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THE METHOD OF TRAJECTORY ROTATION AS THE MONTE CARLO VARIANCE REDUCTION TECHNIQUE

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ABSTRACT

This paper presents review of the variance reduction technique, Method of Trajectory Rotation, applied to solve problems of electron transport. The general description of the method and the algorithm's implementation are illustrated by solutions of critical problems in electron transport simulation.

1. INTRODUCTION

Monte Carlo technique is one of the widely used methods to acquire data on interaction of ionizing radiation with targets (Rogers and Bielajew, 1990). At present, a set of the general purpose Monte Carlo codes, such as EGS (Nelson et al., 1985), PENELOPE (Salvat et al., 1996), ITS (Habbleib et al., 1992) and GEANT (Brun et al., 1987), are used to simulate passage of electron and photon beams in targets. General purpose codes implement the analogue technique of simulation when estimation of quantity based on binary-encounter technique.

Implementing the analogue simulation with the binary-encounter technique widens the usage of Monte Carlo transport simulation codes. This decreases, however, the performance of the code to solve specific problems. If the calculated quantities are characterized by small probabilities of events lots of computational work and time will require to insure statistically representative results in simulation. Is it possible to solve this problem by increasing performance of computers only? To answer this question, let us consider two aspects of analogue technique: statistics and artifacts.

Coming from calculations of quantities in one-dimensional scoring grid to 3D calculations, or to simulation of the passage of wide beams, or radiation field interaction with complex geometrical objects, the amount of simulated particles to ensure adequate statistics increases by few orders of magnitude. Thus, the requirements for simulation are growing so fast that even impressive progress in computer technology is unsatisfactory for these purposes. It seems that the variance reduction technique may be necessary development for many problems mentioned above.

Using variance reduction techniques may reduce the statistical error of a computed quantity without increasing the amount of simulated particles. However, these techniques, in a common opinion, are extremely problem-dependent, and general recipes to minimize the variance cannot be given. It is true, however, that some of the general principles on which one or the other variance reduction techniques are based, may be applied to solve a wide set of problems. One of the good examples is the well-known weight technique, when instead of changing future condition of the particle after sampling event one manipulates its statistical weight. Almost any variance reduction technique uses in some form this procedure.

Let us consider artifacts in simulations based on variance reduction techniques. A set of cutoffs and scoring parameters should be prescribed for Monte Carlo simulation. Transport of electrons is simulated for example, for a range of electron energies, from an initial energy E_0 to a given cutoff energy E_{cut}. Tracing trajectories of electrons until the energy $E_{\rm cut}$ is connected with the limits of validity of the physical models used in computation. The general scoring technique implemented in Monte Carlo codes is the binary-encounter technique. This sets limitations on resolution of simulation results that may lead to the disappearance of physical trends in the case of rapid changes of the scoring function or may introduce artifacts in results of the simulation. The electron range struggling calculations (as well as average energy of electrons penetrating a slab target) illustrate, for example, this phenomenon. In many cases decreases of the size of scoring interval may not be possible (for statistical reason for example) in the case of simulation of penetration particles through thick targets. Thus, to resolve this problem the specific technique of local evaluating is required.

This paper presents the Method of Trajectory Rotation (MTR) developed recently (Lazurik and Moskvin (1996, 1998)) to solve specific problems of electron transport. We render basic principles of the method and implemented algorithms that may be useful to resolve some transport problems also in other type of applications than just a penetration of charged particles in targets.

2. BASICS OF THE METHOD OF TRAJECTORY ROTATION

While using conventional binary-encounter based Monte Carlo technique, the contribution of a given particle trajectory $C_{\rm j}$ into scored value of quantity is the binary random variable ω determined as

$$\omega_j = \omega(C_j) = \begin{cases} 1, \text{ if } C_j \in \{C_D\} \\ 0, \text{ in other case.} \end{cases}, \qquad (1)$$

where $\{C_{\rm D}\}$ is a set of random trajectories C_j that give contribution to calculated quantity. $\{C_{\rm D}\}$ is the subset, of the whole set of simulated trajectories $\{N\}$.

