A model for Multiple Scattering in Geant4

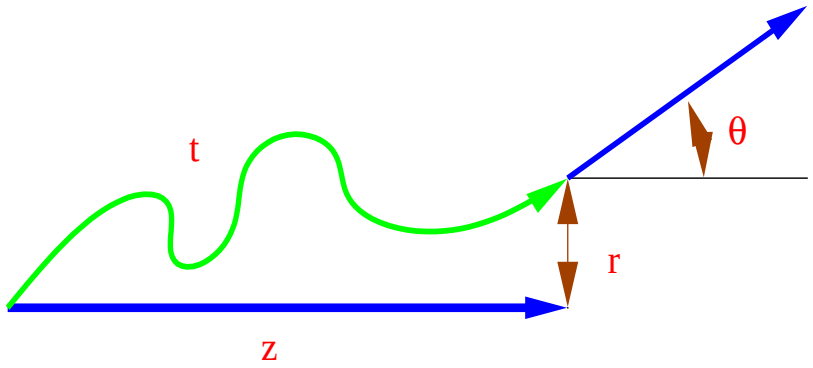
László Urbán

RMKI Research Institute for Physics, Budapest

April 18-21, 2005

Multiple Coulomb scattering

Charged particles traversing a finite thickness of matter suffer repeated elastic Coulomb scattering. The cumulative effect of these small angle scatterings is a net deflection from the original particle direction.



- longitudinal displacement z (or geometrical path length)
- lateral displacement r
- true (or corrected) path length t
- angular deflection θ

The practical solutions of the particle transport can be classified :

- detailed (microscopic) simulation : exact, but time consuming if the energy is not small. Used only for low energy particles.
- condensed simulation : simulates the global effects of the collisions during a macroscopic step, but uses approximations. EGS, Geant3 (both use Moliere theory), Geant4
- mixed algorithms : "hard collisions" are simulated one by one + global effects of the "soft collisions" : Penelope.

Angular distribution

If the number of individual collisions is large enough (> 20) the multiple Coulomb scattering angular distribution is Gaussian at small angles and like Rutherford scattering at large angles.

The Molière theory [Molie48, Bethe53] reproduces rather well this distribution, but it is an approximation.

The Molière theory is accurate for not too low energy and for small angle scattering, but even for this case its accuracy is not too good for very low Z and high Z materials.(see e.g. [Ferna93], [Gotts93])

The Molière theory does not give information about the spatial displacement of the particle, it gives only the scattering angle distribution.

To get a more complete information it is better to start with theory of Lewis which is based on the transport equation of charged particles ([Lewis50, Kawra98]).

The MSC model in Geant4 uses model functions to sample angular and spatial distributions after a step.

The functions are choosen in such a way that they give the same moments than the Lewis theory.

Transport of charged particles

Let $p(r, d, t)$ denote the probability density of finding the particle at the point $r = (x, y, z)$ moving in the direction of the unit vector $\overrightarrow{d}$ after having travelled a path length t.

The transport equation

$$\frac{\partial p(r,d,t)}{\partial t} + \overrightarrow{d}.\overrightarrow{\nabla p(r,d,t)} = n_{at} \int [p(r,d',t) - p(r,d,t)] \frac{d\sigma(\chi)}{d\Omega} d\Omega \quad (1)$$

can be solved exactly for special cases only.

This equation can be used to derive different moments of p.

Transport Mean Free Path

$$\frac{1}{\lambda_k} = 2\pi n_{at} \int_{-1}^{1} [1 - P_k(cos\chi)] \frac{d\sigma(\chi)}{d\Omega} d(cos\chi) \qquad (2)$$

$d\sigma(\chi)/d\Omega$ is the differential cross section of the scattering,
$P_k(cos\chi)$ the k-th Legendre polynomial,
n_{at} the nb of atoms per volume.

The first transport mean free path λ_1, has been calculated by Liljequist et al. for e^- and e^+ in the kinetic energy range 100 eV - 20 MeV in 15 materials [Lilje87], [Lilje90].

The MSC model in Geant4 uses these values, and when necessary, linearly interpolates the transport cross section, $\sigma_1 = 1/\lambda_1$, in atomic number Z and in the square of the particle velocity, β^2.

The ratio $\kappa = \lambda_1/\lambda_2$ is a slowly varying function of the energy: $\kappa \simeq 2$ for $T \sim$ a few keV, and $\kappa \to 3$ for very high energies (see [Kawra98]).

Hence, a constant value of 2.5 is used in the model.

Transport Mean values

Most of the mean properties of MSC computed in the simulation depend only on the first and second transport mean free paths.

At the end of the true step length, t, the scattering angle is θ.
The mean value of $cos\theta$ is

$$\langle cos\theta \rangle = \exp\left[-\frac{t}{\lambda_1}\right] \tag{3}$$

The variance of $cos\theta$ can be written as

$$\sigma^2 = \langle cos^2\theta \rangle - \langle cos\theta \rangle^2 = \frac{1 + 2e^{-2\kappa\tau}}{3} - e^{-2\tau} \tag{4}$$

where $\tau = t/\lambda_1$ and $\kappa = \lambda_1/\lambda_2$.

The mean value of the geometrical path length (first moment) corresponding to a given true path length t is given by

$$\langle z \rangle = \lambda_1 \left[1 - \exp\left(-\frac{t}{\lambda_1} \right) \right] \tag{5}$$

Eqs. 3 - 5 are exact results if the differential cross section has axial symmetry and the energy loss can be neglected.

The transformation between true and geometrical path lengths is called the *path length correction.*

This formula and other expressions for the first moments of the spatial distribution were taken from either [Ferna93] or [Kawra98], but were originally calculated by Goudsmit and Saunderson [Gouds40] and Lewis [Lewis50].

The mean lateral displacement can also be calculated relatively easily and accurately. The square of the mean lateral displacement is

$$\langle x^2 + y^2 \rangle = \frac{4\lambda_1^2}{3} \left[\tau - \frac{\kappa+1}{\kappa} + \frac{\kappa}{\kappa-1} e^{-\tau} - \frac{1}{\kappa(\kappa-1)} e^{-\kappa\tau} \right] \quad (6)$$

($\tau = t/\lambda_1$ and $\kappa = \lambda_1/\lambda_2$)

Here it is assumed that the initial particle direction is parallel to the the z axis.

