Principles of Monte Carlo simulation applied to gamma-ray spectrometry

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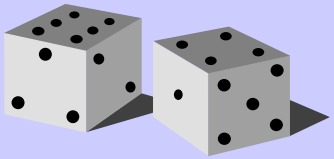
Overview

1. Introduction
2. Sampling of random variables
3. Principles of simulation of radiation transport
4. Simulation of the interactions
5. Variance reduction techniques
6. Physical model, limitations
7. Conclusions

1. Introduction

PRINCIPLES OF THE MONTE CARLO METHOD

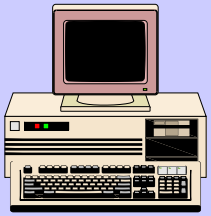
Monte Carlo method – a mathematical simulation method using random numbers



Example: Dice rolling:

Real world experiment:

=> N trials with results $I_1, I_2, .. I_N$; I_k=1 or 2... or 6



Monte Carlo simulation of the experiment:

=> Computer sampling of random numbers r, uniformly distributed in the range (0,1)

=> Establish a correspondence r $\Leftrightarrow$ dice side J

$0 \le r < 1/6 \quad \Rightarrow J=1$

$1/6 \le r < 2/6 \quad \Rightarrow J=2$

$2/6 \le r < 3/6 \quad \Rightarrow J=3$

and so on

=> N random numbers $r_1, r_2, ... r_N \Rightarrow$ the set $J_1, J_2 ... J_N$

The statistical properties of the sets $I_1, I_2, .. I_N$ and $J_1, J_2 .. J_N$ are identical

=> Any estimate computed using $J_1, J_2 .. J_N$ is statistically equal to the same estimate computed using $I_1, I_2, .. I_N$

Monte Carlo simulation is usually applied for solving problems including a random component

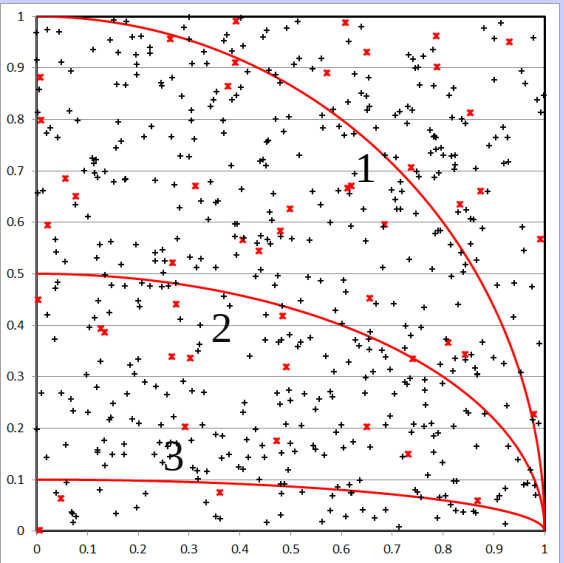
Deterministic problems can also be solved
- by solving a suitable random model corresponding to the deterministic problem;
- using Monte Carlo as a mathematical method without reference to a random model (e.g. computation of multidimensional integrals)

Example: calculation of the area of an ellipse with major axis =2*a* and minor axis =2*b*
- Associate a random model for evaluation of an area A – generate N random uniformly distributed points in a rectangle (area R) encompassing the area of interest; the ratio between the number of points N_i inside the area A to the total number of points is an estimate of the ratio A/R

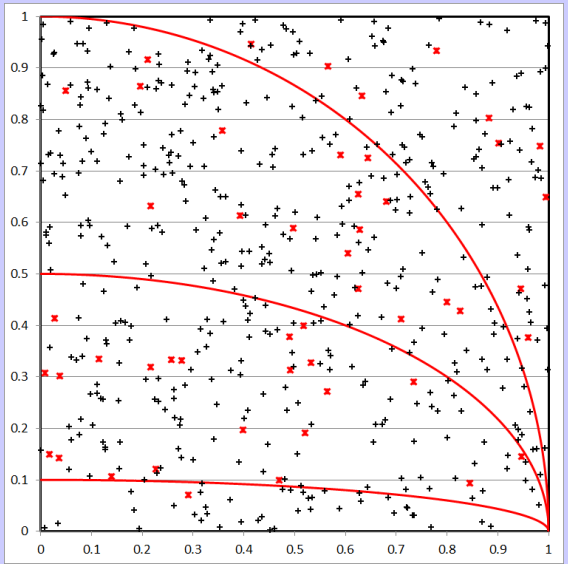
- Cases: $a_1=a_2=a_3=1$, $b_1=1$; $b_2=0.5$; $b_3=0.10$.

Simple calculation in EXCEL with RAND() function, 3 trials

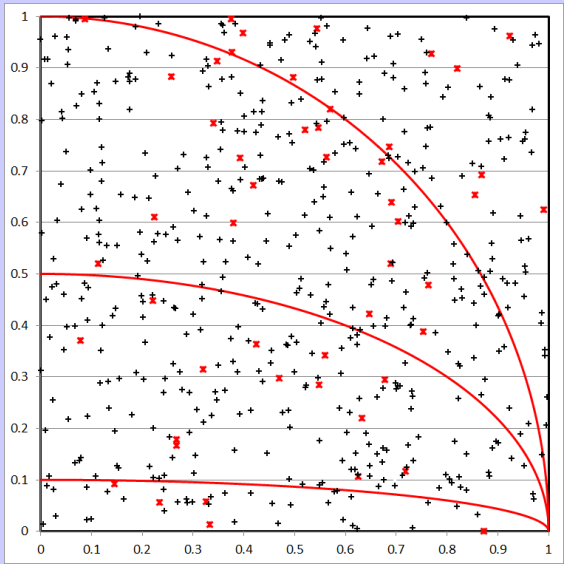
First trial



Second trial



Third trial



Area A of the ellipse estimated by Monte Carlo simulation

N points uniformly sampled in a square with length=1

Results for N=50, N=500 and N=10000:

Ellipse	***a*=1, *b*=1**			***a*=1, *b*=0.5**			***a*=1, *b*=0.10**		
Exact area	**3.1416**			**1.5708**			**0.3142**		
N	**50**	**500**	**10000**	**50**	**500**	**10000**	**50**	**500**	**10000**
A (1st trial)	**2.96**	**3.184**	**3.1368**	**1.36**	**1.68**	**1.5716**	**0.24**	**0.28**	**0.3044**
A (2nd trial)	**3.20**	**3.176**	**3.1436**	**1.84**	**1.376**	**1.5720**	**0.08**	**0.312**	**0.3200**
A (3rd trial)	**3.04**	**3.208**	**3.1464**	**1.44**	**1.608**	**1.5680**	**0.4**	**0.272**	**0.3136**

$\Rightarrow$ The variance of the estimate of the area decreases when N increases

$\Rightarrow$ The variance is higher if the probability of a point in the region of interest decreases

Note:

- In the case of $a=b=1$, the results can be used for the computation of π.
- For a circle of radius 1, area equals π

$\Rightarrow$ The results for $a=1$, $b=1$ from the Table are also estimates of π

Monte Carlo simulation:

• Procedure for sampling random numbers;

• Procedure for establishing a correspondence between the random numbers and the values of the variable of interest;

- The probability distribution of the variable is required – Data base, specific to the problem

• Procedure for the evaluation of the results.