In the theory of Monte Carlo simulation for neutron and photon transport, the variance reduction technique, called the technique of mathematical expectation, was developed (Fano et al., 1959). The idea is that the amount of random trajectories can be vastly increased (or equivalently, sampling may be decreased for given amount of trajectories involved) by

employing analytical methods to calculate the weighted random variable rather than binary random variable. The more detailed description of the procedure will be provided later for the particular application but the general rule can defined as follows. The weight value W_j is determined by a given particle's history and by target parameters so that formula (1) can be transformed into

$$w_j = w(C_j) = \begin{cases} W_j, & \text{if } C_j \in \{\tilde{C}_D\} \\ 0, & \text{otherwise .} \end{cases} \qquad (2)$$

where $\{\tilde{C}_D\}$ is the set of trajectories such that $\{\tilde{C}_D\} \times C_{sym} = C_D$ with C_{sym} being the set of partial trajectories that define the class $\{C_D\}$ after additional simulation is imposed over C_j.

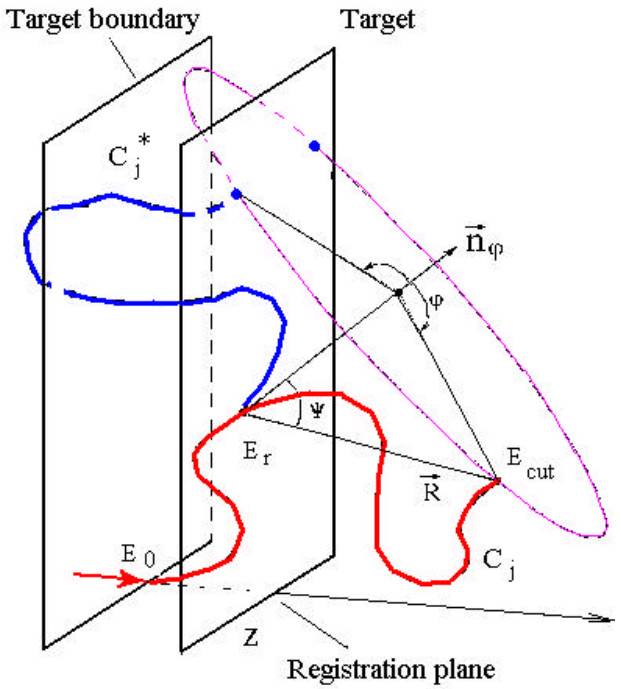

Fig. 1 Method of Trajectory Rotation.

To illustrate the above procedure let us notice that the electron scattering in a uniform media has rotation symmetry in the plane of azimuthal scattering angle. Conventional Monte Carlo algorithms (Berger, 1963) use this symmetry by sampling the azimuthal scattering angle from uniform distribution $j = 2\pi\gamma$, where γ uniformly distributed at the interval [0,1].

In the trajectory rotation technique the sampling of azimuthal angle (in one particular step of trajectory construction) is replaced by a procedure of analytical evaluation of weighting

factors (see Figure 1). This procedure of analytical evaluation is represented by creation of uniform set of trajectories $\{C_{sym} = C_\varphi\}$ by the rotation of the "rest part" of the trajectory around direction of particle movement in a given step and subsequent calculation of mathematical expectation over the set $\{\tilde{C}_D\}$.

In the discretized version of the above described prodedure let us set $\{C_{i,j}\} \equiv \{C_\varphi\}$, so that $\{C_\varphi\}$ consists of i trajectories created by rotation of the trajectory C_j by azimuthal angle $\boldsymbol{j} = 2\boldsymbol{p}$. Each $C_{i,j} \in \{C_{i,j}\}$ has equal probability due to isotropic symmetry of particle scattering and isotropic and translational symmetry of a uniform medium. Probability $P(I)$ of a detection event I for trajectory $\{C_{i,j}\}$ can be written in a form

$$P(I) = \frac{1}{N}\sum_{j=1}^{N}\frac{1}{m}\sum_{i=1}^{m}\boldsymbol{x}_{i,j} \qquad (3)$$

where $\boldsymbol{x}_{i,j}$ is the value of the indicator function of a detection event for trajectory $\{C_{i,j}\}$, i.e. $\boldsymbol{x}_{i,j}$ is, for fixed j, the value of the indicator function of a detection event for trajectory $\{C_{i,j}\}$ under additional sampling.

