International Atomic Energy Agency Technical Visit on

Coincidence summing and geometry correction in gamma spectrometry

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True Coincidence Summing Corrections – Theory Monte Carlo methods

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Layout

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3. Simulation of the decay scheme data
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1. Principle of the Monte Carlo method

Monte Carlo method – a mathematical method of solving problems using computer generated random numbers

- most intuitively applied for stochastic problems
- also for deterministic problems

Ideea of Monte Carlo simulation:

Example – rolling the dice

In real world rolling the dice N times: F_1, F_2, … F_N, where F_k is the total in the k-th experiment; F_1, F_2,… =1, 2,…6

Suppose the computer can provide uniformly distributed random numbers r in (0,1). If for each of the N successive values of r a correspondence with the result of rolling the dice is established like:

$0 < r < 1/6$ => associate face 1
$1/6 < r < 2/6$ => associate face 2
$2/6 < r < 3/6$ => associate face 3
$3/6 < r < 4/6$ => associate face 4
$4/6 < r < 5/6$ => associate face 5
$5/6 < r < 1$ => associate face 6

Then the sequence of the results $S_1, S_2, S_3, \ldots S_N$ of the mathematical experiment has all the statistical properties identical with the statistical properties of the sequence $F_1, F_2, \ldots F_N$

$\Rightarrow$Any conclusion that can be drawn by analyzing the sequence $F_1, F_2, \ldots F_N$ can be equally well drawn by analyzing the sequence of the results $S_1, S_2, \ldots S_N$ of the mathematical experiment

$\Rightarrow$Analog Monte Carlo simulation

=> The results of the Monte Carlo simulation have a statistical uncertainty (as in the real experiment).

=> The relative statistical uncertainty varies like 1/(square root of the number of trials)

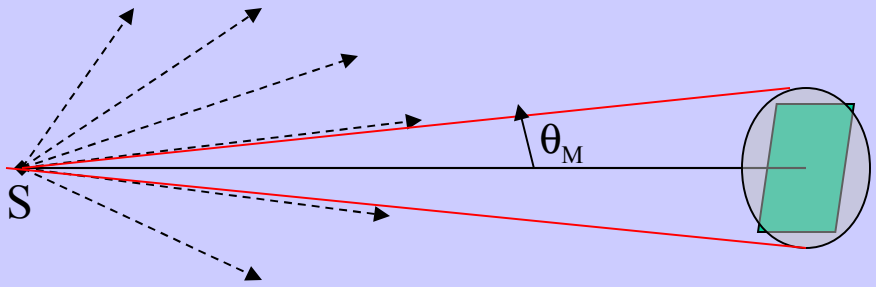
⇒For events with low probability a too big value of N (and a too long computing time) would be required – techniques of accelerating the computation ("variance reduction techniques")

⇒When these techniques are applied, the simulation uses a model with other probabilities than in the real experiment, distorted in order to favor the occurrence of the events of interest

=> Non-analogue Monte Carlo simulation

Example – computation of the solid angle by Monte Carlo

Analog Monte Carlo
-particles isotropically in all directions (NT)
-Count the particles that hit the rectangle (NR)
$\Delta\Omega/4\pi = NR/NT$



Non-analog Monte Carlo
-particles isotropically in the solid angle of the circle (NT')
-Count the particles that hit the rectangle (NR')
$\Delta\Omega/\Delta\Omega_C = NR'/NT'$ with $\Delta\Omega_C=[1-\cos(\theta_M)]/2$ (analytic computation)

Techniques for sampling various probability distribution functions

1. Discrete random variables

Variable x taking the values x_i with probability p_i, i=1,n

Define $S_k=p_1+p_2+..p_k$ then

$0 < r < S_1 \Rightarrow x_1$

$S_1 < r < S_2 \Rightarrow x_2$

$S_2 < r < S_3 \Rightarrow x_3$

$S_3 < r < S_4 \Rightarrow x_4$

……

Very fast if $p_1=p_2=..=p_n=1/n$ (equiprobable x_i values)

r => k=Integer part of (n*r +1), value of the variable x => x_k

=> No need for comparisons, direct sampling of x_k

For the case when the values are not equiprobable, the algorithm proposed by Walker transforms the problem in one with equiprobable distribution.

