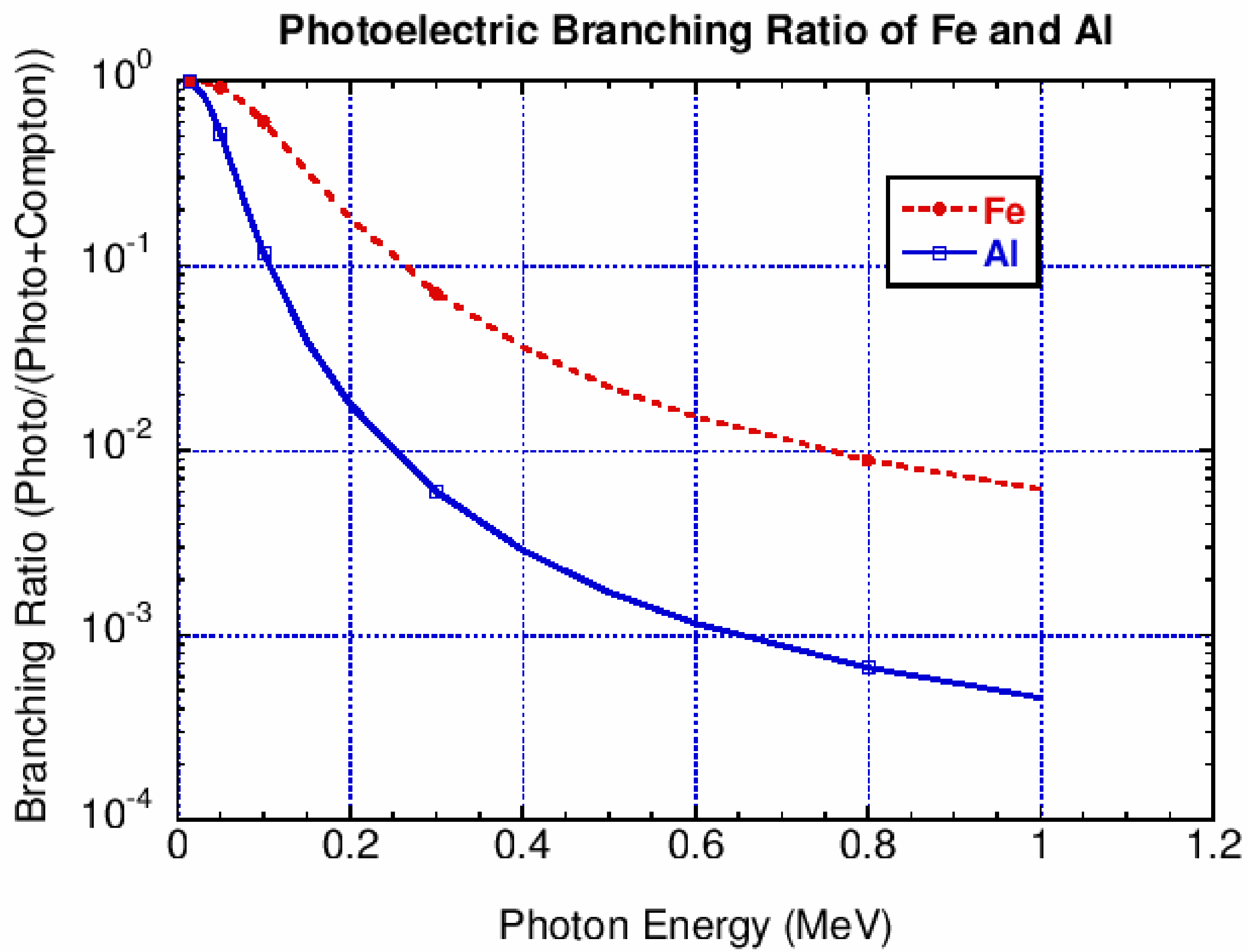
$$E = \frac{E_0}{1 + \left(\frac{E_0}{0.511}\right)(1 - \cos\theta)}$$

Complex, but more realistic, example of photon transport

- Suppose that the azimuthal angle after Compton scattering is 0º or 180º with an equal probability. 0º is 90º left from the particle direction and 180º is 90º right.
- Use the mean free path (mfp) and branching ratio for each photon energy in Fig. 4 and 5.
- Set the cutoff energy of photons to 0.05 MeV.