Let us determine $\Delta\boldsymbol{j}_j \subset [0,\ 2\boldsymbol{p}]$ as an interval of rotation for which a detection event on a trajectory is detected. The estimation (3) may then be written as

$$P(I) = \frac{1}{N}\sum_{j=1}^{N}\frac{\Delta\boldsymbol{j}}{2\boldsymbol{p}}\boldsymbol{x}_j\ , \qquad (4)$$

where $\boldsymbol{x}_j$ is the value of the indicator function of a detection event for trajectory $\{C_j\}$.

It is seen from the general description, that a set of trajectories simulated in a given target is a subset of a full set of trajectories in infinite media. Trajectories traced in uniform infinite medium can be used to estimate characteristics of particle transport in finite target with the use of Method of Trajectory Rotation. The limitation of MTR method is that it is applicable to homogeneous targets, or at least locally homogeneous targets for specific applications.

The partial uniformity and differentiability of function describing the calculated quantity on the spatial coordinates allow deriving equation for analytical part of the estimation (2) to solve problems of local estimation of particle transport characteristics.

3. APPLICATIONS OF THE METHOD OF TRAJECTORY ROTATION

3.1 Electron range-straggling distribution

When using the conventional Monte Carlo techniques, the density of stopped electrons at a given depth in a target cannot be computed as such. The target is divided into a set of depth bins. The particle deposition density at a given depth z is evaluated by the number of electrons

stopped in a depth bin with a given width Δz. As a consequence, the result of computation is the average density of the charge deposited in this depth bin. The range-struggling distribution is fitted using the data on the average density of the deposited charge computed for a set of depth bins. When using the data on the average density of the charge deposited in depth bins, further theoretical assumptions are necessary for fitting the depth-profiles of the primary electrons charge deposition. We have found contradiction between results of different authors in interpretation of calculations of range-struggling distributions ((see discussion in (Lazurik and Moskvin (1998)). To resolve this problem of range-struggling calculations and to produce data on range struggling distribution near the target boundary, we applied Method of Trajectory Rotation (Lazurik and Moskvin (1996, 1998)).

Assume that a layer, depth bin, with the thickness Δz is placed at the depth *z* in a target. The contribution of the base trajectory *Cj* to the average density of the particle stopped in the depth bin is given by an equation

$$W_{\mathrm{D}}^{j} = \frac{1}{2\pi}\left(\frac{\Delta\varphi}{\Delta z}\right)\zeta^{j}\sum_{m=1}^{2}\chi^{j,m} \qquad (5)$$

where ζ^{j} is is the rotation indicator. It equals 1 if the point of the base trajectory $_{t}$ intersects the plane *z* during the full rotation of the trajectory i.e. if the end of the trajectory *Cj* can be placed in a given depth bin after rotation. It equals 0 otherwise. Further, $\chi^{m,j}$ is the region indicator. It equals 1 if all points of the trajectory defined by rotation of the base trajectory *Cj* belong to the target and it equals 0 otherwise. Finally, m is the index to account for the dual intersection of the plane *z* by the base trajectory during rotation.

Let us calculate the weight factor in analytical form. To do this, we suppose that the depth bin width Δz approaches zero size. Going to a limiting case, the ratio ($\Delta\varphi/\Delta z$) converts to the derivative ($\mathrm{d}\varphi/\mathrm{d}z$). The derivative is derived from a formula describing the geometry conditions determined by a trajectory placed in a target and is equal to

$$z = z_r + \gamma_r\left(\vec{R},\vec{n}_j\right)\sqrt{\left(R^2 - \left(\vec{R},\vec{n}_j\right)^2\right)(1-\gamma_r)^2}\,\cos\varphi\,, \qquad (6)$$

In the above z_r is the *z*-coordinate of the rotation point (i.e. the trajectory point with the energy E_r; $\vec{R}$ is the radius-vector from the rotation point to the point of a trajectory where an electron has energy *E*; $\vec{n}_j$, is the rotational axis defined by the direction $\vec{\Omega}_r = (\alpha_r, \beta_r, \gamma_r)$ of electron motion in the rotation point; $(\vec{R},\vec{n}_j)$ is the dot product of $\vec{R}$ and $\vec{n}_j$.