Monte Carlo results have an intrinsic statistical disperison:

relative uncertainty ~ $1/(N^{1/2})$

better results for large N, but this implies longer computing time

$\Rightarrow$ methods to reduce the computing time

- Technical solution: Improve the algoritm for simulation of events

Simple example: faster simulation of the dice experiment:

Instead of:	*Apply directly:*
$0 \le r < 1/6 \Rightarrow J=1$	$J=\text{IntegerPart}(6 \cdot r)+1$
$1/6 \le r < 2/6 \Rightarrow J=2$	
$2/6 \le r < 3/6 \Rightarrow J=3$	
and so on	

=> no comparison required

=> much faster if the random variable takes a large number of values

- More complex solutions: variance reduction techniques

Analog (imitative) vs non-analog (non-imitative) simulation:

- Analog simulation: the probabilities applied in the model simulation are exactly the same as in the physical experiment

=> every feature of the physical experiment can be analyzed using the simulation

=> long computing time

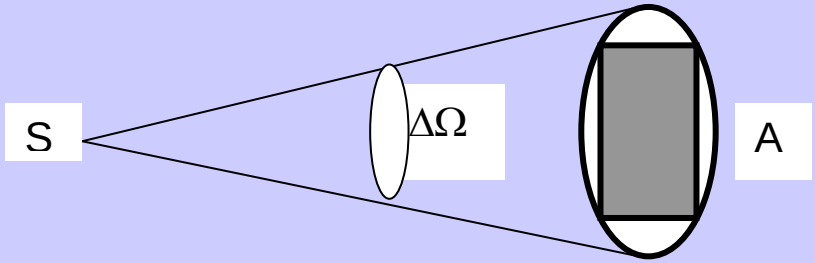
-Non-analog simulation: distorted probabilities applied in the model simulation to increase the occurrence of events of interest

=> probability distortion accounted for in the analysis by using weights

=> smaller variance of the results in a shorter computing time – variance reduction

=> most important in the simulation of low probability events

Example: Evaluation of the solid angle Ω_A subtended by area A as seen from point S



Analog simulation:

shot isotropically N_0 particles from S (random directions); count the particles (N_1) which hit A

$f = N_1/N_0 = \Omega_A/4\pi \Rightarrow \Omega_A = 4\pi \cdot N_1/N_0$

Non-analog simulation:

shot isotropically N_0 particles restricted to solid angle $\Delta\Omega$; count the particles (N_1) which hit A

$N_1/N_0 = \Omega_A/\Delta\Omega \Rightarrow \Omega_A = \Delta\Omega \cdot N_1/N_0 = (\Delta\Omega/4\pi) \cdot 4\pi \cdot N_1/N_0$

- $\Delta\Omega$ is known [can be computed analytically = $2\pi(1-\cos(\theta_{max})]$; $\Delta\Omega/4\pi$ = weight factor for each particle hitting A

- Benefits vs costs – simulation focused on useful events; no information about particles emitted in the real experiment outside $\Delta\Omega$.

For the same value of N_0 the uncertainty in the non-analog simulation is smaller

Particles emitted outside $\Delta\Omega$ are not included in the simulation – more efficient simulation, no time spent in sampling trajectories of no interest

The distortion in the probability distribution used in the simulation is compensated by assigning the weight factor ($\Delta\Omega/4\pi$) to each counted particle.

2. Sampling of random variables

Discrete variables

Random variable x: $(x_1\ p_1)$; $(x_2\ p_2)$; … $(x_n\ p_n)$

- General procedure:

  $S_k = \sum_1^k p_i$

  $0 \le r < S_1 \Rightarrow x_1$

  $S_1 \le r < S_2 \Rightarrow x_2$

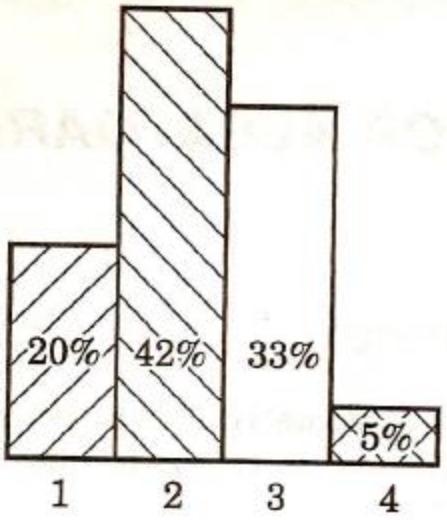
  $S_2 \le r < S_3 \Rightarrow x_3$

  and so on

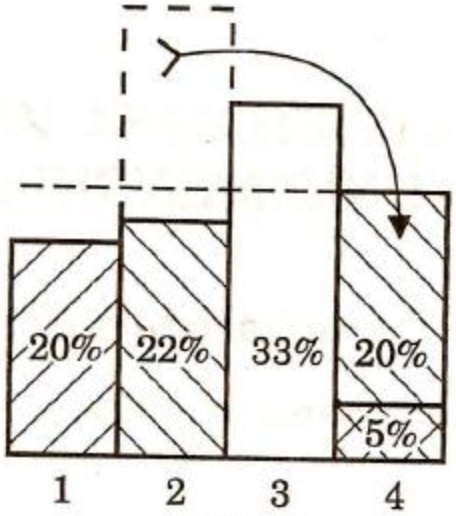
If $p_1 = p_2 = \ldots = p_n = 1/n \Rightarrow k = \text{IntegerPart}(n \cdot r)+1$, much faster for high n.

