The Monte Carlo Method: Versatility Unbounded In A Dynamic Computing World
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THE MONTE CARLO SAMPLING OF ELECTRON TRANSPORT BY INDIVIDUAL COLLISION TECHNIQUE

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ABSTRACT

The problem of electron transport is of the most interest in all fields of modern science. To solve this problem the Monte Carlo sampling has to be in use. The transport of electrons is characterized by a large number of individual interactions. To simulate electron transport, the "condensed history" technique may be used, where a large number of collisions are grouped into a single step to be randomly sampled. Another kind of Monte Carlo sampling is the individual collision technique. In comparison with condensed history technique researcher has the incontestable advantages. For example one doesn't need to give parameters altered by condensed history technique like upper limit for electron energy, resolution, number of sub-steps etc. Also the condensed history technique may lose some very important tracks of electrons because of its limited nature by step parameters of particle movement and due to weakness of algorithms for example energy indexing algorithm. There are no these disadvantages in the individual collision technique. This report presents the new version of code BRAND where above mentioned technique is used. All information on electrons was taken from ENDF-6 files. They are the important part of BRAND. These files have not been processed but directly taken from electron information source. Four kinds of interaction like the elastic interaction, the bremsstrahlung, the atomic excitation and atomic electroionization were considered. In this report some results of sampling are presented after comparison with analogs. For example the endovascular radiotherapy problem (P2) of QUADOS2002 was presented in comparison with another techniques solves.

Key Words electron transport problem, electron interactions, ENDF-6 format, individual collision technique, QUADOS2002

1 INTRODUCTION

For precision solving of electron transport problems exactly computing of emission transfer in complex geometry form fields the Monte-Carlo statistical tries technique is convenient and reliable. In foundation of it the elementary interaction emission act probable character use lies. Moreover macroscopically cross-section of emission interaction with substance interprets like probability of collision with material atom on unit path of particle. It follows that the mathematical statistical laws applying for radiation field analysis is possible. In particular the statistical rule of vary particle (neutron, photon, electron and other) amount behavior is defined by analysis of their small quantity.

Although the application of Monte-Carlo method demands of using high-speed computer techniques the simplicity of composing program codes for compute by this way suborns. The disadvantage is the receiving result only for some restricted area of detectors (points, intervals of energy and angle) but not for all emission field like in many others approaches. However, these

manners adaptability is less effective for solving of complex geometry problems than Monte-Carlo. For your attention *the individual collision technique* is introduced.

Offered sampling of electron transport process by Monte-Carlo technique is based on the solve of the emission transport integral form equation in assumption of binary interactions model:

$$\psi = K\psi + f\,. \tag{1}$$

To solve the equation (1) it is adequate to estimate its answer. For that the evaluation is embedded:

$$I = (\psi, h) = \int_G \psi(\vec{\mathbf{X}}) h(\vec{\mathbf{X}}) d\vec{\mathbf{X}} = \sum_{n=0}^{\infty} (K^n f, h), \tag{2}$$

where $h(\vec{\mathbf{X}})$ is linear functional.

2 FREE LENGTH OF ELECTRON

For the put transport problem solving the free length is defined by formula:

$$l = -\frac{1}{\Sigma_N} ln(\gamma) + \sum_{k=1}^{N-1} T_k \cdot \left(1 - \frac{\Sigma_k}{\Sigma_N}\right), \tag{3}$$

where Σ_k is total macro cross-section for material involved with number k, T_k is depth of material k by beam, and $\gamma \sim U(0, 1)$.

The reaction type that particle taken is chosen by each trace step. It depends on micro cross-sections given for substance which particle is inside. While researching of the electron transport problem the sampling of reaction type is founded on ENDF-6 estimated data file.

3 INTERACTIONS

Four possible kinds of electron interactions (in accordance with formulism accepted in ENDF-6 standards) are accounted for: elastic interaction, bremsstrahlung, atomic excitation, and atomic electroionization with next relaxation [2].