Equation (5) can be rewritten for the discussed case of the Method of Trajectory Rotation as follows. The contribution of the base trajectory C_J (after its rotation) to the density of electrons at depth *z* is given by

$$W_{\mathrm{D}}^{j} = \frac{1}{2\pi}\left(\frac{d\varphi}{dz}\right)\zeta^{j}\sum_{m=1}^{2}\chi^{j,m} \qquad (7)$$

where $(d\varphi/dz)$ is given in an analytical form as

$$\left(\frac{d\varphi}{dz}\right)_{z} = \frac{1}{\sqrt{\left(R^{2}-(\vec{R},\vec{n}_{j})^{2}\right)(1-\gamma_{r})^{2}-\left(z-\left(z_{r}+\gamma_{r}(\vec{R},\vec{n}_{j})\right)\right)^{2}}} \qquad (8)$$

The density of particles stopped in a given depth z is calculated by averaging the contributions over the N base trajectories from the set $\{\tilde{C}_{D}\}$.

Notice that, the weight factor tends to infinity as a trajectory during rotation approaches maximum or minimum coordinate z. However, a total contribution of the base trajectory C_j defined by the integration, is less than (or equals to) 1. Therefore, the divergence is integrable and it can be removed by conventional procedures.

As we see the method discussed depends only on a set of quantities, which describe the motion of an electron in a target. Consequently, the method can be applied to any Monte Carlo scheme that traces trajectories of electrons.

The algorithm of the method proceeds as follows:

1. An electron trajectory C_j is simulated in an infinite medium from initial energy E_0 to the cut-off energy E_{cut} and stored in the memory as a set of (x_i, y_i, z_i ,E_i), where i is the index of the trajectory steps.

2. The trajectory C_j is placed in a target D (see Figure 1).

3. The point of the trajectory where the electron has a given energy E_r is a point of trajectory rotation. The direction of the electron motion at this point is considered to be the axis of rotation. Note that any value can be taken for E_r except E_0 and E_{cut}.

4. The part of the trajectory where electron has the energy $E < E_r$ is selected. A set of trajectories is created by rotating this part of the base trajectory around the rotation axis.

5. The registration plane z is considered. If the indicator of rotation $\zeta^{j}(z)$ for a given depth z is 1, then go to 6; if $\zeta^{j}(z)$ equals 0 it is necessary to consider another z.

6. A weight factor of the trajectory C_j in scoring the density of stopped particles is calculated.

Figure 2 shows that the profile $D(z,E_{\mathrm{cut}}\})$ describing the range-struggling distribution of electrons in a target decreases drastically near the surface of a target with the cutoff energy E_{cut}

decrease. The value of range straggling distribution approaches 0 at the boundaries of a target. Considering a region near the surface of a finite target, it is found that the uncertainty in the conventional Monte Carlo depends dramatically on the distance to a target boundary. Detailed analysis of the physics of the boundary effect, caused by vanishing of the equilibrium of slowing down electrons near the target vacuum interface, we presented in (Lazurik and Moskvin, 1998).

The reason for difficulty of Monte Carlo modeling mentioned above has to be analyzed. The use of simple approaches for fitting the profiles near the boundaries of semi-infinite targets cannot lead to advance. Moreover, existing contradictions between results of different authors have just been caused by such simplistic analysis of results of computations. It seems likely that the improper handling of algorithms in studying range-struggling distribution, or charge deposition, along with the energy deposition calculations, can lead to anomalous results known as "interface artifacts". The presence of depth bin in conventional Monte Carlo leads to artifacts in simulation and incorrect conclusions concerning behavior of the range-struggling distribution near the target boundary.