Walker algorithm:

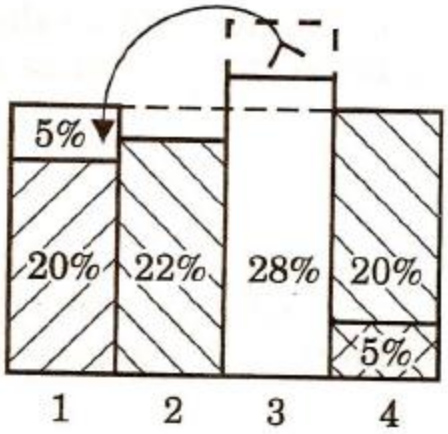
- general discrete variable ($p_i \neq p_j$), a single comparison needed, irrespective to the number of values



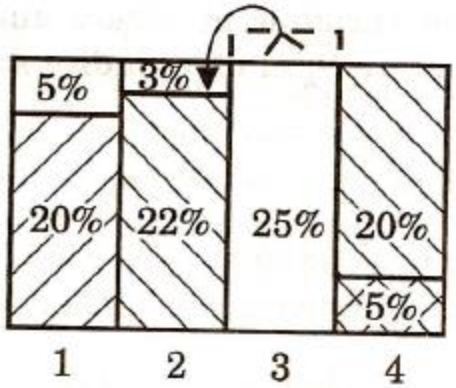
(a)



(b)



(c)



(d)

(b): $q_4=5/25$
$j_4=2$

(c): $q_1=20/25$
$j_1=3$

(d): $q_2=22/25$
$j_2=3$

$k = \text{IntegerPart}(4 \cdot r)+1$; If $r<q_k \Rightarrow x=x_k$; otherwise, $x=x_{j_k}$

Continuous random variables

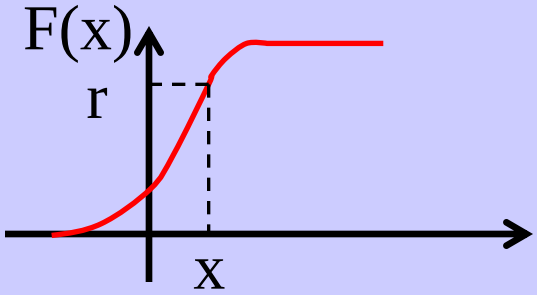
Random variable x characterized by:
Probability density function p(x): $p(x)\cdot\Delta x=\text{Prob}(\text{var}\in(x,x+\Delta x)$
Distribution function $F(x)=\text{Prob}(\text{var}\leq x)$

$$F(x) = \int_{-\infty}^{x} p(x')dx'$$

F(x) monotonically increasing function, lim F(x)=0 at -∞, lim F(x)=1 at +∞

a. Method of inverse function

x is obtained by solving the equation r=F(x), r random number => $x=F^{-1}(r)$
useful if F(x) is a convenient function and the equation is easily solved
Example:
$p(x)=\mu\cdot\exp(-\mu x)$ => $F(x)=1-\exp(-\mu x)$ => $1-\exp(-\mu x)=r$ => $x=-1/\mu\cdot\ln(1-r)$
Or
$x=-1/\mu\cdot\ln(r)$, because r and 1-r have identical distributions
Application: pathlength to the next interaction, time until decay (λ instead of μ)



b. The composition method

Useful if the probability density function p(x) can be written as

$p(x) = a_1 \cdot p_1(x) + a_2 \cdot p_2(x) + \ldots + a_n \cdot p_n(x)$, with

$p_1(x), p_2(x), \ldots p_n(x)$ probability density functions for the variable x that can be conveniently sampled e.g. by the method of the inverse function

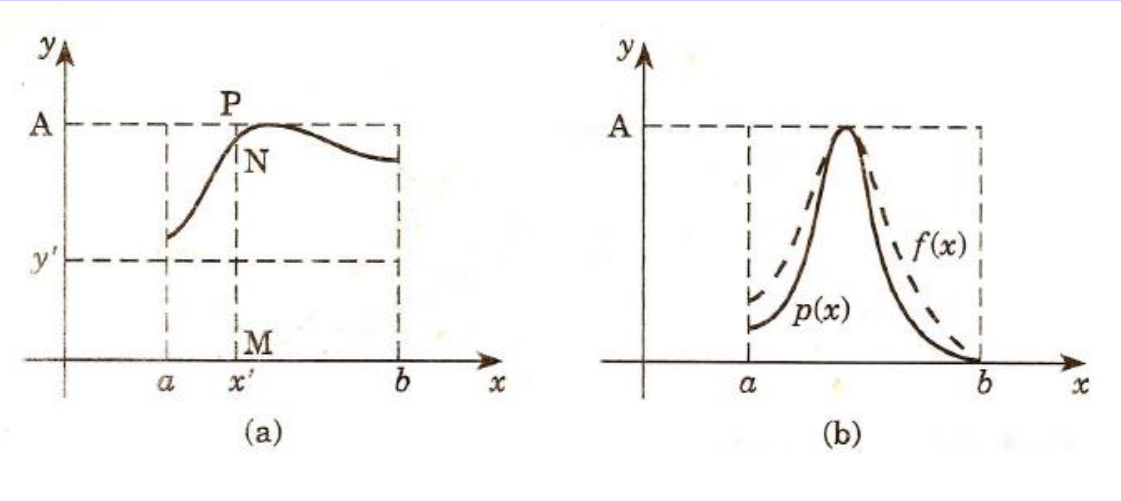
$a_1, a_2, \ldots a_n > 0$; then clearly their sum equals 1

Procedure: using $a_1, a_2, \ldots a_n$ as probabilities of a discrete variable, one of the terms 1, 2, … n is selected, say k; after that, x is sampled from the pdf $p_k(x)$

=> Very useful if sampling from $p_k(x)$ can be done efficiently

=> Can be applied efficiently also for complex functions, if the coefficient of the term described by the complex function $p_j(x)$ is $a_j << 1$.

=> the complex function will be sampled very rarely (with the probability a_j), thus the total simulation time is not much affected



c. Rejection method (Von Neumann)

Variable x defined in (a,b), and max(p(x))=A

Step 1: sample x uniformly distributed in (a,b), say $x' = a + (b-a) \cdot r$.

Step 2: sample a new random number r; if $r \cdot A < p(x')$ then $x=x'$ (x' is accepted), while if $r \cdot A > p(x')$ then x' is rejected => go to step 1

Efficiency=1/[A·(b-a)]

Improved rejection method: required when A·(b-a)>>1

Find $f(x) \geq p(x)$, construct $q(x)=K \cdot f(x)$ as a probability density function

Step 1: sample x' according to q(x) (thus x' is not uniformly sampled, but closer to the probability density function p(x)).

Step 2. sample a random number r; if $r \cdot f(x') < p(x')$ => $x=x'$, otherwise => Step 1

Improved efficiency of the procedure

F(x) not required!