3.1 Elastic interaction

Because of the very large mass of the residual atom with respect to the mass of the electron, it is assumed that the electron scatters without a change of energy, and there is no energy transfer to the residual atom. Electron continue its traffic with some another direction to be simulated by estimated nuclear data files. Secondary particles are not achieved. The sampling parameter is cosine of electron deflection angle between given and original motion direction.

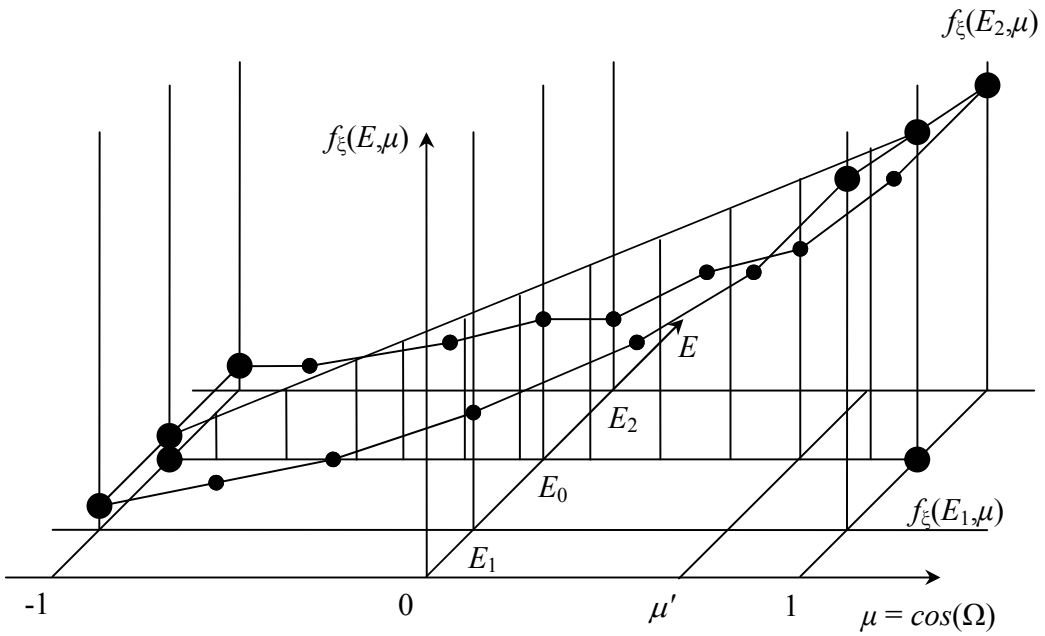

Figure 1.
Finding of the probability angle distribution density function

For sampling of outgoing electron deflection angle cosine it is known some densities of angle distribution $f_\xi(E, \mu)$ that depend on electron energy and with E_0 give the angle distribution density function cosine-dependent only (μ=cos(Ω)). Since distribution density functions are not uninterruptedly but energy discretely than in the beginning energies that given E_0 is between are defined, i.e. . $E_1 \le E_0 \le E_2$. One comes in two functions $f_\xi(E_1,\mu)$ and $f_\xi(E_2,\mu)$ between $f_\xi(E_0,\mu)$ desired lies, $f_\xi(E_1,\mu) \le f_\xi(E_0,\mu) \le f_\xi(E_2,\mu)$. These angle distribution density functions are shown on **fig.1**.

After angle distribution density functions are defined it is necessary to find μ_0 according to simulated random number F. Therefore $\mathrm{F} = \int_{-1}^{\mu_0} f_\xi(E_0,\mu)d\mu = \int_{-1}^{\mu_1} f_\xi(E_1,\mu)d\mu = \int_{-1}^{\mu_2} f_\xi(E_2,\mu)d\mu$. We solve this proposition in two cases for functions $f_\xi(E_1,\mu)$ и $f_\xi(E_2,\mu)$ and then find two solutions μ_1 and μ_2 respectively. It is certain $\mu_1 \le \mu_0 \le \mu_2$. And it is also known that points (E_1,μ_1), (E_2,μ_2), (E_0,μ_0) are on line. Because of that μ_0 follows from formula $\mu_0 = \dfrac{\mu_1 \cdot (E_2 - E_0) + \mu_2 \cdot (E_0 - E_1)}{E_2 - E_1}$.

