Simulation of Multiple Coulomb scattering in GEANT4

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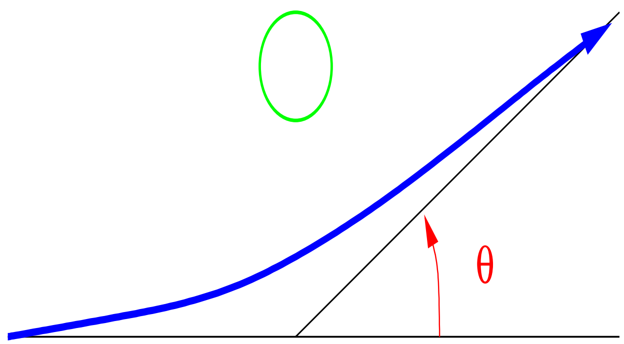
Single Coulomb scattering

Single Coulomb deflection of a charged particle by a fixed nuclear target.

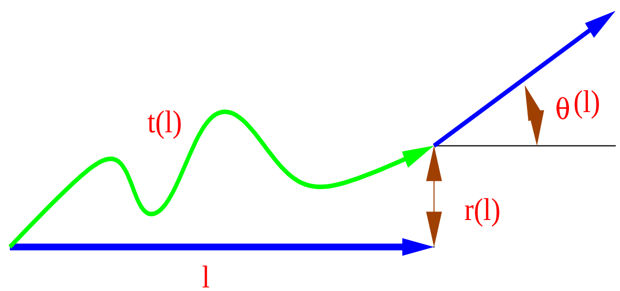


The cross section is given by the Rutherford formula

$$\frac{d\sigma}{d\Omega} = \frac{r_e^2 z_p^2 Z^2}{4} \left(\frac{mc}{\beta p}\right) \frac{1}{\sin^4 \theta/2}$$

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.



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 reproduces rather well this distribution. [Mol48, Bethe53]

Gaussian approximation

The central part of the spatial angular distribution is approximately

$$P(\theta)\,d\Omega = \frac{1}{2\pi\theta_0^2}\ \exp\left[-\frac{\theta^2}{2\theta_0^2}\right]\ d\Omega$$

with

$$\theta_0 = \frac{13.6\ \mathrm{MeV}}{\beta\,pc} z\,\sqrt{\frac{l}{X_0}}\left[1 + 0.038 \ln\left(\frac{l}{X_0}\right)\right]$$

where l/X_0 is the thickness of the medium measured in radiation lengths X_0 ([Highland75]).

This formula of θ_0 is from a fit to Molière distribution. It is accurate to $\leq 10\%$ for $10^{-3} < l/X_0 < 10^2$

note: the appearance of X_0 in the formula is only for convenience.

Others formulas for θ_0 have been developed, starting from the Molière theory. [Lynch91]

related quantities

- lateral displacement $r(l)$
- true (or corrected) path length $t(l)$
- projected angular deflection $\theta_{proj}(l)$

they are correlated random variables, for instance needed in Monte Carlo simulation.

Neither the Moliere theory nor the Gaussian approach of MSC give information about the spatial displacement of the particle, they give the scattering angle distribution only.To get a more complete information it is better to start with theory of Lewis which based on the transport equation of charged particles ([Lewis50, Kawrakow98]).

The MSC model used in GEANT4 uses the Lewis theory to simulate the transport of charged particles.In this approach model functions are used to sample the spatial and angle distributions after a step, the theory gives constraints for these model functions (the model functions should give the same moments of the distributions then the theory).The details of the MSC model can be found in the GEANT4 Physics Reference Manual ([PRM])

Transport of charged particles

A charged particle starts from a given point (origin of the reference frame), moving in a given direction (dir. of the z-axis).

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 d after having travelled a path length t.

The transport is governed by the transport equation :

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

which can be solved exactly for special cases only.

But this equation can be used to derive different moments of p.

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 [Fer93].