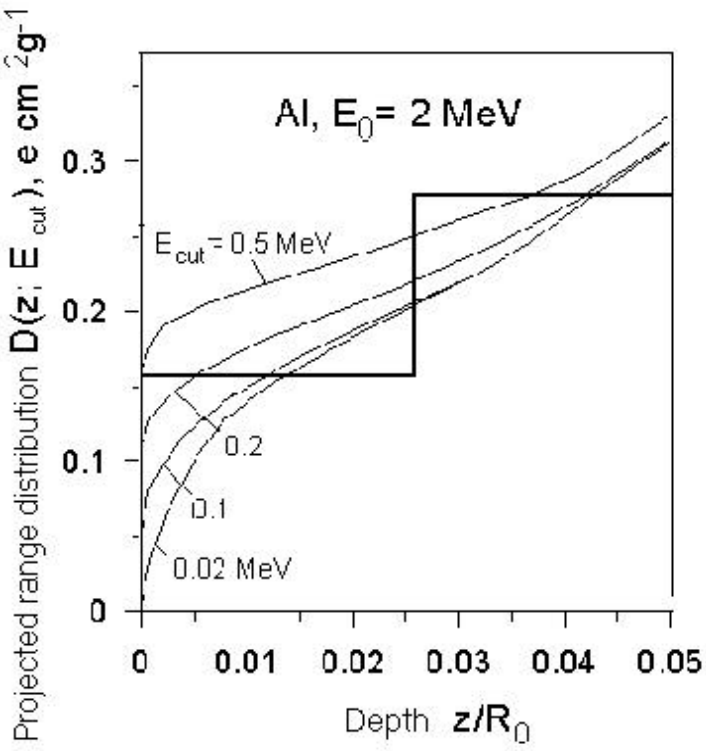

Fig. 2 Range struggling distribution of 2 MeV electrons in semi-infinite target near the target boundary calculated for different cutoff energies E_{cut}. Solid line is MTR calculations. Histogram is the ITS calculations (Tabata et al., 1994) R_0 is the CSDA range of electrons.

Evaluation of the efficiency of the MTR in a problem of range-struggling calculations shows the considerable improvement in efficiency of calculations of electron density in small spatial regions. Considering the non-local implementation of the method given by (5), the calculations with MTR for a given depth with the been size selected to be 0.01 of CSDA (continuous slowing down approximation) of range R_0 of electrons depends on the choice of the rotation point E_r. The choice of rotation point close to end of trajectory or near the entering point (for normal incidence) will give the performance almost the same as the analogous Monte Carlo simulation. The reasonable choice is the point on the trajectory where particle already experienced sufficient scattering but its residual range is comparable with initial range. When we consider the point on the trajectory with energy of $0.9E_0$, we get evaluation of performance of the MTR. The amount of primary MTR trajectories that are needed to reach the same statistics as conventional Monte Carlo method can be reduced from order of 10^6 to 10^3. The use of MTR increases the time for one trajectory processing by about a factor of 2; thus the efficiency of the MRT is about a factor of 500 in comparison to the conventional Monte Carlo technique. The decrease in the depth of the bin size leads to a considerable increase in the method's performance (relative to the original Monte Carlo simulation).

3.2 Deep electron penetration simulation

For semi-empirical modeling of electron depth-dose curves, the knowledge on the average energies of transmitted electrons and transmission coefficients for different target materials is essential (Tabata and Moskvin, 1999). The same knowledge is also important in the measurement and the use of electron beams. However, poor statistics in conventional Monte Carlo calculations for deep penetration of electron beams produces unsatisfactory results. For example, the general-purpose Monte Carlo codes, using the binary-encounter technique, yield average energies of transmitted electrons with strange behavior or artifacts in deep regions of a target (see Figure 3).

To decrease such effects one may combine the use of symmetry in uniform media and information contained in trajectories to improve the efficiency of evaluation by Monte Carlo codes. One specific technique of this type is also the Method of Trajectory Rotation (MTR).