This formulation is the solution of combined equations derived from geometry of **fig.2**:

$$\begin{cases} \mu_0 = a \cdot E_0 + b \\ \mu_1 = a \cdot E_1 + b \\ \mu_2 = a \cdot E_2 + b \end{cases} \text{, hence } \begin{cases} \mu_0 - \mu_1 = a \cdot (E_0 - E_1) \\ a = \dfrac{\mu_2 - \mu_1}{E_2 - E_1} \end{cases} .$$

In result we come to $\mu_0 = \mu_1 + \dfrac{\mu_2 - \mu_1}{E_2 - E_1} \cdot (E_0 - E_1)$, and from here desired formula succeeds.

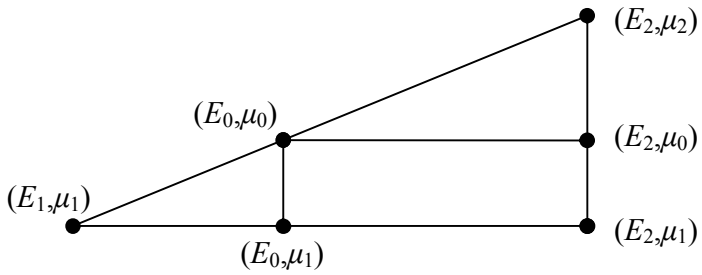

Figure 2.
Triangle finding of the scattering electron angle component

The angle distribution density function is formed discretely on segment $[-1,\mu']$ (note that $\mu' = 0.999999$ in ENDF-6) for that reason segment $[\mu',1]$ is filled analytic density function:

$$f_\xi(E,\mu) = \frac{A}{(\eta + 1 - \mu)^2}. \tag{4}$$

Quantity A may be expressed explicitly through η:

$$A = f \cdot (\eta + 1 - \mu')^2, \tag{5}$$

where $f = f_\xi(E,\mu')$ is value of the angle distribution density function at point μ'. In turn parameter η is calculated by Seltzer formula:

$$\eta = \frac{1}{2} \cdot \left(\frac{\alpha \cdot m \cdot c}{0.885 \cdot p} \right) \cdot Z^{2/3} \cdot \left[1.13 + 3.76 \cdot (\alpha \cdot Z/\beta)^2 \cdot \sqrt{\frac{\tau}{\tau + 1}} \right], \tag{6}$$

$$\text{where } \beta = \frac{v}{c} = \sqrt{1 - \left(\frac{1}{\tau + 1} \right)^2}, \ \tau = \frac{E}{mc^2}, \ p = \frac{1}{c} \cdot \sqrt{E \cdot (2mc^2 + E)}, \tag{7}$$

and α is fine structure constant, m, p, v are rest mass, momentum, velocity of electron correspondently, and Z is atomic number.

3.2 Bremsstrahlung

At bremsstrahlung electron continue its traffic with energy loss but in the straight-ahead direction. Also photon moving with some energy and some different way from original is produced. The sampling characteristics are electron energy, and energy, cosine of outgoing photon.

A) <u>For sampling of produced photon energy</u> similar to elastic scattering some angular distribution densities $f_\xi(E, E_p)$ that depend on incident electron energy are specified. In defined value E_0 these functions give some energy distribution density which is up to the outgoing photon energy (E_p) only. Analogously to elastic we rewrite all formulas with changing μ to E_p. Remember that $E_1 \le E_0 \le E_2$. Resulting to two functions $f_\xi(E_1,E_p)$ and $f_\xi(E_2,E_p)$ between these borders the value of desired function lies, i.e. $f_\xi(E_1,E_p) \le f_\xi(E_0,E_p) \le f_\xi(E_2,E_p)$. These discrete energy distribution density functions are shown on **fig.3**.