MSC model in Geant4, notations

- true path length or ’t’ path length is the total length travelled by the particle. All the physical processes restrict this ’t’ step.
- geometrical or ’l’ path length is the straight distance between the starting and endpoint of the step, if there is no magnetic field. The geometry gives a constraint for this ’l’ step.
- path length correction(transformation) : $t \Longleftrightarrow l$
  $t \Longrightarrow l : F(l, t, \lambda)$
  $l \Longrightarrow t : G(t, l, \lambda)$
- scattering angle distribution: $f(cos\theta, t, \lambda)$
- lateral displacement : $R(t, \lambda)$.

Physics input of the model

first transport mean free path :

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

where $d\sigma(\chi)/d\Omega$ is the differential cross section of the scattering, n_{at} is the nb of atoms per volume.

i-th transport mean free path is defined similarly with the substitution : $(1 - cos\chi) \Longrightarrow (1 - P_i(cos\chi))$, (i-th Legendre polynomial).

Instead of using the cross section directly the model uses λ and λ_2 to calculate the different (spatial and angle) distributions.
Basic assumption of the model: the scattering/transport depend on the physics through a dependence on the t/λ and t/λ_2 variables.

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

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

STEP 1

1. take the smallest step length coming from the step limitations given by the physics processes (all but MSC)
   $t = min(t_{proc1}, t_{proc2}, ..., t_{procn})$
2. do the $t \rightarrow l$ transformation $F(l, t, \lambda) \Longrightarrow l_{phys}$
   done by AlongStepGetPhysicalInteractionLength() of MSC
3. ask step limit l_{geom} from geometry
4. take the final (geom.) step size as $l_{step} = min(l_{phys}, l_{geom})$
5. compute the corresponding true step length
   $G(t, l_{step}, \lambda) \Longrightarrow t_{step}$
   done by AlongStepDoIt() of MSC

Model function $F(l, t, \lambda)$

Distribution with the theoretical mean values.

$$F(l,t,\lambda) = [(k+1)/t]\ (l/l_0)^k \quad \text{for } l < l_0$$
$$F(l,t.\lambda) = [(k+1)/t]\ [(t-l)/(t-l_0)]^k \quad \text{for } l \geq l_0 \qquad (3)$$

where

$$l_0 =< l > +d\ (t- < l >) \qquad (4)$$

where $< l >$ is the mean value of l, d is a constant model parameter.

The value of the exponent k is computed from the requirement that $F(l, t, \lambda)$ should give the theroretical mean value for l

$$k = \frac{2 < l > -t}{l_0 - < l >} \qquad (5)$$

The geometrical path length ⇒ true path length transformation is performed using the mean values

$$t =< t >= -\lambda * log \left(1 - \frac{l}{\lambda} \right) \qquad (6)$$

This trasformation should be done at volume boundaries only when the final step length comes from the geometry. In all the other cases MSC can take the original value of the true path length !

STEP 3, performed by PostStepDoIt() of MSC

Sample θ from the model distribution $f(x,t,\lambda)$ $(x = cos\theta)$.

$$f(x,t) = q*\{p*f_1(x,t,\lambda)+(1-p)*f_2(x,t,\lambda)\}+(1-q)*f_3(x,t,\lambda) \quad (7)$$

$p, q \in [0,\ 1]$

$f_i(x,t,\lambda)$ are relatively simple functions of x and the variable $\tau = t/\lambda$.