The method described in previous section can also be applied to evaluate the weight of the contribution by a given trajectory to the average energy E_{av} at depth z (we set axis z to be normal to a target). The algorithm of the MTR works in this case as follows (Moskvin et al., 2000)

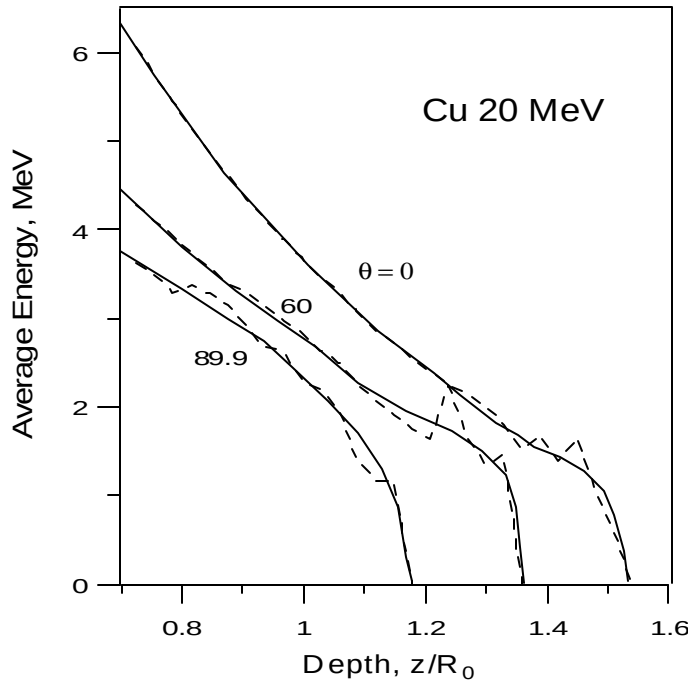

Fig. 3 Strange behavior of average energy of electrons as a function of target thickness at deep penetration for different angles of beam incidence. Solid lines represent MTR calculations.

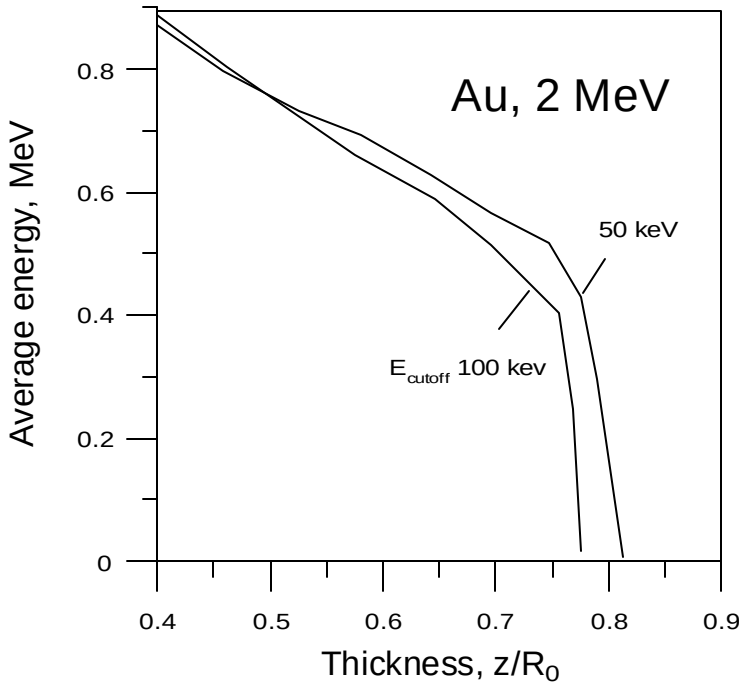

Fig. 4 Average energy of electrons transmitted through thick targets vs. thickness of the target calculated with 100 keV and 50 keV cutoff energies.

1. An electron trajectory C_j is simulated in an infinite medium from initial energy E_0 to the cut-off energy E_c and stored in memory as a set of (x_i, y_i, z_i ,E_i), where i is the index of the trajectory steps.