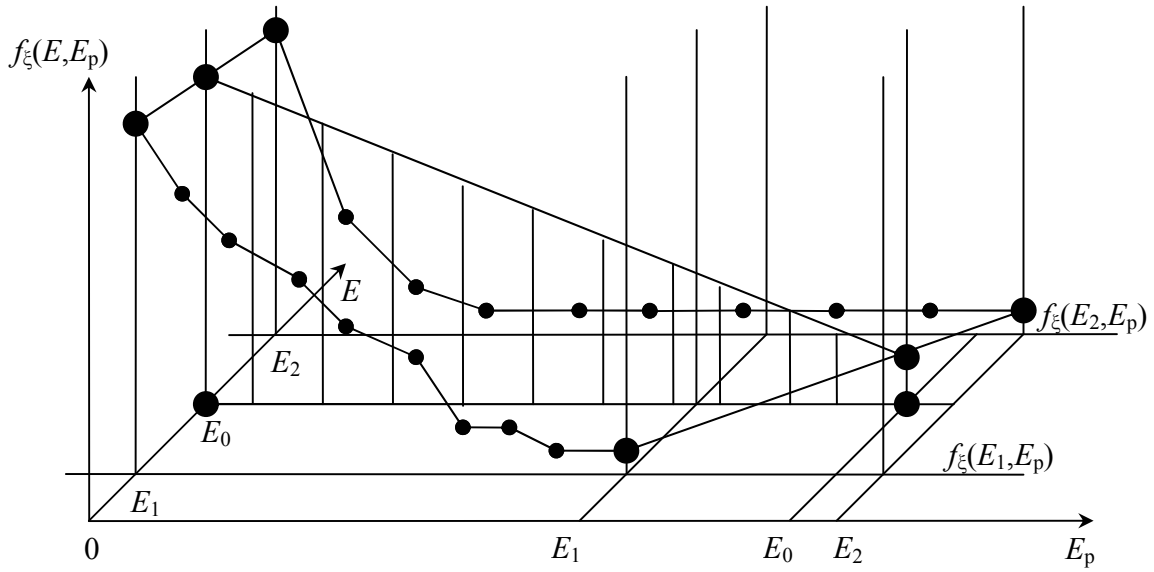

Figure 3.
Finding of probability energy distribution density function

After energy distribution density functions are defined it is essential to find E_{p0} in dependence from simulated random number F. Moreover

$$\mathrm{F} = \int_0^{E_{p0}} f_\xi\left(E_0, E_p\right)dE_p = \int_0^{E_{p1}} f_\xi\left(E_1, E_p\right)dE_p = \int_0^{E_{p2}} f_\xi\left(E_2, E_p\right)dE_p \,. \tag{8}$$

If we consider this predicate in two cases, i.e. for two distribution density functions $f_\xi(E_1,E_p)$ and $f_\xi(E_2,E_p)$, then we will find two solutions E_{p1} and E_{p2} respectively. It is known that $E_{p1} \le E_{p0} \le E_{p2}$. It is also certain that points (E_1,E_{p1}), (E_2,E_{p2}) and (E_0,E_{p0}) lie on line. And so E_{p0} is found on rule $E_{p0} = \dfrac{E_{p1}\cdot\left(E_2 - E_0\right) + E_{p2}\cdot\left(E_0 - E_1\right)}{E_2 - E_1}$ which is resulted from solution of combined equations derived from geometry of **fig.2** (if you change μ to E_p):

$$\begin{cases} E_{p0} = a\cdot E_0 + b \\ E_{p1} = a\cdot E_1 + b \\ E_{p2} = a\cdot E_2 + b \end{cases} \text{, hence } \begin{cases} E_{p0} - E_{p1} = a\cdot\left(E_0 - E_1\right) \\ a = \dfrac{E_{p2} - E_{p1}}{E_2 - E_1} \end{cases} .$$

In total we come to $E_{p0} = E_{p1} + \frac{E_{p2} - E_{p1}}{E_2 - E_1} \cdot (E_0 - E_1)$ and from this to desired formulation.