Sampling of random vectors

Random vector: e.g. (x,y,z) with given probability density function p(x,y,z)

Sampling by constructing unidimensional variables, e.g.

$$p(x,y,z) = p(x) \cdot p(y|x) \cdot p(z|x,y)$$

$$p(x) = \iint p(x,y,z)dydz$$

$$p(y|x) = \frac{\int p(x,y,z)dz}{p(x)}$$

$$p(z|x,y) = \frac{p(x,y,z)}{p(x) \cdot p(y|x)}$$

The order of sampling can be important

3. Principles of simulation of radiation transport

Radiation propagation and interaction in matter – sequence of random events
Complex phenomenon, however based on many individual relatively simple events
=> Monte Carlo method – ideal tool for the simulation of radiation transport

Today many computer codes are available

- *General simulation codes:*
  - Advantages: realistic description of physics processes, well tested
  - Disadvantage: computing time, maybe require user intervention
  - Examples:
    - GEANT 4 (GEANT3.21)
    - PENELOPE
    - MCNP, MCNPX
    - EGS (EGS4, EGSnrc)
    - ITS - CYLTRAN
    - …

- *Specific purpose simulation codes:*
  - Advantages: optimized for the particular problem, user friendly, faster
  - Disadvantage: sometimes limited validity

Proper choice of the code, correct application require:

$\Rightarrow$ Basic understanding of the Monte Carlo simulation

$\Rightarrow$ Correct definition of the problem

$\Rightarrow$ Good understanding of the functionality of the code

$\Rightarrow$ Correct, well understood, input data and code parameters

$\Rightarrow$ Correct interpretation of the output

- **Preparatory phase for Monte Carlo simulation:**

Definition of the problem, geometry, materials (including interaction coefficients)

- **Typical steps in simulation (repeated many times):**

Simulation of the source, simulation of radiation propagation and interaction, evaluation of the results

- **Simulation of one history**

Simulation of the source

Simulation of the emission point, then:

- single particle emission: type, direction of propagation, energy, polarization
- Full decay: put the characteristics of each particle in a particle stack (bank) – include additional relevant information (e. g. angular correlations)

Example: a uniformly distributed source in a cylinder of radius R, height H

Simulation of the emission point x, y, z

Variables ρ, ϕ, z [$x=\rho\cdot\cos(\phi)$, $y=\rho\cdot\sin(\phi)$]

The z coordinate uniformly distributed between 0 and H: $z= r\cdot H$, r a random number uniformly distributed in (0,1)

Frequent error: the radial coordinate ρ uniformly distributed between 0 and R,
$\rho = r \cdot R$
Why wrong?
Number of emission points with $\rho<R/2$, $N(\rho<R/2)$, equal to the number of random numbers $r<1/2$, i.e. equal to $1/2 \cdot N_t$
$\Rightarrow N(\rho<R/2)=1/2 \cdot N_t$
$\Rightarrow N(\rho<R/2)= N(\rho \geq R/2)$, whereas the corresponding volumes are: $\pi(R/2)^2 \cdot H=\pi \cdot R^2 \cdot H/4$ and $\pi[R^2-(R/2)^2] \cdot H=3 \cdot \pi \cdot R^2 \cdot H/4$
$\Rightarrow$Emission points not uniformly distributed: half of them are distributed in the volume $\pi \cdot R^2 \cdot H/4$, the other half in the bigger volume $3 \cdot \pi \cdot R^2 \cdot H/4$.

Correct sampling: $\rho = R \cdot \sqrt{r}$

Sampling the angle ϕ: $\phi=2\pi \cdot r$

Final coordinates of the emission point
=> $x=\rho \cdot \cos(\phi)$, $y= \rho \cdot \sin(\phi)$, $z=r \cdot H$

Simulation of the direction of propagation: isotropic distribution

Direction described by the angles θ, φ

Sampling φ: $\varphi = 2\pi \cdot r$, uniformly distributed between 0 and 2π

Sampling θ

Frequent error: $\theta = \pi \cdot r$; wrong, this does not correspond to isotropy!

Isotropy: the probability per solid angle should be proportional to the solid angle

=> $\cos(\theta)$ uniformly distributed in (-1, 1), not θ uniformly distributed between 0 and π

Sampling: $\cos(\theta) = 1 - 2 \cdot r$

Propagation along trajectory better described by the direction cosines:

$$u = \sin(\theta) \cdot \cos(\varphi),\ v = \sin(\theta) \cdot \sin(\varphi),\ w = \cos(\theta)$$

u, *v*, *w*: projection of the unit vector parallel to the trajectory on the coordinate axes

- **Simulation of radiation propagation:**

Propagation along the trajectory from (x_0,y_0,z_0) to (x,y,z):

$$x = x_0 + u \cdot l,\ \ y = y_0 + v \cdot l,\ \ z = z_0 + w \cdot l,$$

l the length of the trajectory from the initial point to the current point

l – distance to the next interaction or to the boundary of the current volume

Distance to the boundary:

- Geometric computation

Distance to the next interaction

Example: photons of energy E, linear attenuation coefficient μ

Probability density function for the distance l to the interaction: $p(l)=\mu\cdot\exp(-\mu\cdot l)$

Distribution function: $F(l)= 1 - \exp(-\mu\cdot l)$

Sample l with the method of the inverse function: $\Rightarrow l=-\ln(r)/\mu$

- **Simulation of the interactions (see next section)**

- **place all radiations except one in particle stack for further transport;**
- **start simulation of the history of the selected radiation**

- **Stack interrogation – when current history is completed**

- Current history is completed: radiation is absorbed, or energy falls below the threshold, or it escape from the simulation domain; then

$\Rightarrow$ extract one particle from the stack and start the simulation for this particle until its history is completed

$\Rightarrow$ Track similarly all the secondary particles from the particle stack

- **Evaluation of the energy deposited in the sensitive volume of the detector**

- **Repeat the simulation for many histories**

- **Summarize the results**

4. Simulation of the interactions

- Interactions have a probabilistic nature

- The probability of interaction and the state of the system after interaction depend on the nature of radiation, on the energy, on the properties of the medium

- Characterization of the system after interaction:
  - Components: number, type
  - Energy, momentum, polarization, etc.

  $\Rightarrow$ Probability distribution of the parameters characterizing the final state computed using physics laws

  $\Rightarrow$ Data bases

- After interaction one radiation is selected for immediate simulation, the parameters of the other relevant radiations are saved (particle stack)

Photon simulation

Photon interactions of interest are: photoelectric (μ_{Ph}), Compton (μ_{Co}), production of a pair electron-positron (μ_{Pair}), Rayleigh (μ_R) (usually less important).