2. The trajectory C_j is placed in a set of thick targets D (see Figure 1).

3. 3. The point of the trajectory where the electron has a given energy E_r is a point of trajectory rotation. The direction of the electron motion at this point is considered to be the axis of rotation. Note that any value can be taken for E_r except E_0 and E_{cut}. We have chosen E_r = 0.9 E_0 based on the discussion presented in (Lazurik and Moskvin, 1998).

4. The part of the trajectory where electron has the energy $E < E_r$ is selected. A set of trajectories is created by rotating this part of the base trajectory around the rotation axis.

5. The deeper region of the target is considered. If the indicator of rotation (see below) $\zeta^j(E, z)$ for a given depth z and energy E on the trajectory is 1, then go to 6; if $\zeta^j(E, z)$ equals 0 it is necessary to consider another z and E.

6. A weight factor of the trajectory C^j in scoring the spectrum of electrons transmitted through the target of thickness z is calculated as

$$W_S^j(E;z) = \frac{1}{2\pi}\left(\frac{d\sigma}{dE}\right)_z \zeta^j(E,z) \sum_{m=1}^{2} \chi^{j,m}(E) \tag{9}$$

$\left(d\sigma/dE\right)$ can be written for uniform isotropic media as

$$\left(\frac{d\sigma}{dE}\right)_z = \left(\frac{d\sigma}{dz}\right)_z \frac{\left|\gamma^m\right|}{\left(\frac{dE}{dl}\right)_E} \tag{10}$$

where σ is the rotation angle, γ^m is the directional cosine relative to z-axis (normally directed to a target), $(dE/dl)_E$ is a linear stopping power of electron with an energy E.

The binary indicator of rotation $\zeta^j(E, z)$ determines the intersection of a given trajectory created by rotation of the basic trajectory with a set of trajectories that produce contributions to a spectrum of transmitted electrons. $\chi^{m,j}(E)$ is the binary region indicator which determines boundary conditions for a given trajectory created by rotation.

The indicator of rotation $\chi^{m,j}(E)$ can be written as

$$\zeta^j = \begin{cases} 1, & \text{if } \left(\left(R^2 - (\vec{R},\vec{n}_j)^2\right)(1-\gamma_r)^2 - \left(z - \left(z_r + \gamma_r(\vec{R},\vec{n}_j)\right)\right)^2\right) \geq 0; \\ 0, & \text{in other case} \end{cases} \tag{11}$$

7. The average energy E_{av} of transmitted electrons is calculated as the average of the transmitted electron spectrum:

$$E_{av} = \frac{1}{N} \int_0^{E_0} \sum_{j=1}^{N} W_S^j (E; z) dE \qquad (12)$$

The algorithm described above was implemented in a FORTRAN subroutine and integrated with PENELOPE code (Salvat et al., 1996), and the efficiency of the usage of the MTR was evaluated.

A set of calculations of average energy for thick targets shows the high efficiency of the MTR in providing data for deep penetration of electrons. The amount of primary MTR trajectories that are needed to reach the same statistics as conventional Monte Carlo method can be reduced by a factor of 50 for depths of the order of one CSDA (continuous slowing down approximation) range R_0 of electrons. Since the MTR increases the time for one trajectory processing by about a factor of 2, the efficiency of the MRT is about a factor of 25 in comparison to the conventional Monte Carlo technique.

The reason for such an efficiency increase is the fact that when using the MRT, we create an additional set of trajectories that may also reaches deeper regions in a target. The artificiality of these trajectories is weighted by the weight factor given by (9)

We compared data on average energy E_{av} of electrons penetrating thick targets calculated by the use of PENELOPE in conventional binary Monte Carlo mode with the data provided by the MTR technique. Figure 3 shows how much the statistical uncertainty of the results can be reduced by the MTR technique (solid lines). The data given by the dashed line are the results of conventional calculations that have been presented in (Tabata et al., 1999). The number of primary electrons has been 100,000 in the calculation by the conventional Monte Carlo method, while it has been 5,000 with the application of the MTR.