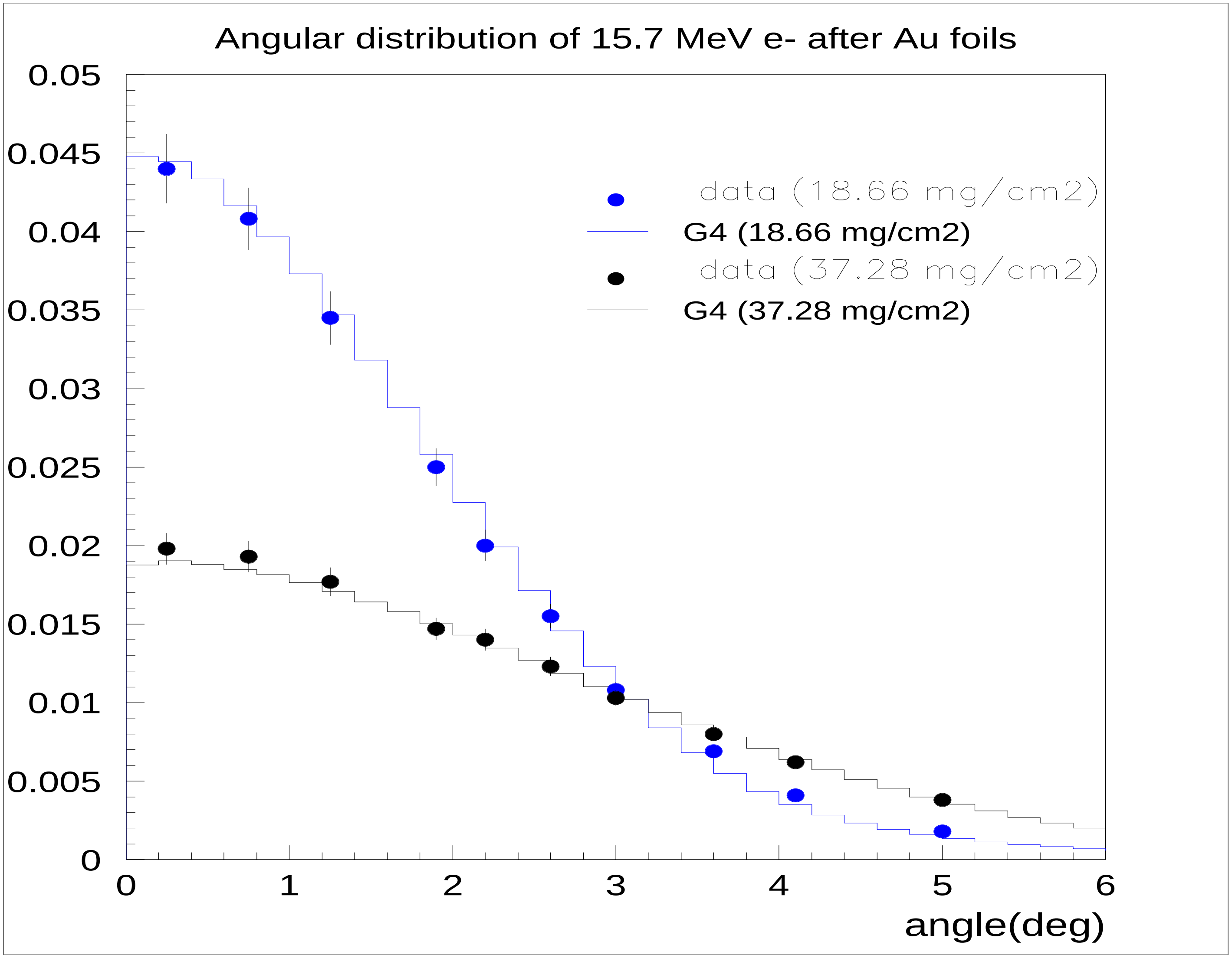
($f_1 \approx$ Gaussian for small angle, f_2 has a Rutherford-like tail, $f_3 = const$).