Energy Dependence

If the energy loss along the step cannot be neglected, Eqs. 3-5 must be modified :

$$\langle cos\theta \rangle = \exp\left[- \int_0^t \frac{du}{\lambda_1(u)} \right] \tag{7}$$

$$\langle z \rangle = \int_0^t \langle cos\theta \rangle_u \; du \tag{8}$$

In order to compute Eqs. 7-8 the t dependence of the transport mean free path must be known. λ_1 depends on the kinetic energy of the particle which decreases along the step. All computations in the model use a linear approximation for this t dependence:

$$\lambda_1(t) = \lambda_{10}(1 - \alpha t) \tag{9}$$

The constant α can be expressed using λ_{10} and λ_{11}, the values of the transport mean free path at the beginning and at the end of the step :

$$\alpha = \frac{\lambda_{10} - \lambda_{11}}{t\lambda_{10}} \tag{10}$$

It is worth noting that Eq. 9 is *not* a crude approximation. It is rather good at low (< 1 MeV) energy. At higher energies the step is generally much smaller than the range of the particle, so is the change in energy.

Using Eqs. 7 - 9 the explicit formula for $\langle cos\theta \rangle$ is :

$$\langle cos\theta \rangle = (1 - \alpha t)^{\frac{1}{\alpha\lambda_{10}}} \tag{11}$$

Mean geometrical path length: $\langle z \rangle$

Using Eqs. 7 - 9 the explicit formula for the geometrical path length z can be written as

$$\langle z \rangle = \frac{1}{\alpha(1+\frac{1}{\alpha\lambda_{10}})}\left[1-(1-\alpha t)^{1+\frac{1}{\alpha\lambda_{10}}}\right] \tag{12}$$

For a step with small relative energy loss the formula of $\langle z \rangle$ gives back the expression 5 :

$$\langle z \rangle = \lambda_{10}\left[1-\exp\left(-\frac{t}{\lambda_{10}}\right)\right] \tag{13}$$

Eq. 12 or 13 gives the mean value of the geometrical step length for a given true step length.

Sampling the geometrical path length: z

The actual geometrical path length is sampled according to the simple probability density function defined for $v = z/t \in [0, 1]$:

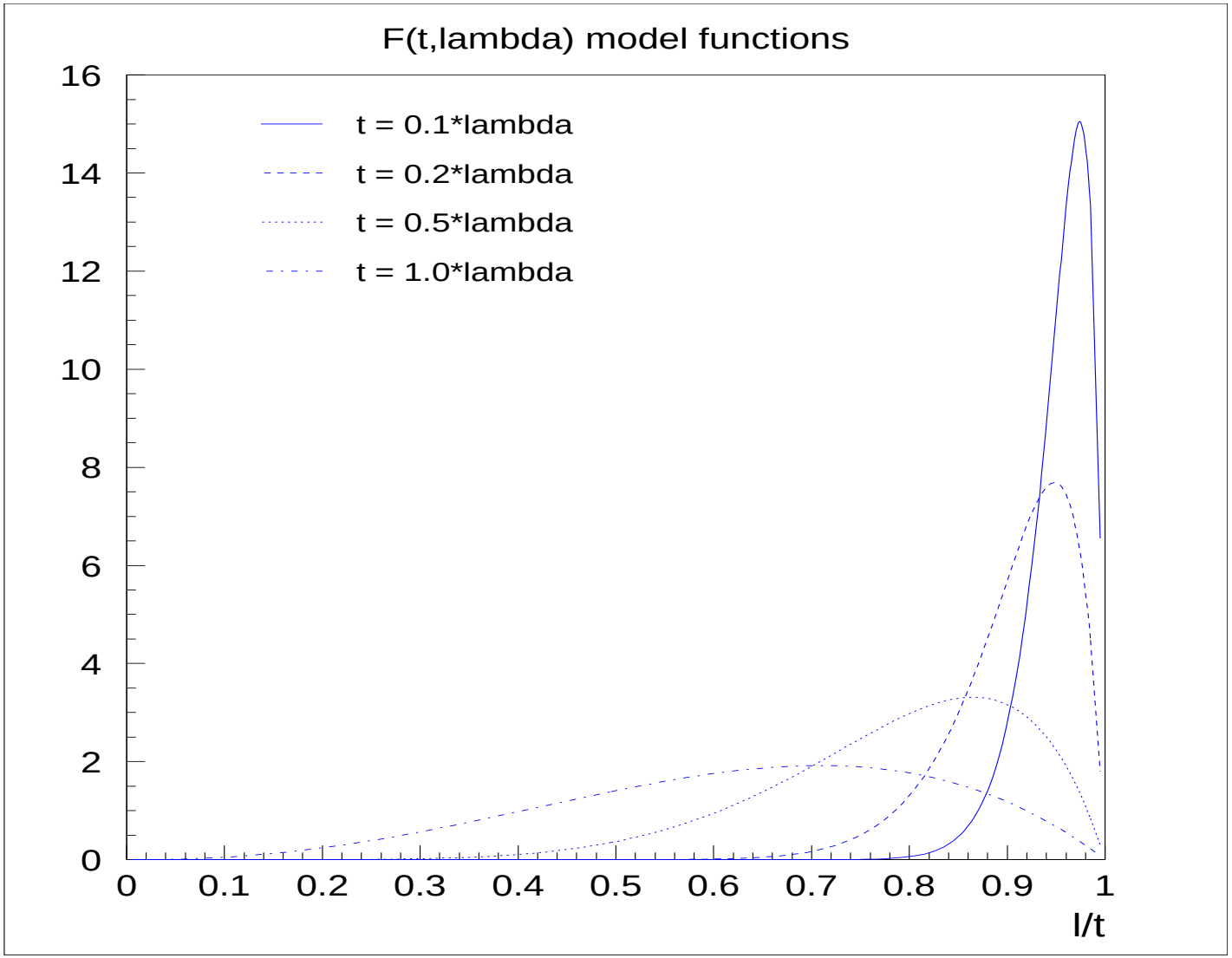
$$f(v) = (k+1)(k+2)v^k(1-v) \tag{14}$$

The value of the exponent k is computed from the requirement that $f(v)$ must give the same mean value for $z = vt$ as eq. 12 or 13. Hence :

$$k = \frac{3\langle z\rangle - t}{t - \langle z\rangle} \tag{15}$$

The value of $z = vt$ is sampled using $f(v)$ if $k > 0$, otherwise $z = \langle z\rangle$ is used.