The behavior of the curve describing the dependence of E_{av} on target thickness at deep penetration is determined by the range of struggling electrons. The slope of this curve becomes steeper at a large thickness, but this is an artifact associated with the energy cutoff used as a set-up parameter of the Monte Carlo simulation. The cut-off energy of 100 keV was used in the present calculations. The decrease of the cut-off value from 100 keV to 50 keV leads to a slight shift of the position of the change of the slope (see Figure 4). Ideally the dependence of average energy on target thickness should be studied with a cut-off energy comparable to the energy of electron thermalisation in solids. The use of a low cut-off energy increases the computation time, so that the application of the MTR would also be effective in reducing the artifact of the type described above as well as the artifact due to statistical fluctuations.

3.3 Detection of b-radiation from distributed sources.

It is common known problem of simulation detection of radiation from spatial distributed sources. One of the typical tasks is the detection of radiation from incorporated ***b***-sources in nuclear medicine.

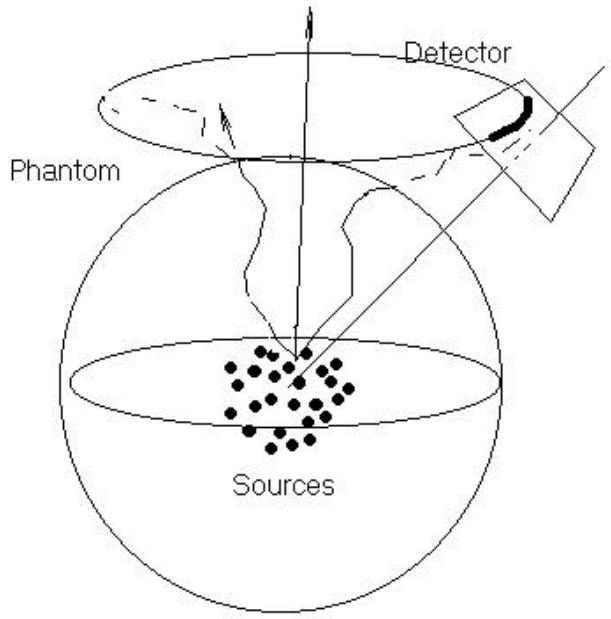

Fig. 5 MTR simulation of radiation from incorporated β-sources

The algorithm of MTR application for problems of distributed sources can be described as follows:

1. Sampling initial position of the source from source distribution, direction of the particle movement and energy from ***b***-spectrum.

2. An electron trajectory C_j is simulated in an infinite medium from initial energy E_0 to the cut-off energy E_c and stored in memory as a set of (x_i, y_i, z_i ,E_i).

3. The trajectory C_j is placed in a phantom (see Figure 5).

4. The initial point of the trajectory may be chosen as a point of trajectory rotation. The direction of the electron motion at this point is considered as a rotation axis.

5 The part of the trajectory C_j, where electron has the energy $E < E_r$ is selected. A set of trajectories is created by rotating this part of the base trajectory around the rotation axis.

6. The detector position is considered. If the indicator of rotation of rotation 1 (trajectory intersects detector during a given rotation), then go to 6; if $\zeta^j(E, z)$ equals 0 it is necessary to consider another trajectory.

7. Detection of the particle.

We simulated a detection of β radiation from 50 sources randomly distributed in the center of spherical phantom with the radius of 15 cm. The size of the detector placed on the surface of the phantom was 2x2 cm. Comparison with the analogue simulation gives a factor 15 for MTR performance. Increase in efficiency may be reached if additional rotations will be applied for a trajectory.

4. CONCLUSION

The *Method of Trajectory Rotation* (MTR) relies on rotational and translational symmetry of a uniform medium. A set of trajectories is created by rotation of the part of the trajectory around the direction of electron movement at some arbitrary point of the track. This set of trajectories is used to evaluate the weight of the contribution by a given trajectory to computed value of quantity.

We have shown that the general principles of the Method of Trajectory Rotation are applicable for a wide set of problems. Solutions of these problems that rely on purely analog techniques can be very difficult, if at all tractable. The Method of Trajectory Rotation shows also that principles of symmetry may be of crucial importance for any variance reduction techniques.

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