Note that cosine of photon motion direction μ_p is defined by formula:

$$\mu_p = \frac{2\gamma - 1 - \beta}{2\gamma\beta - 1 - \beta}, \tag{9}$$

where $\gamma \sim U(0,1)$, a $\beta = \frac{v}{c}$ (see **Eq. 7**), v is velocity of electron. [1]

B) For simulating of outcome electron energy the values of energies to be subtracted from incident electron original energy (E_0) are given. To specify subtract energy it is made the retrieval of two neighboring energies E_1 and E_2 to E_0 on predetermined discrete function. On **fig.4** the finding of E_1 and E_2 from given energy E_0 is shown.

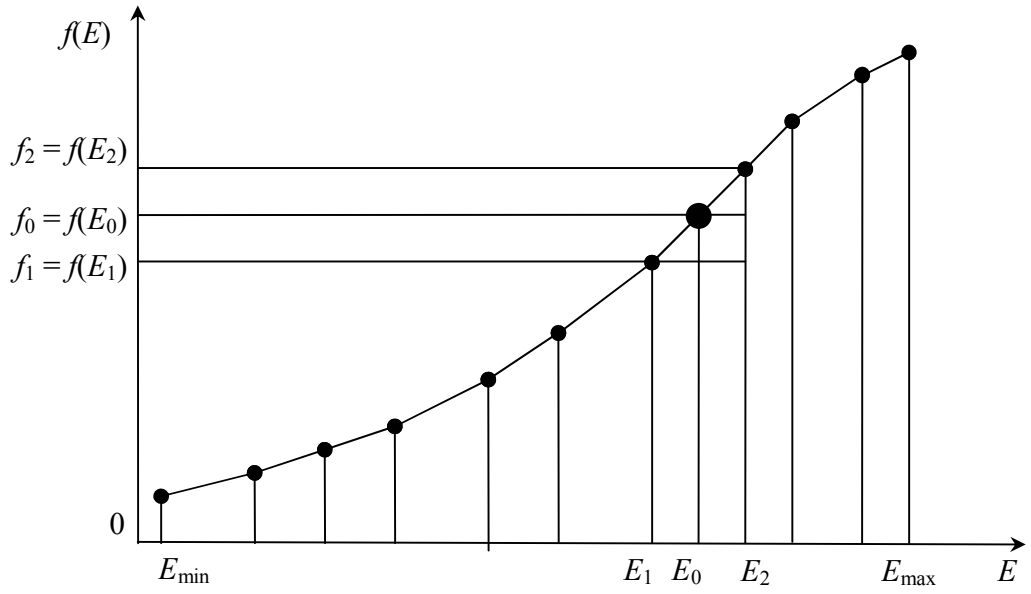

Figure 4.
Finding of probability energy distribution density function by incident electron energy

For given triangle (similarly **fig.2** if you change μ to f) we calculate desired quantity f_0=$f(E_0)$ from next formula $f_0 = f_1 + \frac{f_2 - f_1}{E_2 - E_1} \cdot (E_0 - E_1)$. In result $E_e = E_0 - f_0$.

3.3 Atomic excitation

Excitation occurs when the incident electron losses some of its energy by exciting the outer electrons of the atom to higher energy states. The energy transfer to the residual atom is scattered. The electron is assumed to continue in the straight-ahead direction. The variety factor is energy loss.

Reasoning for electron energy loss sampling in given case are the same as in the item **B)** of topic **3.2 "Bremsstrahlung"** because of identically data given.