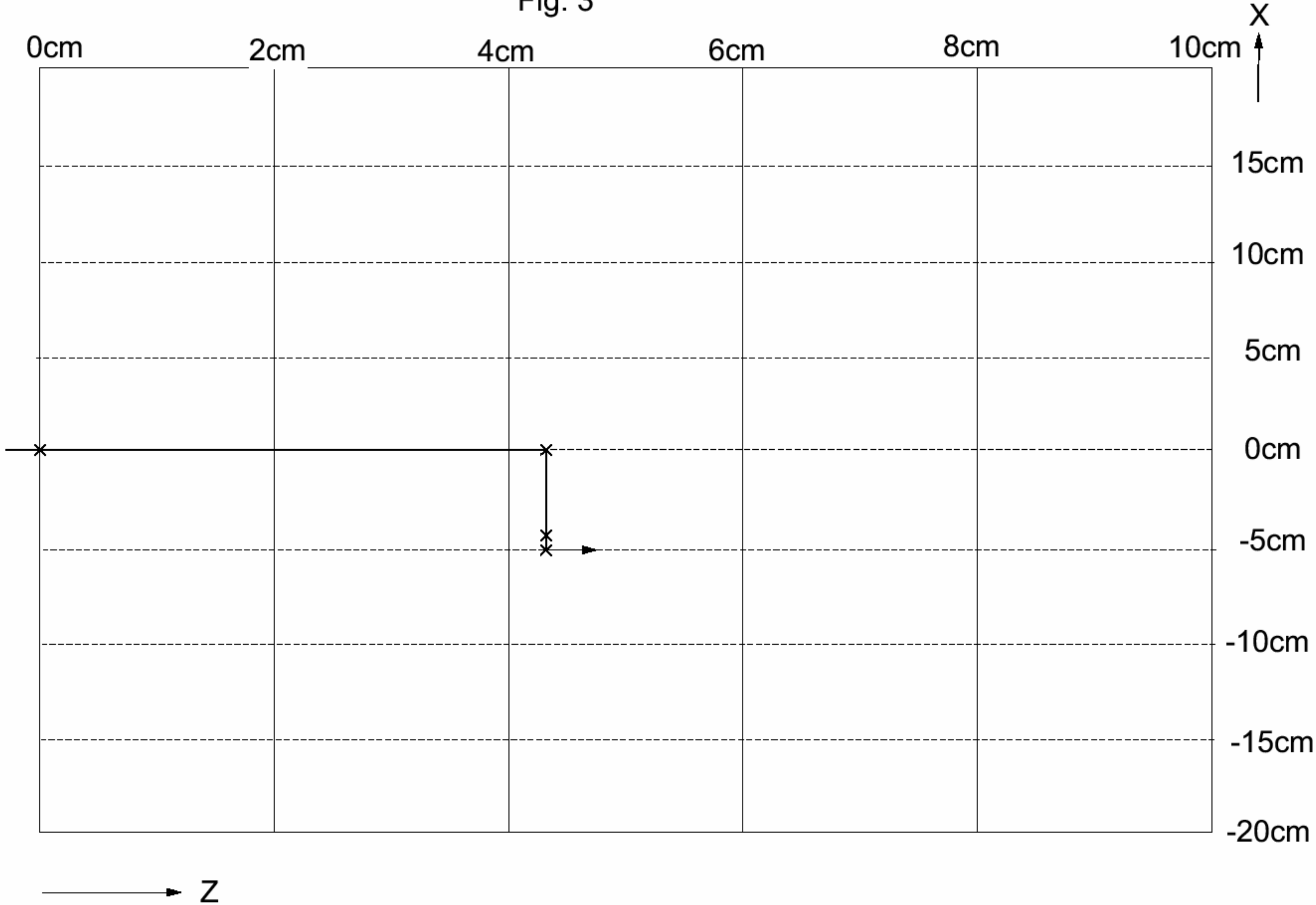


Mfp of Al and Fe
Mean Free Path (cm)
10^1
10^0
10^-1
10^-2
0
0.2
0.4
0.6
0.8
1
1.2
Photon Energy (MeV)
Fe
Al



Photoelectric Branching Ratio of Fe and Al
Branching Ratio (Photo/(Photo+Compton))
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
0
0.2
0.4
0.6
0.8
1
1.2
Photon Energy (MeV)
Fe
Al

Fig. 3


0cm
2cm
4cm
6cm
8cm
10cm
X
15cm
10cm
5cm
0cm
-5cm
-10cm
-15cm
-20cm
Z