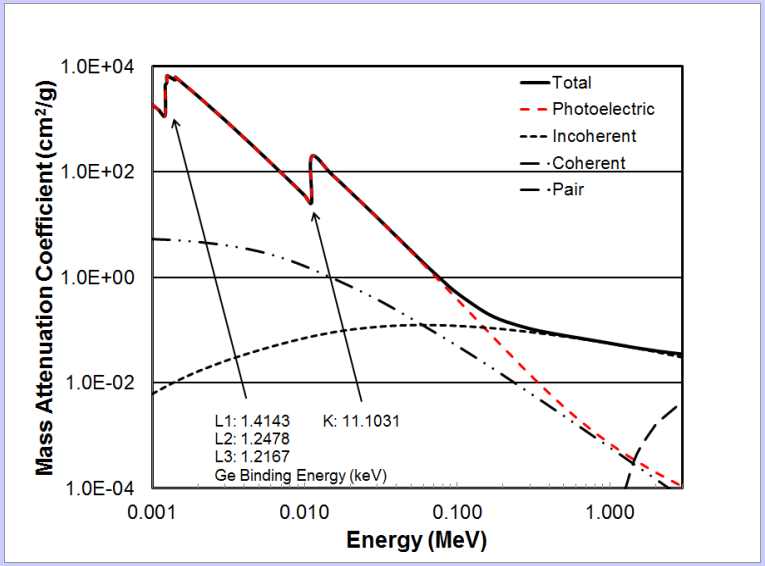
The linear attenuation coefficients depend on the energy of the photon and on the medium (can be computed e.g. by XCOM)

Sampling of the interaction:

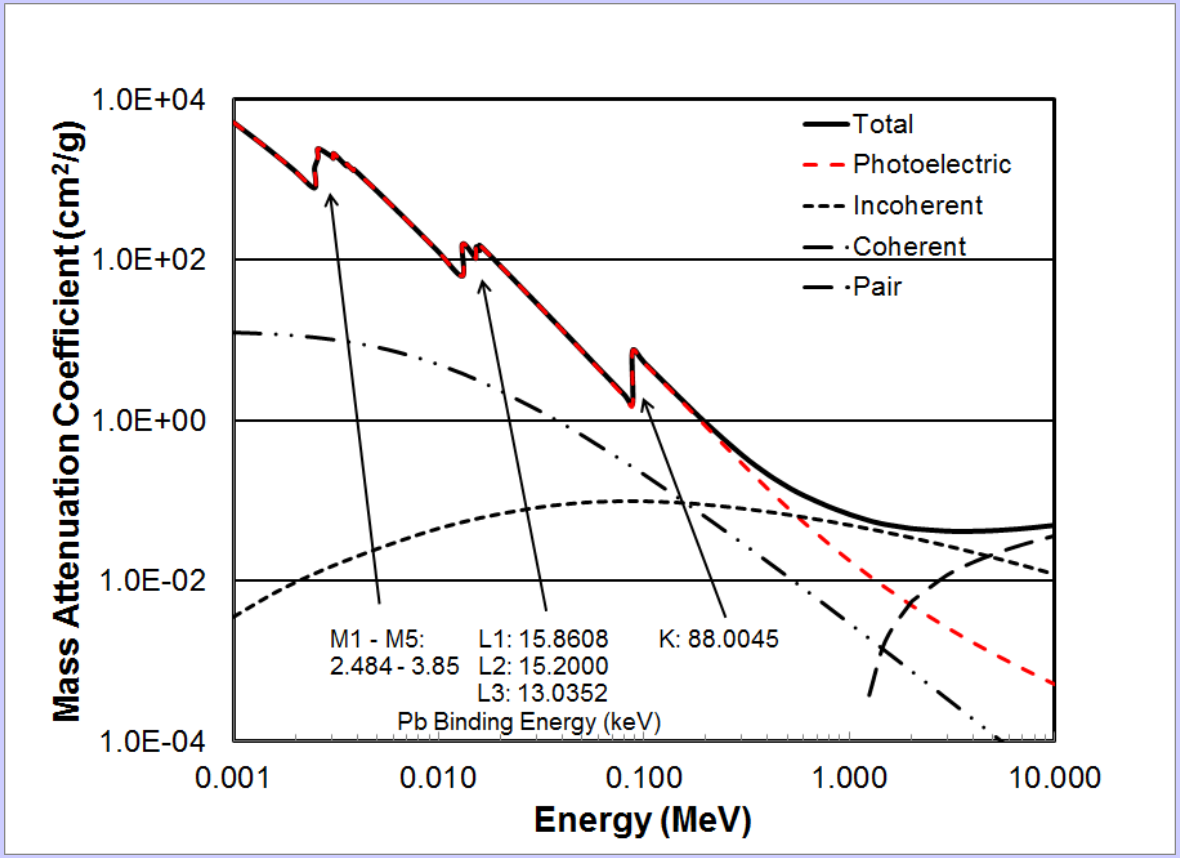
$0 < r < \mu_{Ph}/\mu$ => photoelectric effect is selected

$\mu_{Ph}/\mu < r < (\mu_{Ph}+\mu_{Co})/\mu$ => Compton effect is selected

$(\mu_{Ph}+\mu_{Co})/\mu < r < 1$ => Pair production effect is selected



Interaction coefficients in Ge (XCOM)



Interaction coefficients in Pb (XCOM)

Distance to the next interaction – based on total attenuation coefficient
Sampling of the interaction type – based on individual attenuation coefficients

Photoelectric effect:

⇒ the incident photon is absorbed;

⇒ a photoelectron is produced;

⇒ the atom relaxation follows.

Simulation requires:

⇒ the probability of photoelectric effect on various shells (photoionization cross sections); energy threshold: $E=E_{bi}$, E_{bi}=binding energy on shell (subshell) i

⇒ the angular distribution of the emitted photoelectron

⇒ the probability of emission of characteristic X rays

⇒ the probability of emission of Auger electrons

Energy conservation:

Photoelectron energy

$E_e=E-E_{bi}$ (ionization on shell i)

X-Ray energy:

$E_X=E_{bi}-E_{bj}$ (transition from j to i)

Auger electron energy:

$E_A=E_{bi}-E_{bj}-E_{bk}$ (bound electron transition from j to i, Auger electron emitted from k)

Incoherent scattering:

⇒ photon scattered at an angle θ

⇒ part of the energy and momentum transferred to an electron

Scattering on a free electron – Compton Scattering

$$E' = \frac{E}{1 + \frac{E}{m_0 c^2}(1 - \cos\theta)} \; ; \; E' \in \left[\frac{E}{1 + 2\frac{E}{m_0 c^2}} , \; E \right]$$

$$E_e = E - E' \; ; \; E_e \in \left[0 , \; \frac{E}{1 + \frac{m_0 c^2}{2E}} \right]$$

$$\operatorname{tg}\psi = \frac{\operatorname{ctg}\frac{\theta}{2}}{1 + \frac{E}{m_0 c^2}} \; ; \; \psi \in \left[0 , \; \frac{\pi}{2} \right]$$

E = photon energy before

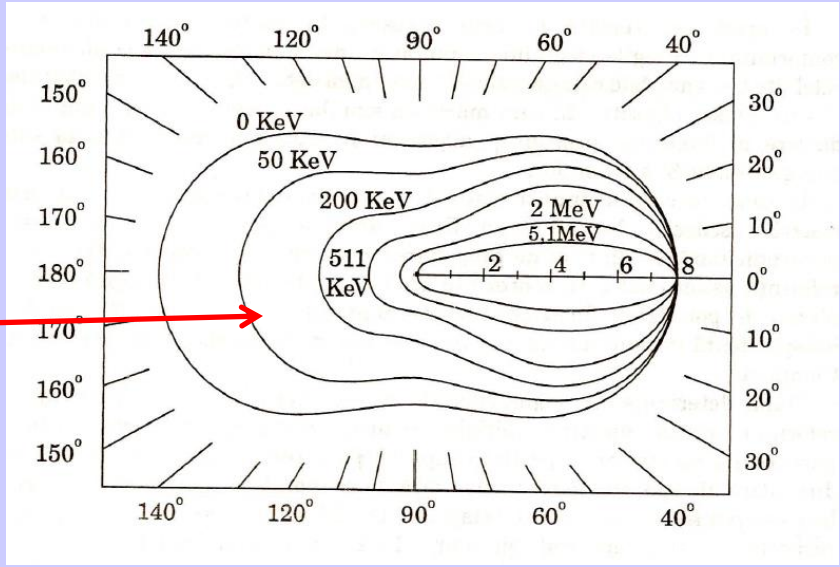
E′ = photon energy after scattering

θ = photon scattering angle

ψ = electron recoil angle

m_0c^2=511 keV = electron rest energy

Display of the cross section on a free electron at rest (units 10^{-26} cm^2) - Klein Nishina



Electron binding in atom:

⇒ cross section decreases at low energies

⇒ angular distribution is changed

Pair production:

$\Rightarrow$ A photon with E>1.022 MeV is absorbed (in the field of a nucleus)

$\Rightarrow$ A pair of electron-positron is produced

Simulation of pair production effect:

=> simulation of the energies E^- of the electron and E^+ of the positron, related by:

$$E=E^-+E^++2m_0c^2$$

m_0c^2=511 keV rest energy of electron

=> simulation of the directions of movement;

=> simulation of electron and positron transport;

=> simulation of positron annihilation

=> energies and directions of the annihilation photons (very much simplified if positron annihilation in flight is negligible, two photons with E=511 keV emitted isotropically in opposite directions)

Triplet production:

$\Rightarrow$ A photon with E>2.044 MeV is absorbed (in the field of an electron)

$\Rightarrow$ A pair of electron-positron is produced

$\Rightarrow$ Besides the pair, the recoil electron may require simulation (3 particles in the final state)

Electron and positron simulation

Elementary processes:
- Elastic scattering
- Inelastic scattering
- Bremsstrahlung emission

Cross sections much higher than for photons
=> too many interactions, generally impossible to be simulated individually

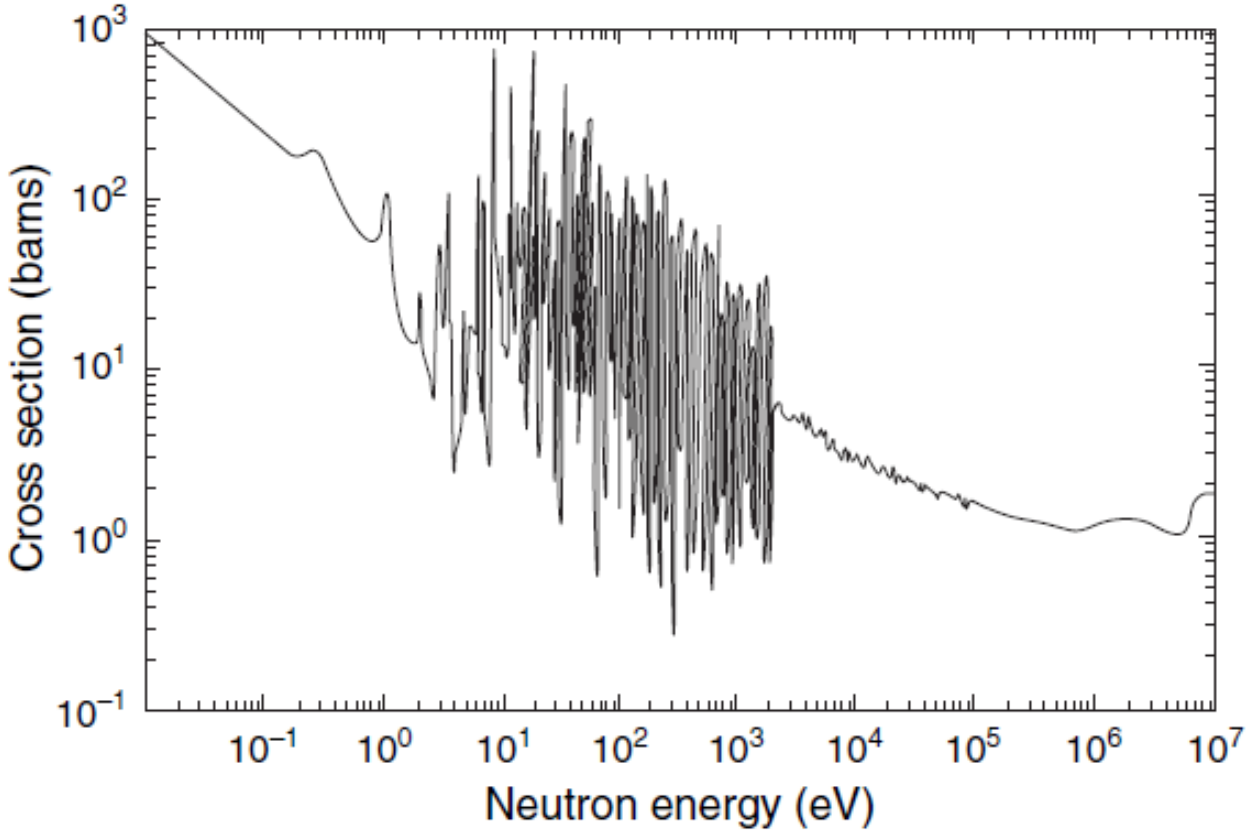
Solution: condensed history schemes
- All the interactions grouped together – energy distributions, direction distributions and position distributions based on the result of multiple interactions
or,
- Interactions resulting in a high energy loss or in a high angle scattering described individually, the others condensed together