The sampling function: $f(v)$



Computing the true path length: t

The $z \rightarrow t$ transformation is performed using mean values.
The transformation is the inverse of eq. 12 :

$$t(z) = \frac{1}{\alpha}\left[1 - (1 - \alpha w z)^{\frac{1}{w}}\right] \tag{16}$$

where

$$w = 1 + \frac{1}{\alpha\lambda_{10}}$$

If the step is small, the expression is simply (inverse of eq. 13) :

$$t(z) = \langle t \rangle = -\lambda_1 \log\left(1 - \frac{z}{\lambda_1}\right) \tag{17}$$

This transformation is needed when the particle arrives at a volume boundary, causing the step to be geometry-limited.
Then the true path length must be recomputed in order to have the correct energy loss of the particle after the step.

Angular Distribution

$u = cos\ \theta$ is sampled according to a model function $g(u)$:

$$g(u) = p\ [q\ g_1(u) + (1-q)\ g_3(u)] + (1-p)\ g_2(u) \qquad (18)$$

where $0 \leq p, q \leq 1$, and the g_i are simple functions of $u = cos\theta$, normalized over the range $u \in [-1,\ 1]$.

The functions g_i have been chosen as :

$$g_1(u) = C_1 \quad e^{-a(1-u)} \qquad u \in [u_0,\ 1] \qquad (19)$$

$$g_2(u) = C_2 \quad \frac{1}{(b-u)^d} \qquad u \in [-1,\ u_0] \qquad (20)$$

$$g_3(u) = C_3 \qquad u \in [-1,\ 1] \qquad (21)$$

a, b, d, u_0 and the weights p, q are the parameters of the model.
C_i are normalization constants.

It is worth noting that

- at small angle, $g_1(u)$ is nearly Gaussian

$$exp\left(\frac{-\theta^2}{2\theta_0^2}\right) \tag{22}$$

  with $\theta_0^2 = 1/a$

- for large θ, $g_2(u)$ is a Rutherford-like tail if $b \approx 1$ and $d \sim 2$.

Determination of the Model Parameters - 1

- $g(u)$ and its first derivative must be continuous at $u = u_0$
- $g(u)$ must give the same $\langle \cos\theta \rangle$ as the theory (eq. 11) :

$$q\ p\ \langle u \rangle_1 + (1-p)\ \langle u \rangle_2\ = [1 - \alpha\ t]^{\frac{1}{\alpha \lambda_{10}}} \qquad (23)$$

  where $\langle u \rangle_i$ is the mean value of u computed from the distribution $g_i(u)$.

- The value of u_0 and d has been chosen as

$$u_0 = 1 - \frac{3}{a} \qquad d = 2 + \frac{t}{\lambda_1} \qquad (24)$$

Determination of the Model Parameters - 2

The parameter a was chosen according to a modified Highland formula for the width of the angular distribution :

$$a = \frac{0.5}{1 - cos(\theta_0)} \tag{25}$$

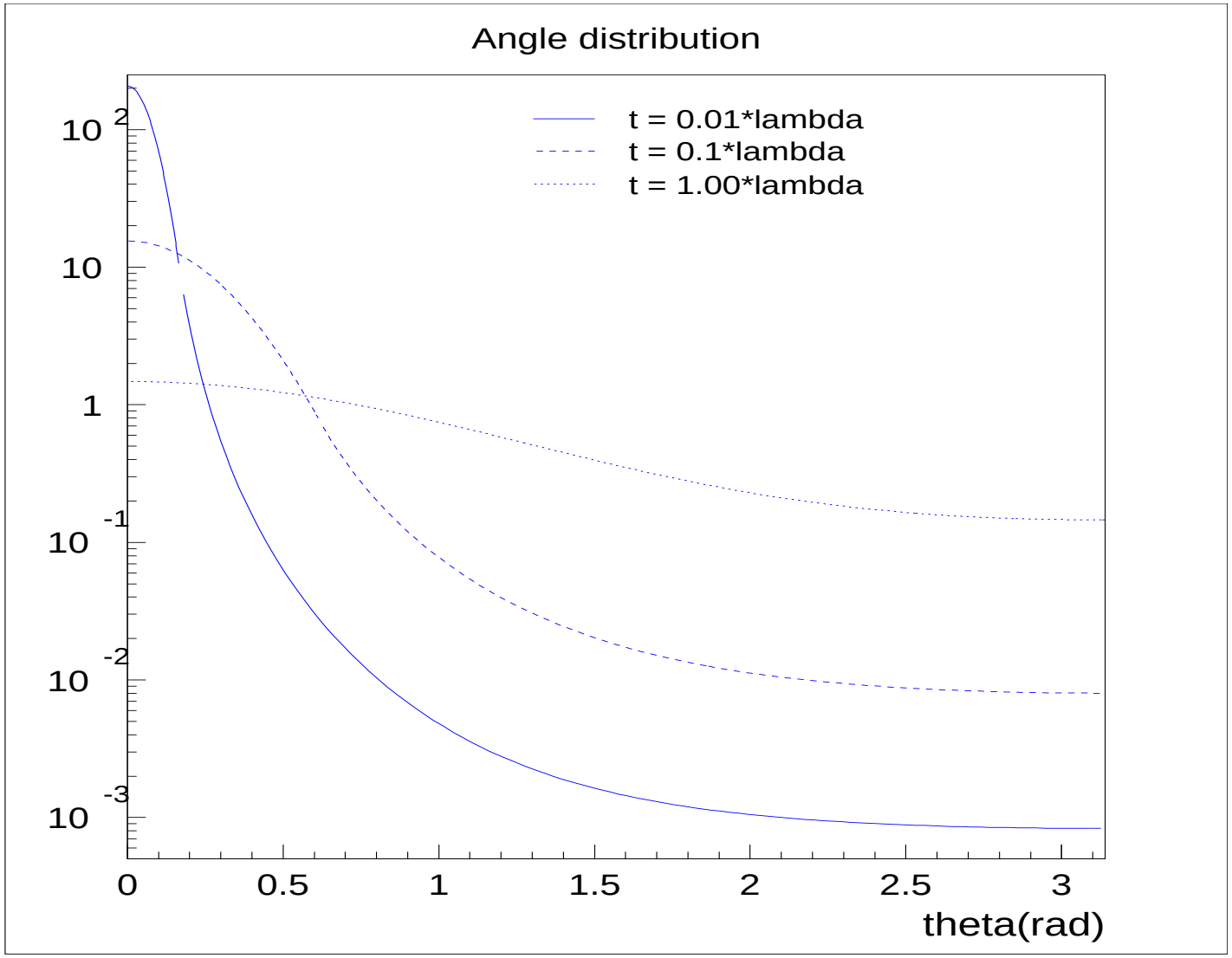
where θ_0 is

$$\theta_0 = \frac{13.6MeV}{\beta cp} z_{ch} \left[\frac{t}{X_0}\right]^{0.555} \tag{26}$$

Here $\theta_0 = \theta_{plane}^{rms}$ is the width of the approximate Gaussian projected angle distribution.