2. Continuous variables

Variable x, p(x) probability density function (pdf), F(x) distribution function

a. The method of the inverse function

Solve the equation F(x)=r =>x

b. The composition method

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

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

$a_1, a_2, \ldots a_n > 0$;

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

Then: 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 $p_k(x)$

c. Rejection method (Von Neumann)

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

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

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

Improved rejection method: in step 1 x' is not uniformly sampled, but closer to the probability density function p(x). Improved efficiency of the procedure

2. Schematic simulation of radiation transport

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

Simulation of the source
Simulation of the emission point, of the direction of propagation, of the energy.

Simulation of the emission point
Example – a uniformly distributed source in a cylinder of radius R, height H
The z coordinate uniformly distributed between 0 and H: z= r*H, r a random number uniformly distributed in (0,1)
Frequent mistake: the radial coordinate ρ uniformly distributed between 0 and R, ρ = r*R
⇒This is not uniformly distributed: half of the emission points have ρ<R/2 half have ρ>R/2; so the number of points sampled in the cylinder of radius R/2 is half the number from the cylinder of radius R, while in a uniformly distributed source ¼ from the total are in the cylinder of radius R/2, not ½!

Correct solution: $\rho = R * \text{square root}(r)$
The angle $\phi=2*\pi*r$
$x=\rho*\cos(\phi)$, $y= \rho*\sin(\phi)$, $z=r * H$

Simulation of the direction of emission
Angles θ, ϕ for an isotropic distribution
The angle $\phi=2*\pi*r$
Frequent mistake: $\theta=\pi*r$; this is not isotropic!
Isotropic: the probability per solid angle should be constant, not per θ angle!
Solution: $\cos(\theta)$ uniformly distributed in (-1, 1):
$\cos(\theta) = 1- 2*r$
Direction cosines: $u=\sin(\theta)\cos(\phi)$, $v= \sin(\theta)\sin(\phi)$, $w= \cos(\theta)$

Simulation of photon propagation:
Propagation along the trajectory from (x_0,y_0,z_0) to (x,y,z):
$x=x_0 + u*l$, $y=y_0 + v*l$, $z=z_0 + w*l$,
l the length of the trajectory from the initial point to the current point

Distance to the next interaction for photons

Photons of energy E and linear attenuation coefficient μ

Pdf for the distribution of the distance to the interaction is $p(x)=\mu*\exp(-\mu*x)$

The distribution function is $F(x)= 1 - \exp(-\mu*x)$

Sample x with the method of the inverse function => $x= - \ln(1-r)/\mu$ or equivalently but computed faster: $x= - \ln(r)/\mu$

Simulation of the interactions

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

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

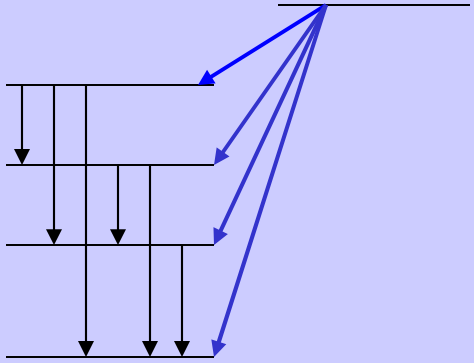
Simulation of the photoelectric effect => the incident photon is absorbed; a photoelectron is produced; the atom relaxation follows

Simulation of the Compton effect => simulation of the scattering angle (several algorithms available), computation of the energy of the scattered photon, of the direction cosines; of the energy of the recoil electron, of the direction cosines for electron

Simulation of pair production effect => simulation of the energies of the electron and positron, of the directions of movement; simulation of electron and positron transport; simulation of positron annihilation (very much simplified if positron annihilation in flight is negligible) => energies and directions of the annihilation photons