Neutron simulation

Individual interactions:

- Elastic scattering
- Inelastic scattering
- Radiative capture
- (n,p), (n, α) reactions
- fission

Small cross sections, individual interactions may be described, but additional complications



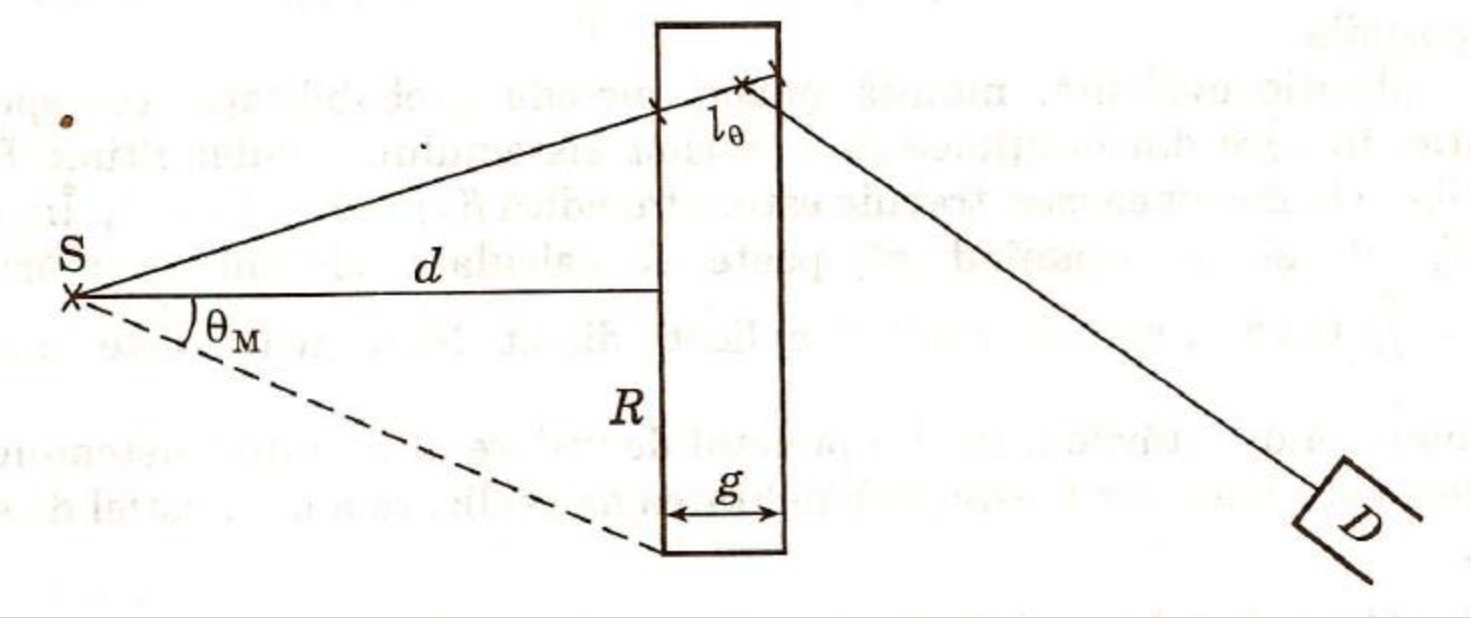
Complications:

- Cross sections dependence on energy – too many histories required to sample adequately the effect of the energy dependence of the cross sections in the resonance regions
  - Multigroup cross sections
- In nuclear reactor core: the source is not known before the simulation
  - The method of successive generations (with/without regularization)

5. Variance reduction techniques

Purpose: achieving results with lower variance in a shorter computation time

The probability method (the mean value method)
Example: interactions in a thin disc
Problem: a point source located far from a thin disc emits photons which may suffer Compton scattering in the disc. Purpose of simulation: evaluation of the probability of registering a scattered photon in a detector located off axis.



1. Photons are emitted only towards the disc => θ is sampled isotropically up to θ_M:
   $\cos(\theta)=\cos(\theta_M)+[1-\cos(\theta_M)]\cdot r$
   - A weight factor $w_1=\Delta\Omega/(4\pi)=[1-\cos(\theta_M)]/2$ is assigned to each photon

2. The photons directed towards the disc are forced to interact; an additional weight factor is introduced, $w_2=P(l(\theta))=1-\exp[-\mu\cdot l(\theta)]$ (the actual probability of interaction on the trajectory in the disc)

3. The point of interaction is sampled from the distorted probability density function restricted to $l<l(\theta)$: $P_d(l)=P(l|l(\theta))=\{1-\exp(-\mu\cdot l)\}/\{1-\exp[-\mu\cdot l(\theta)]\}$
$\Rightarrow l=-1/\mu\cdot\ln\{1-r[1-\exp(-\mu\cdot l(\theta))]\}$

4. Compton scattering is forced, and an additional weight factor $w_3=\mu_C/\mu$ is introduced

5. If the scattered photon interacts with the detector, the weight factor $w=w_1\cdot w_2\cdot w_3$ is cumulated

Finally, after emitting a big number N of photons, the required probability per source photon is p=W/N, with W the cumulated weight

Russian roulette and particle multiplication

Russian roulette avoids spending time with particles with a too low weight.