3.4 Atomic ionization

Electroionization consist of two parts to be simulated. First there are two electrons coming out of each ionization reaction: the scattered electron and the recoil electron. Because these two particles are identical, it is arbitrarily assumed that the particle with the lower energy is the "recoil" electron, and the one with the higher energy is the "scattered" electron (E_0). It is assumed that both the scattered and the recoil electrons continue in the direction of the incident electron, and that no kinetic energy is transferred to the residual atom. The sampling rate is "recoil" electron energy.

Here it is necessary to refer to energy repartition in relaxation of atom with next possible process of outcome X-rays and atomic "knock-out" electrons from atom shell. Later there are more details of this procedure in topic **3.5 "Atomic relaxation"**.

The simulating scheme of "recoil" electron (E_e) repeat the item **A)** of topic **3.2 "Bremsstrahlung"** for produced photon (see **fig.3**, if E_p is changed to E_e, the last energies (axis E_e) for given energy distribution density functions are $E_1/2$, $E_0/2$, $E_2/2$ correspondently, the minimal distribution function energy is E_{bin}). That is why let see main aspects of sampling. They are as follows:

$$E_1 \le E_0 \le E_2,$$

$$f_\xi(E_1, E_e) \le f_\xi(E_0, E_e) \le f_\xi(E_2, E_e),$$

$$F = \int_{-1}^{E_{e0}} f_\xi(E_0, E_e)dE_e = \int_{-1}^{E_{e1}} f_\xi(E_1, E_e)dE_e = \int_{-1}^{E_{e2}} f_\xi(E_2, E_e)dE_e ,$$

$$E_{e1} \le E_{e0} \le E_{e2}.$$

Using **fig.2** (if you change μ to E_e) we find desired $E_{e0} = \dfrac{E_{e1} \cdot (E_2 - E_0) + E_{e2} \cdot (E_0 - E_1)}{E_2 - E_1}$.

The scattering electron energy is put by expression:

$$E_{e'} = E_0 - E_{bin} - E_{e0}, \tag{10}$$

where E_{bin} is the minimal energy that is need to electron for knocking out of atomic electron from given atom subshell. Atom is ionized with its quantity of energy.

3.5 Atomic relaxation

The relaxation of the residual atom left after ionization results in the emission of additional X-rays and electrons. The process will continue by filling the new holes from higher levels, *etc*., until all the ionization energy has been accounted for by the emission of X-rays and electrons.

The electrons produced by this atomic relaxation can be used as a source for a subsequent electron transport calculation, or their energy can just be added to the local heating. The X-rays can be transported elsewhere to cause additional photo-atomic reactions. In general, the use of relaxation is indicated when high-Z materials are present and photon energies of less than 1 MeV are of interest. Data file is provided to give the information necessary to compute the emission of X-rays and electrons associated with atomic relaxation cross section. It is based on EADL, the Evaluated Atomic Data Library developed by D. E. (Red) Cullen at the Lawrence Livermore National Laboratory (LLNL).

The first energy and atomic subshell from what electron was “knock out” are defined beforehand they are known from atomic electroionization reaction in given case. Scheme of atomic relaxation appears in the following way. Atomic relaxation file (File 28 [2]) data contain tables of transitions for each atomic electron level. Possible energy transitions by electron levels with indication of level number, given transition probability, electron count of neutral atom, and extracted energy are shown in these data.

Radiative transitions are appeared in the beginning of transition table and enclose one number of higher atomic level electron be taken from. In addition photon is produced with energy equals to energy quant between subshells. It is possible that there are no allowed transitions from higher subshells to a particular subshell.

An alternative path is to bring down an electron from a higher level with the simultaneous emission of an electron from that level or a higher one. And these non-radiative transitions are located lower and contain information about two atomic level numbers. One of them will replace the “knock-out” electron another will be irradiated by atom. After substitution original energy has to be reduced by value equals to energy quant between these levels. This value is given in transition table. If vestigial energy is still positive the replacement process continue from one of levels electron brought from. The choice of level is defined by the rule of preferring lower level to the rest. If further transitions are unacceptable and vestigial energy is still positive then atomic relaxation simulating process should be stopped. Moreover residual energy must be transit to atom, i.e. substance.