This formula gives much smaller step dependence in the angular distribution and describes the available electron scattering data better than the Highland form.

Angular distribution: $f(cos\theta)$



Additional Comments

- In this model there is no step limitation originated from multiple scattering.
- The sum of the 'true' step lengths of the particle does not depend on the length of the steps.
  (Most algorithms used in simulations do not have these properties)
- For heavy charged particles (μ, π, p, etc.) λ_1 is calculated from the electron or positron values with a scaling : λ_1 depends only on the variable $p\beta c$
- In its present form, only the mean value of the lateral displacement is computed and the correlations are neglected. However, the model is general enough to incorporate other random quantities in the future.

Nuclear Size Effects

The effect of the finite nuclear size is estimated in Born approximation ([Lilje87]). Then, the scattering cross section can be factorised as

$$\frac{d\sigma(\chi)}{d\Omega} = \frac{d\sigma_B(\chi)}{d\Omega} F(\chi) \tag{27}$$

where $d\sigma_B/d\Omega$ is the Born cross section for a screened point-like nucleus and $F(\chi)$ is the squared nuclear form factor. $F(\chi) \approx 0$ if $\chi > \chi_{max}$ where

$$sin(\frac{\chi_{max}}{2}) = \frac{1}{kR} \tag{28}$$

where k is the particle wave number and R is the nuclear radius. This correction means that $\sigma(\chi)$ decreases, so λ_1 defined by

$$\frac{1}{\lambda_1} = 2\pi n_a \int_{cos\chi_{max}}^{1} [1 - P_1(cos\chi)] \frac{d\sigma_B(\chi)}{d\Omega} F(\chi) d(cos\chi) \tag{29}$$

increases for larger energies.

MSC Algorithm

Steps of MSC algorithm (are essentially the same for many condensed simulations) :

1. selection of step length $\Longleftarrow$ physics processes + geometry (MSC performs the $t \Longleftrightarrow z$ transformations only)
2. transport to the initial direction : (not MSC business)
3. sample scattering angle θ
4. compute lateral displacement, relocate particle

Boundary Crossing Algorithm

Low energy particles entering a new volume penetrate deeply in it in the first step and then - because of energy loss - they are not able to reach again the boundary in backward direction. The backscattering rate is underestimated.

A very simple boundary crossing algorithm has been implemented : restrict the step of particles entering in a new volume :

$$t = f_r \cdot max\{r, \lambda_1\} \tag{30}$$

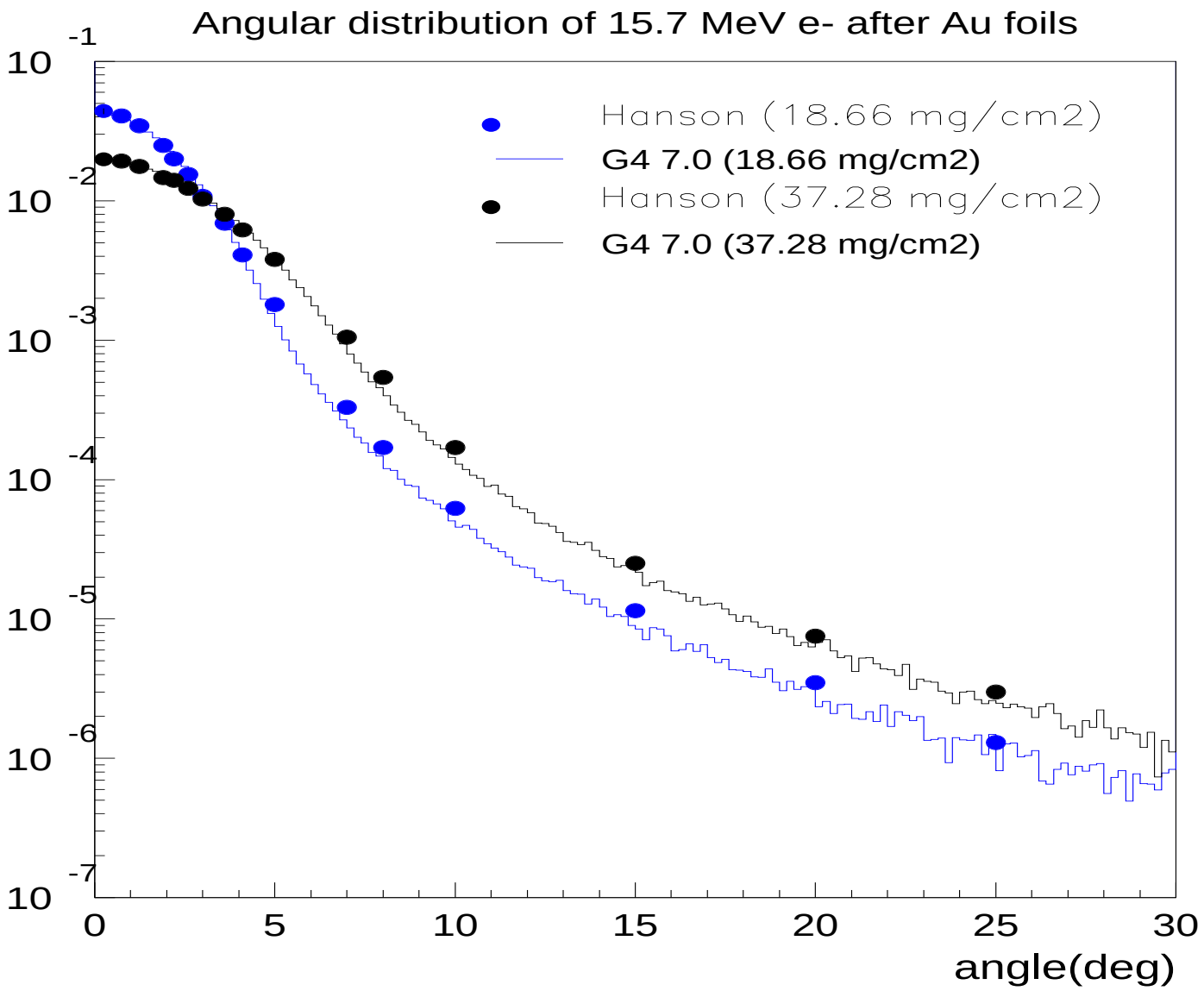
where r is the range of the particle, f_r is a constant ($f_r \in [0, 1]$) (taking the max of r and λ_1 is an empirical choice).