3. Simulation of the decay scheme data

Simulation of the decay



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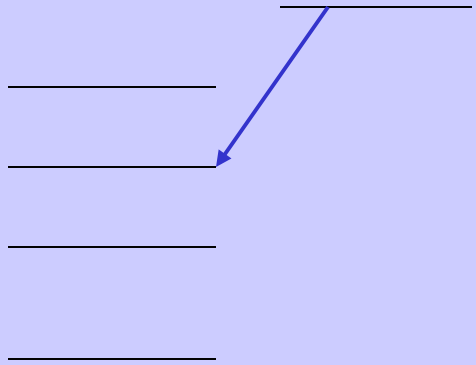

Simulation of the decay

– sampling of the level of the daughter nuclide on the basis of branching ratios of the decay on various levels

-simulation of the radiations emitted (beta particles – either average energy, or random according to the spectrum; X ray emission and/or Auger electron emission in EC decays etc)

-place the radiations of interest on stack for further transport

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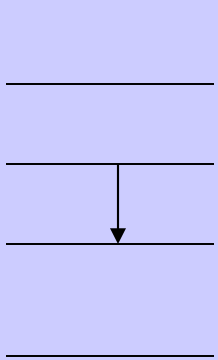

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Simulation of deexcitation of the nucleus:

-sampling of the final level for transition

-sampling of photon emission, conversion electron emission or internal pair conversion; if gamma emission, sample the energy and direction (frequently isotropic); if conversion electron transition sample atomic relaxation process (X rays, Auger electrons)

-place the emitted radiations on stack for further transport

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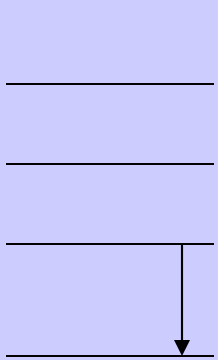

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-place the emitted radiations on stack for further transport;

-repeat sampling until the ground level is reached

Laedermann and Décombaz, ARI 52 (2000) 419; Décombaz et al., NIMA 312 (1992) 152; the subroutine SCH2FOR, implemented in GEANT 3.21
Application: García-Talavera et al., ARI 54 (2001) 769; Capogni et al., ARI 68 (2010) 1428
Berlizov and Tryshyn, JRNC 264 (2005) 169; Berlizov and Solovyeva, JRNC 276 (2008) 663; full simulation of the decay path (including L X rays, angular correlation) then coupled with MCNP
Less elaborated simulations: Dias et al., ARI 56 (2002) 105; Byun et al., NIMA 553 (2004) 674; García-Toraño et al., NIMA 544 (2005) 577; Johnston et al., ARI 64 (2006) 1323.

Advantages of random sampling of the decay path:
-realistic
-easily programmed
-naturally coupled with Monte Carlo computation of the efficiencies

The disadvantages of random sampling of the decay path in comparison with deterministic computation of joint emission probabilities:
-longer computing time
-statistical uncertainty of the final result increased due to sampling of the decay
-difficulties to sample low probability decay paths

4. Simulation of the efficiencies

Correlated transport of the radiations emitted on a decay path

Simultaneous evaluation of the ideal count rate in the peaks and of the real, coincidence-summing affected, count rate

In GESPECOR variance reduction techniques to improve the computation speed; e.g. for coincidence losses from the peak of a main photon:
-focused emission, attenuation approximation, forced first collision in the detector for the main photon;
-Stop the simulation when the first interaction occurs in the detector for the accompanying photons

Validation of the computation required:
-input data of the detector
-interaction coefficients
-Specific features of the detector (e.g. poor charge collection)
-Restriction of the uncertainty of the detector parameters if peak efficiency is known => good uncertainty of the coincidence correction factors (Arnold and Sima, ARI 61 (2004) 117)

5. Summary and conclusions

Monte Carlo simulation can provide realistic descriptions of the phenomena related to the HPGe spectroscopy (efficiency, self-attenuation, coincidence summing corrections)

Validation of the input data and of the code is required

Several Monte Carlo packages dealing with radiation transport, with a varying degree of sophistication, friendliness and scope, are available. The general purpose codes should be adapted for solving problems in gamma ray spectrometry, while specific codes can be directly applied to this purpose.