For example, if an incident electron of energy E ionizes the K subshell with binding energy EK, the atom will emit an electron with some energy (see above topic **3.4 “Atomic ionization”**), and the atomic structure will be left ionized, with a "hole" in the K subshell. After that the atom can proceed to fill this hole is to bring down an electron from a higher energy level, for example L1, with the simultaneous emission of an X-ray of energy EK-EL1. In this way obviously relaxation process is not stopped because energies EK and EL1 are not equal. In a like manner next ionization of subshell L1 will occur with energy EL1. Another case should be considered if non-radiative process is taken place. As an example, you might see an emitted electron of energy EK-EL1-EM1, and one which fills the vacancy in the K shell and leave new holes in the L1 and M1 shells. Then ionization procedure of these levels is continued. First the subshell L1 selected by the rule of preferring is undergone. If there is energy left after that proceeding we carry on relaxation with other levels.

4 SIMULATION

In ending it is essential to present BRAND simulating compares with researches. As we see on **fig.5** there is a close approximation of modeling with experimental data [3], some additional compares with experiments were presented in [5].

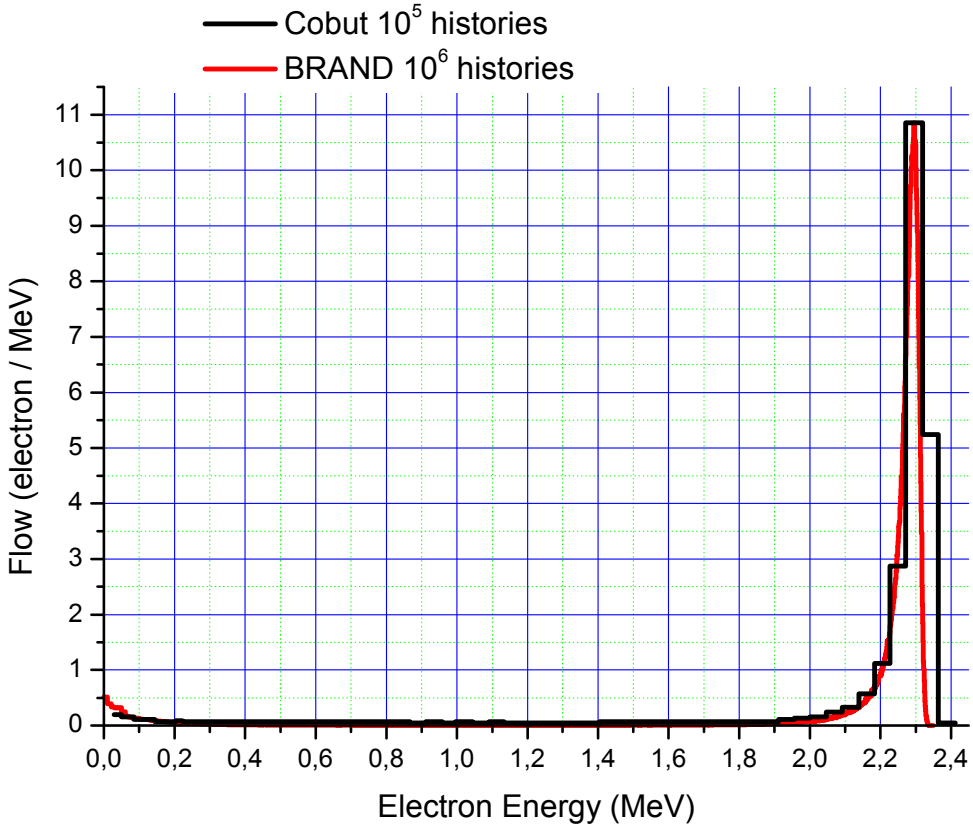

Figure 5.
Flow rate simulation results for 2.43-MeV electrons slowing down in a 0.48085 cm thick silicon slab

As another demonstration of simulation the endovascular problem solve example is adduced on **fig.6** (Problem P2, QUADOS2002, Bologna, 2002) [4]. As we see the BRAND result is sufficiently close to MCNP simulating.