It can be easily seen that this kind of step limitation means a real contraints for low energy particles only.

The choice of the parameter f_r is a question related with performance. By default $f_r = 0.2$ is used as a compromise between performance and physics.

When a better backscattering simulation is needed, one must use a smaller value for $f_r (< 0.01)$.

However, this model is too simple and it can reproduce the backscattering data approximately only.


Angular distribution of 15.7 MeV e- after Au foils
Hanson (18.66 mg/cm2)
G4 7.0 (18.66 mg/cm2)
Hanson (37.28 mg/cm2)
G4 7.0 (37.28 mg/cm2)
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
10^-7
0
5
10
15
20
25
30
angle(deg)

In Fig.2 the lateral spreading of a 2.5 MeV proton beam is shown after mylar foils of different thicknesses. The spreading is measured in a distance 6.3 mm after the foils, the line representing the experimental data have been taken from [Miche01], the squares are the simulation results. The lateral spreading of the beam is directly connected with the angle distribution of the beam after the mylar absorber, so this result is a benchmark comparison for the angle distribution.

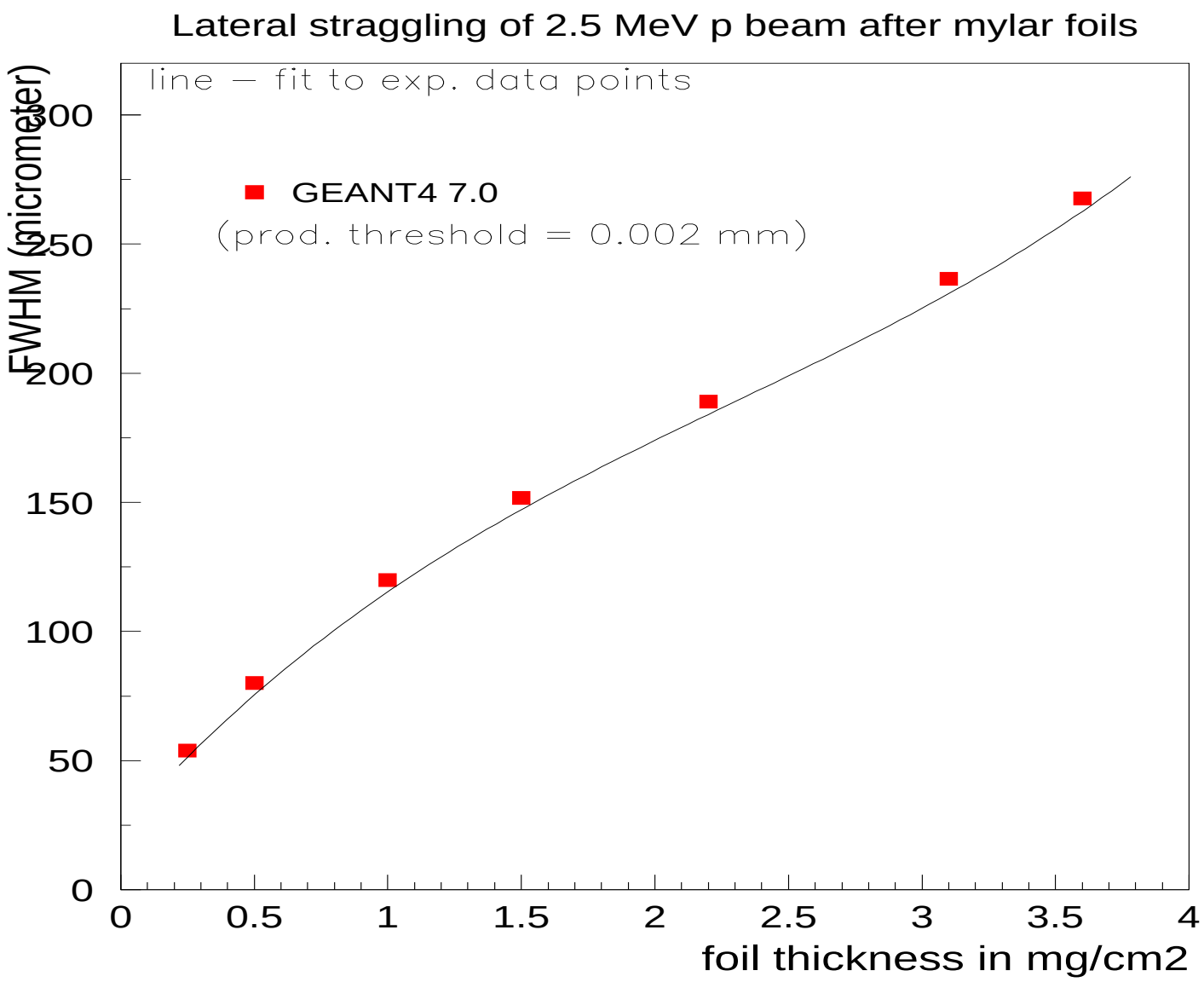
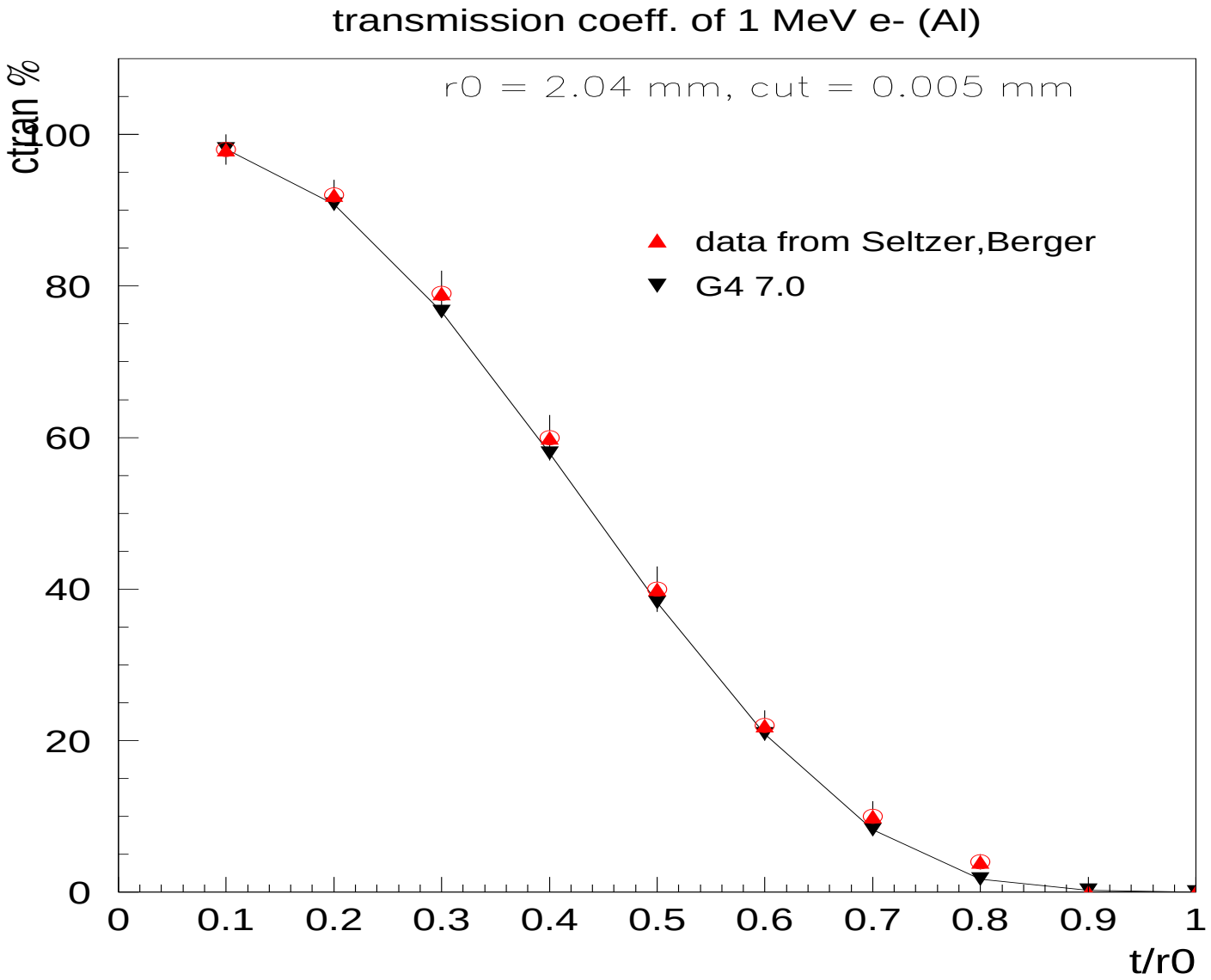
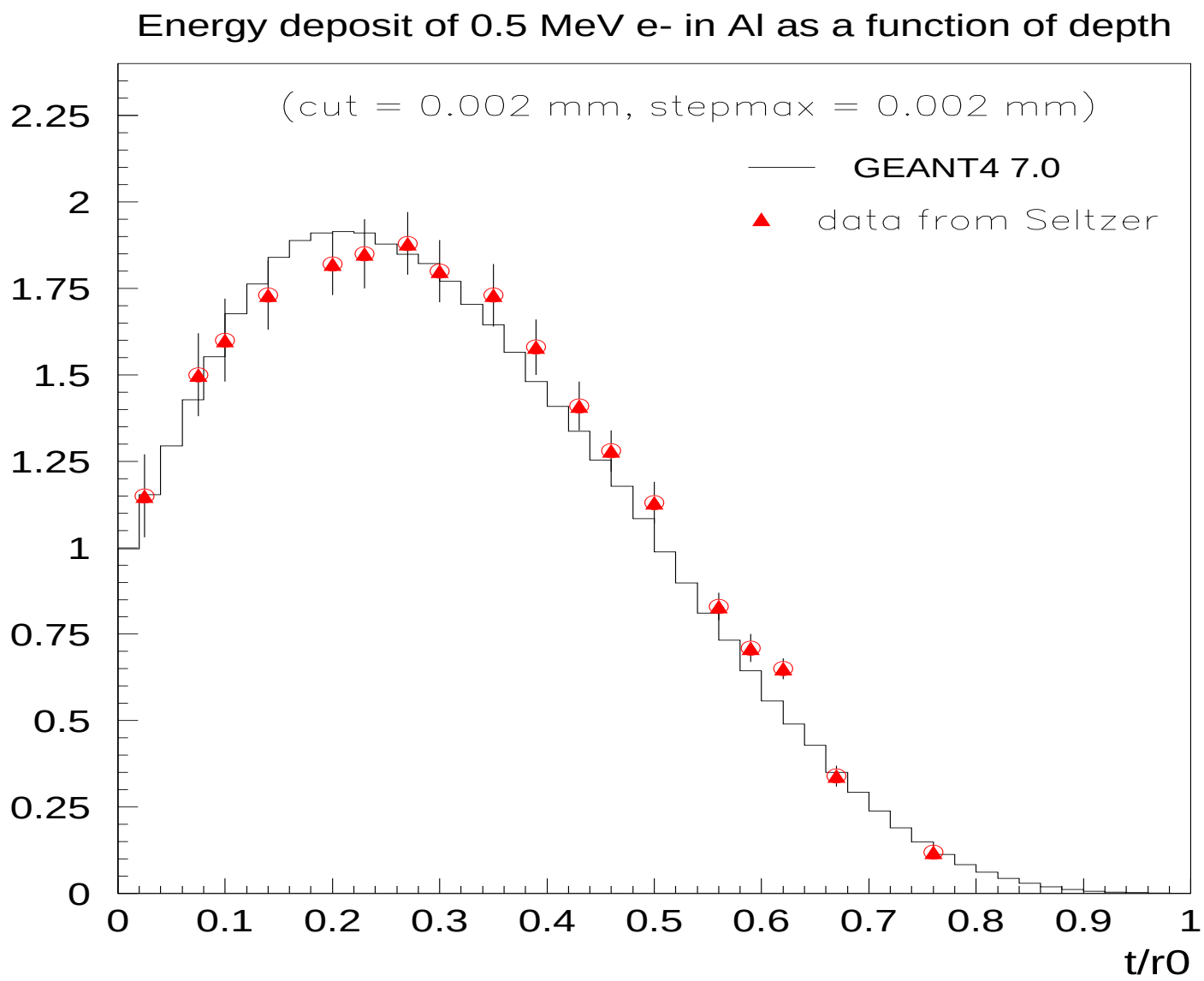
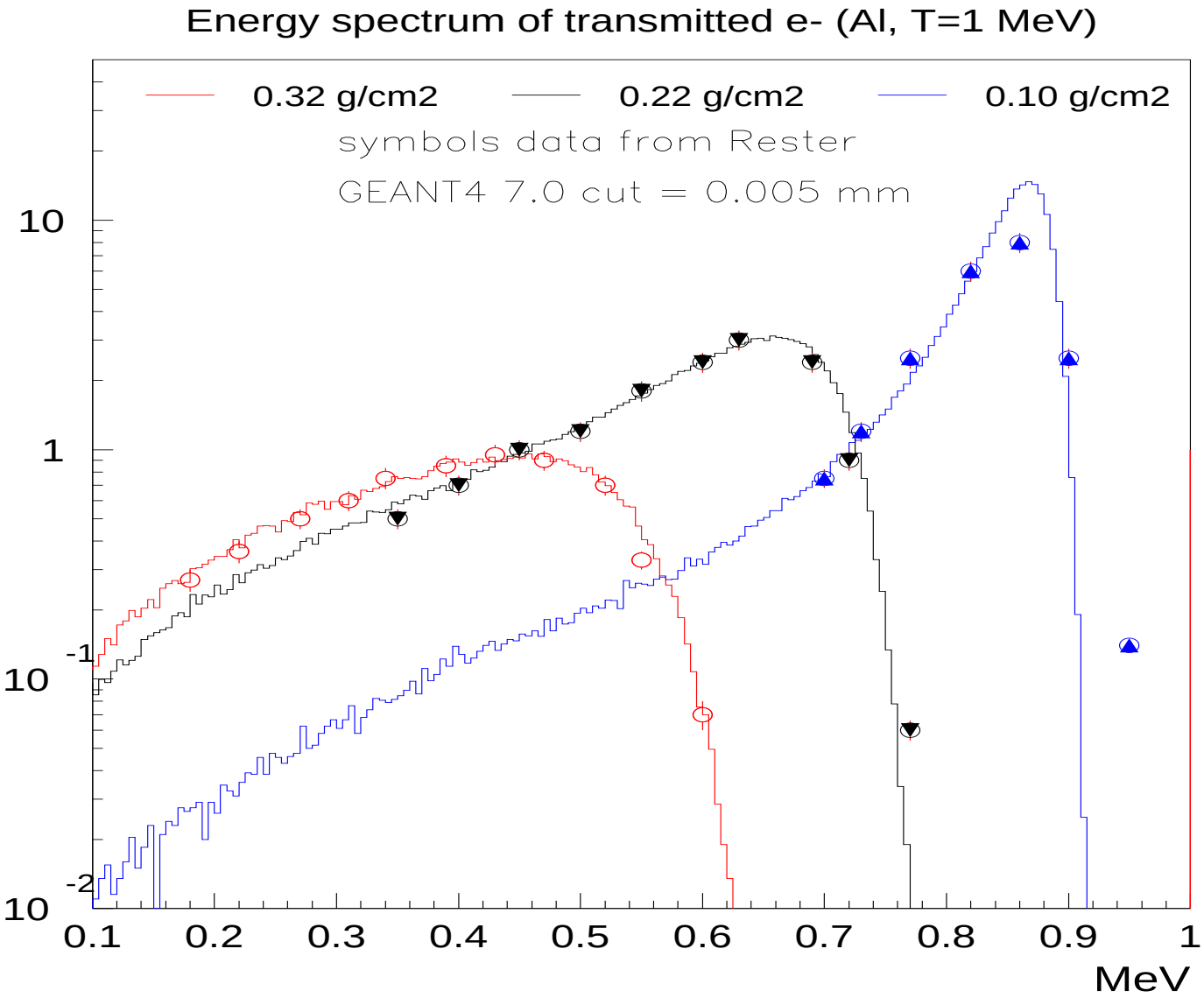