Two weight limits are set, $W_L << W_S$

If $w > W_L$ normal simulation, w the weight of the particle

If $w < W_L$, then if $r > w/W_S$ the particle is killed, otherwise the weight becomes W_S

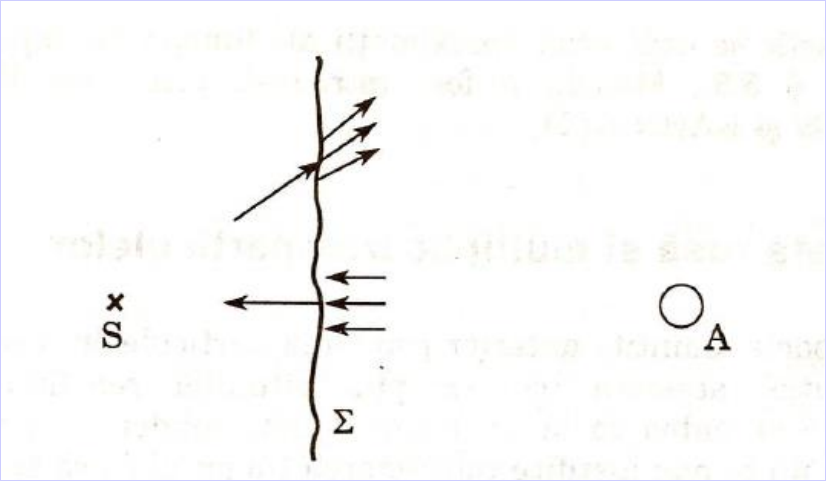
=> Because w/W_S is small when $w < W_L$, very rarely $r < w/W_S$, thus most frequently the particles with low weight ($w < W_L$) are killed

=> The average weight remains unchanged

Particle multiplication:

- Better description of details for events of interest

1 particle of weight w replaced by n particles of weight w/n each



Example: evaluate the energy deposited in the small volume around A, far from the source S

- Particles going towards A are multiplied, with reduced weight each – chance of A being hit by a particle increases
- Particles departing from the region of A are frequently killed when passing the surface Σ

Useful features

$\Rightarrow$ Particle simulation algorithms do not require modifications

$\Rightarrow$ The parameters can be optimized after a learning simulation

Importance sampling

Example: purpose of simulation: the mean value of y=f(x), where x is a random variable with probability density function p(x)

Standard simulation:

Mean of y is estimated by sampling n values $x_1, x_2, \ldots x_n$ of x, according to p(x)

$\Rightarrow$ estimator: $1/n \cdot \Sigma f(x_i)$

Importance sampling

Construct a distorted probability distribution function q(x), ideally $q(x)=K \cdot |f(x)| \cdot p(x)$, K normalization constant

Construct a new function $g(x)=p(x)/q(x) \cdot f(x)$

Simulation: sample n values $x_1, x_2, \ldots x_n$ of x, according to q(x)

$\Rightarrow$ estimator: $1/n \cdot \Sigma g(x_i)$

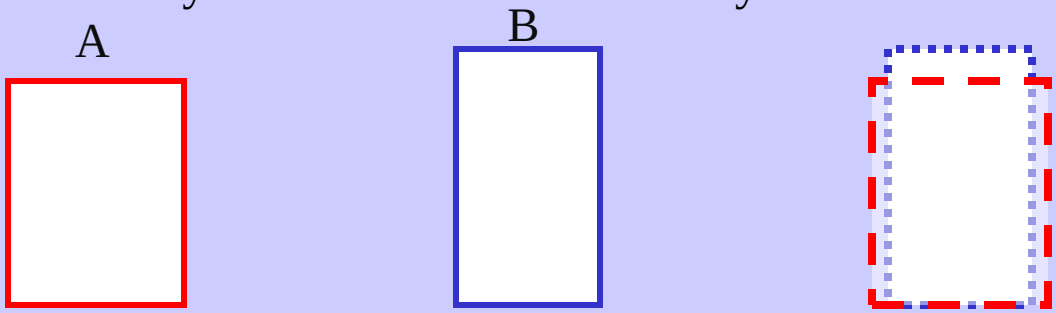
$\Rightarrow$ Particle simulation algorithms should be changed (another pdf, q(x) instead of p(x))

$\Rightarrow$ Specific applications in reactor physics

Correlated sampling

- Best to evaluate the effect of small (or not so small) changes
- The variance of correlated variables is lower

Example: efficiency transfer = ratio of efficiency for source A to efficiency for source B



- In the simulation of radiations emitted by nuclides belonging to the common part of the volumes (intersection of the two volumes), use the contribution of that history for the evaluation of the efficiency for both sources
- Variance of the ratio of the efficiencies (efficiency transfer factor) due only to points belonging only to a single volume (outside of the common part)

Example: coincidence summing effects

- Evaluate simultaneously the contribution to the full energy peak efficiency in the absence of summing and with summing

6. Physical Model - limitations

Definition of quantities

- Precise specification of what should be simulated is required
  - Should variance reduction be included?
  - Or only analog simulation, for obtaining also the distribution?
    - Personal preference: best estimate and its uncertainty, distribution due to statistics of the number of decays evaluated separately
    - Variance reduction techniques acceptable, however used with caution
- In gamma spectrometry, precise definition of the full energy peak efficiency (FEPE) as used in measurement is required
  - Experimental FEPE is obtained by Gaussian integration, or by summing the counts in the spectrum e.g. between 1/10 limits of the peak height?
  - Small angle Compton scattering is included?
    - If yes, FEPE depends on the environment
  - How is FEPE obtained in simulation?
    - Full spectrum simulation with or without Gaussian broadening?
    - Simulation only of potential cases when the complete energy is deposited in the crystal?
      - Faster simulation, more efficient (focalized emission, forced interaction in the sensitive volume, exponential attenuation outside detector)
  - Balance between details included in the simulation model and the time required (affecting the variance of results)

Description of the phenomena – is it sufficiently detailed?

- Coincidence summing:
  - Angular correlations are included?
  - Groups with multiple photons are treated?
  - Volume sources integration or quasi point source approximation?
- Efficiency:
  - Geometry of the source is realistic? e.g.
  - Solution in ampoule – presence of meniscus (depending on solution)?
    - Radon diffusion, radon decay products deposited on surfaces?
  - Granularity?
    - Definition of the volume – free surface of the sample is not really a plane
    - Inhomogeneity effects?
- Self-attenuation:
  - Homogeneity approximation?

Physical Model

- Interactions – cross sections
  - Description
    - Tables of values and interpolations – energy range, number of values
  - Electron and positron interactions – condensed history
  - Neutron interactions – multigrup cross sections
    - Problems also for photons at absorption edges
  - Knowledge of cross sections – e.g. very high energy cosmic rays
- Medium properties
  - Charge collection (commonly not included in simulation)
    - Structure of the dead layer
    - Different dead layer thickness for peak efficiency than for total efficiency (p-type detectors)
- Experimental configuration
  - Detector geometry

- Validation required

7. Conclusions

- Monte Carlo simulation is a very powerful method with many applications in gamma-ray spectrometry

- Many computer codes are available, complex calculations are currently done
  - Generally the codes are user friendly, but be careful!
  - Sometimes approximations are implemented, the validity domain insufficiently documented
  - Good understanding of the basics and of the specific tool very useful

- Still incomplete models

$\Rightarrow$ Validation required for well defined cases

- Preferably apply Monte Carlo simulation for the evaluation of correction factors

$\Rightarrow$ Best results in calibration: combination of experiment and Monte Carlo simulation