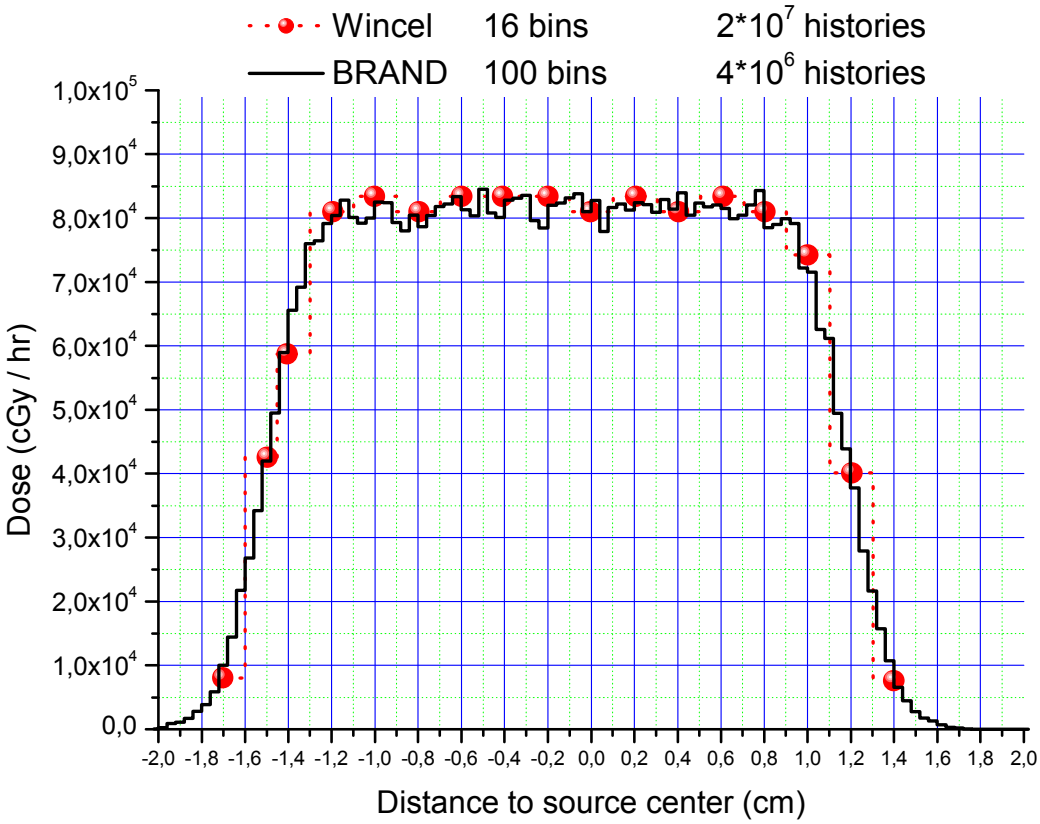

Figure 6.
Electron absorbed dose rate along the source longitudinal axis,
at a depth of 1mm into the artery wall from the inside surface without plaque
(source width is 2.7cm, source strength is 7GBq)

5 CONCLUSIONS

The creating of sampling algorithms need ENDF-6 evaluated data format files, in particular, the Secondary Distributions for Photo- and Electro- Atomic Data file (File 26) and Atomic Relaxation Data file (File 28) are in use. The sampling algorithms of four main reactions and the atomic relaxation were developed.

All algorithms were composed into Fortran-90 codes. Codes are built by module principle that include a number of functions and procedures for evaluated data file information reading and writing into convenient simulating format. The efforts resulted in new version of program complex BRAND 6.5 allowed to precisely solve electron transport problems.

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