Lateral straggling of 2.5 MeV p beam after mylar foils
line — fit to exp. data points
GEANT4 7.0
(prod. threshold = 0.002 mm)
FWHM (micrometer)
foil thickness in mg/cm2
0
50
100
150
200
250
300
0
0.5
1
1.5
2
2.5
3
3.5
4

Fig. 3 shows the number transmission coefficient T as function of the foil thickness for 1 MeV electrons in aluminium. The thickness is measured in units of the continuous slowing down range, the data originated from different measurements have been taken from the review paper of Seltzer and Berger ([Seltz74]).

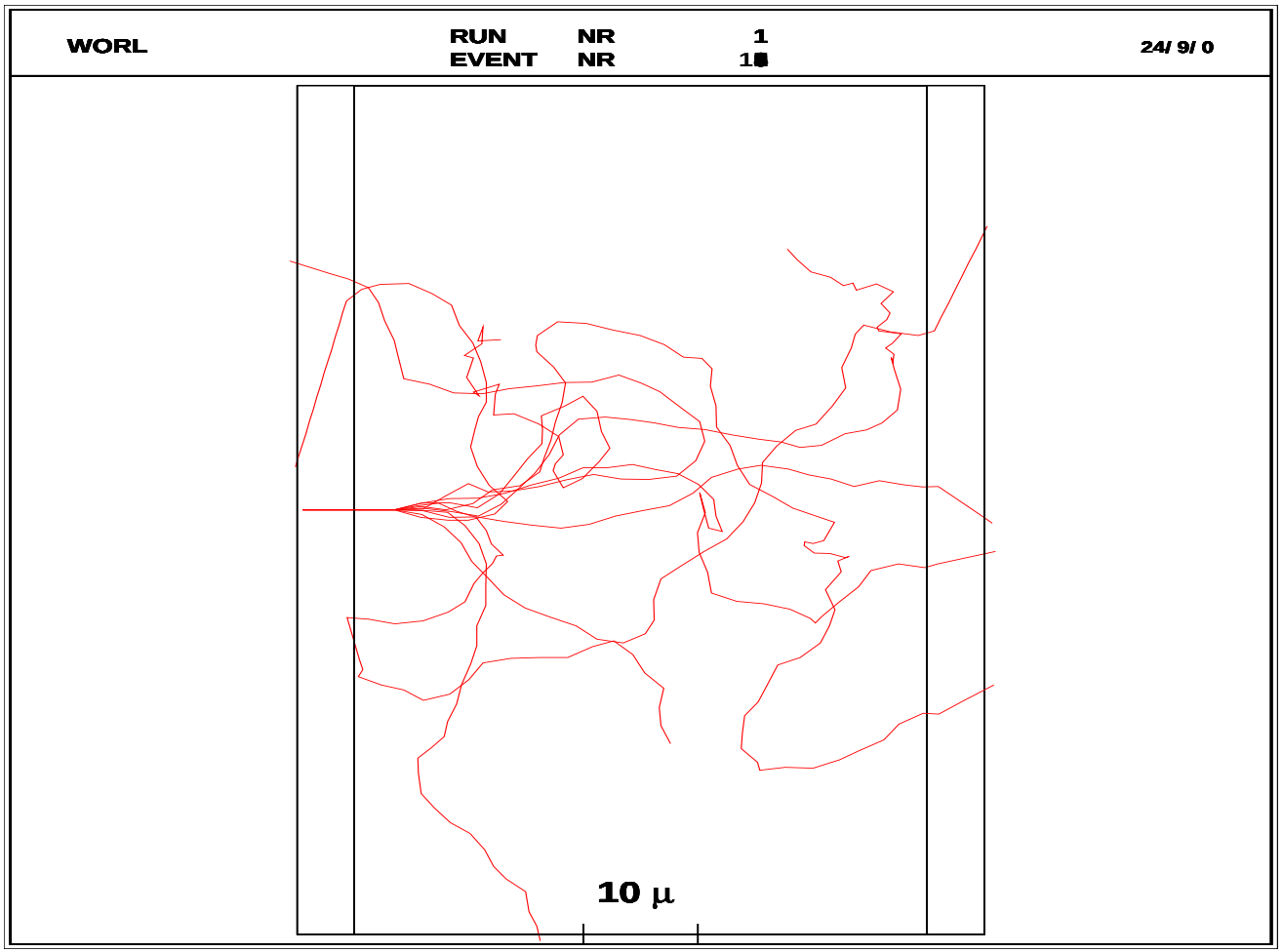

transmission coeff. of 1 MeV e- (Al)
r0 = 2.04 mm, cut = 0.005 mm
ctran %
100
80
60
40
20
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
t/r0
data from Seltzer,Berger
G4 7.0

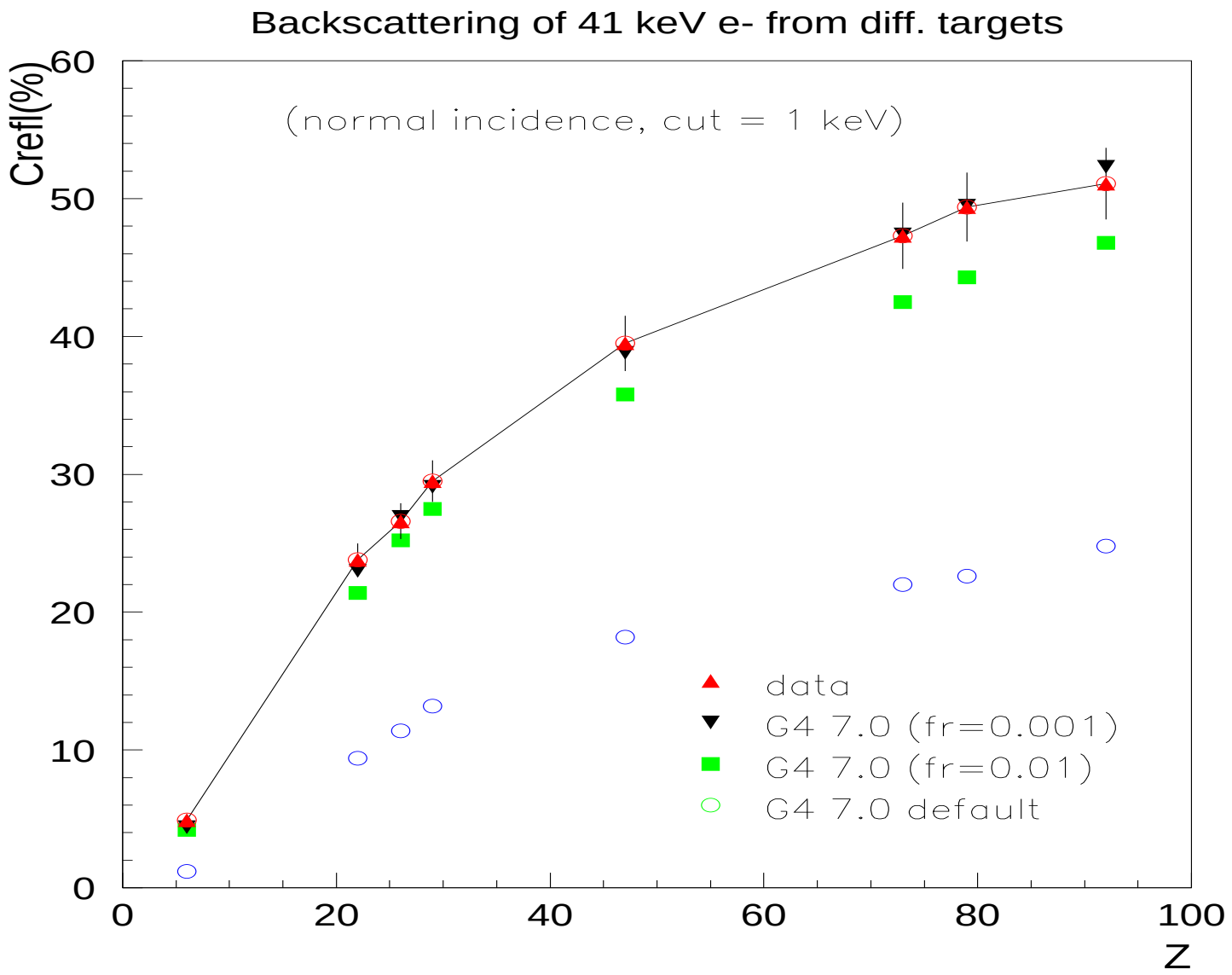

Energy deposit of 0.5 MeV e- in Al as a function of depth
(cut = 0.002 mm, stepmax = 0.002 mm)
GEANT4 7.0
data from Seltzer
2.25
2
1.75
1.5
1.25
1
0.75
0.5
0.25
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
t/r0

The energy spectra of 1 MeV electrons transmitted through aluminium foils is shown in Fig. 5. The experimental points are from a measurement of Rester and Derrickson ([Reste70]). The simulation again are quite close to the data.


Energy spectrum of transmitted e- (Al, T=1 MeV)
0.32 g/cm2
0.22 g/cm2
0.10 g/cm2
symbols data from Rester
GEANT4 7.0 cut = 0.005 mm
10
1
10 -1
10 -2
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
MeV

backscattering of low energy electrons The incident beam is 10 electrons of 600 keV entering in 50 μm of Tungsten.
4 electrons are transmitted, 2 are backscattered.




Backscattering of 41 keV e- from diff. targets
(normal incidence, cut = 1 keV)
Crefl(%)
Z
data
G4 7.0 (fr=0.001)
G4 7.0 (fr=0.01)
G4 7.0 default
0
10
20
30
40
50
60
0
20
40
60
80
100

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