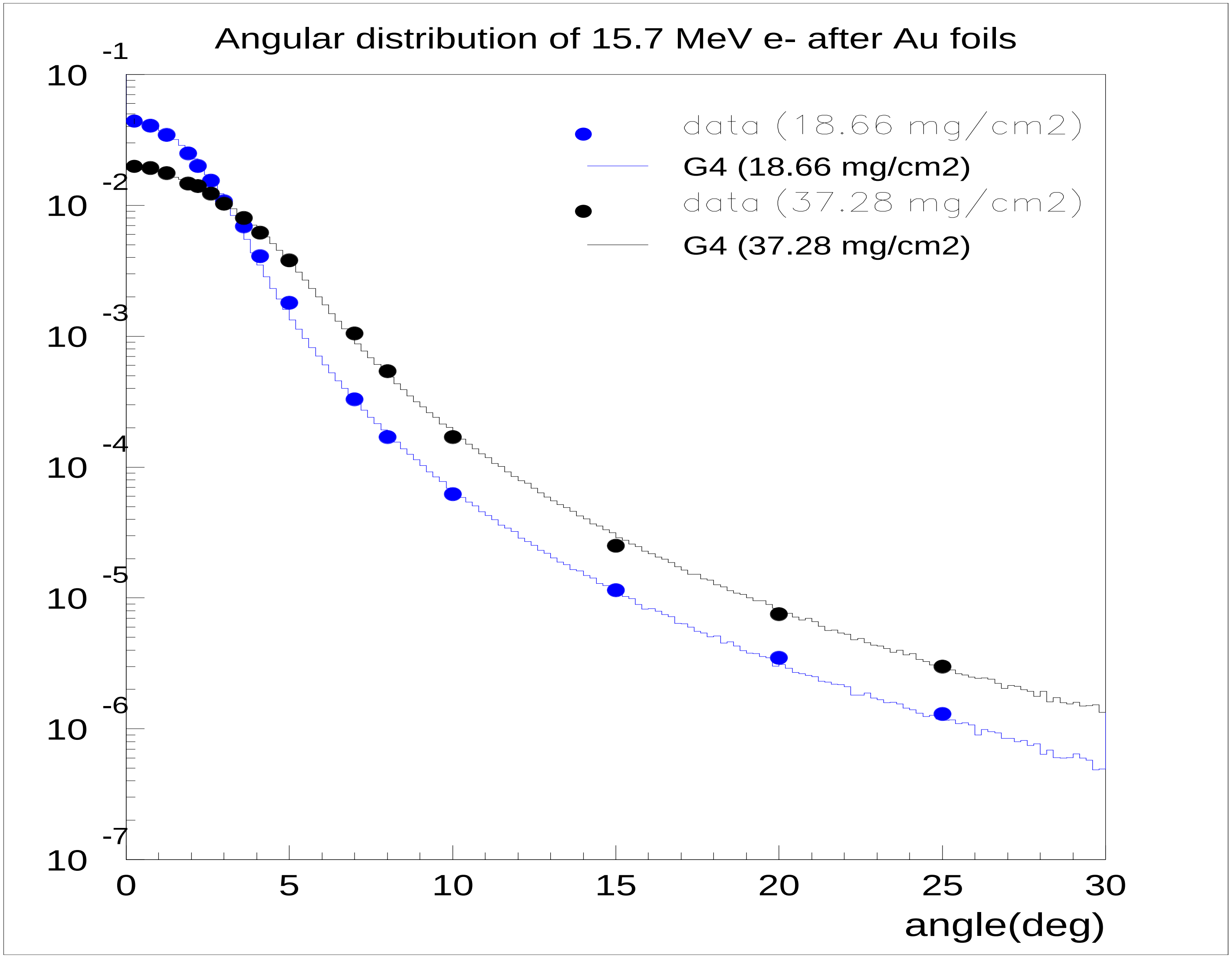
STEP 4, performed by PostStepDoIt() of MSC
compute the mean lateral displacement according to the theoretical formula and change the position of the particle correspondingly.
note: this step is executed only if the particle is 'far' from the boundary of the volume.
MSC is a ContinuousDiscreteProcess, until now we have seen AlongStepGetPhysicalInteractionLength() AlongStepDoIt() PostStepDoIt().
What is the task for PostStepGetPhysicalInteractionLength() ?
It sets only a ForceFlag in order to ensure that PostStepDoIt() is called at every step.

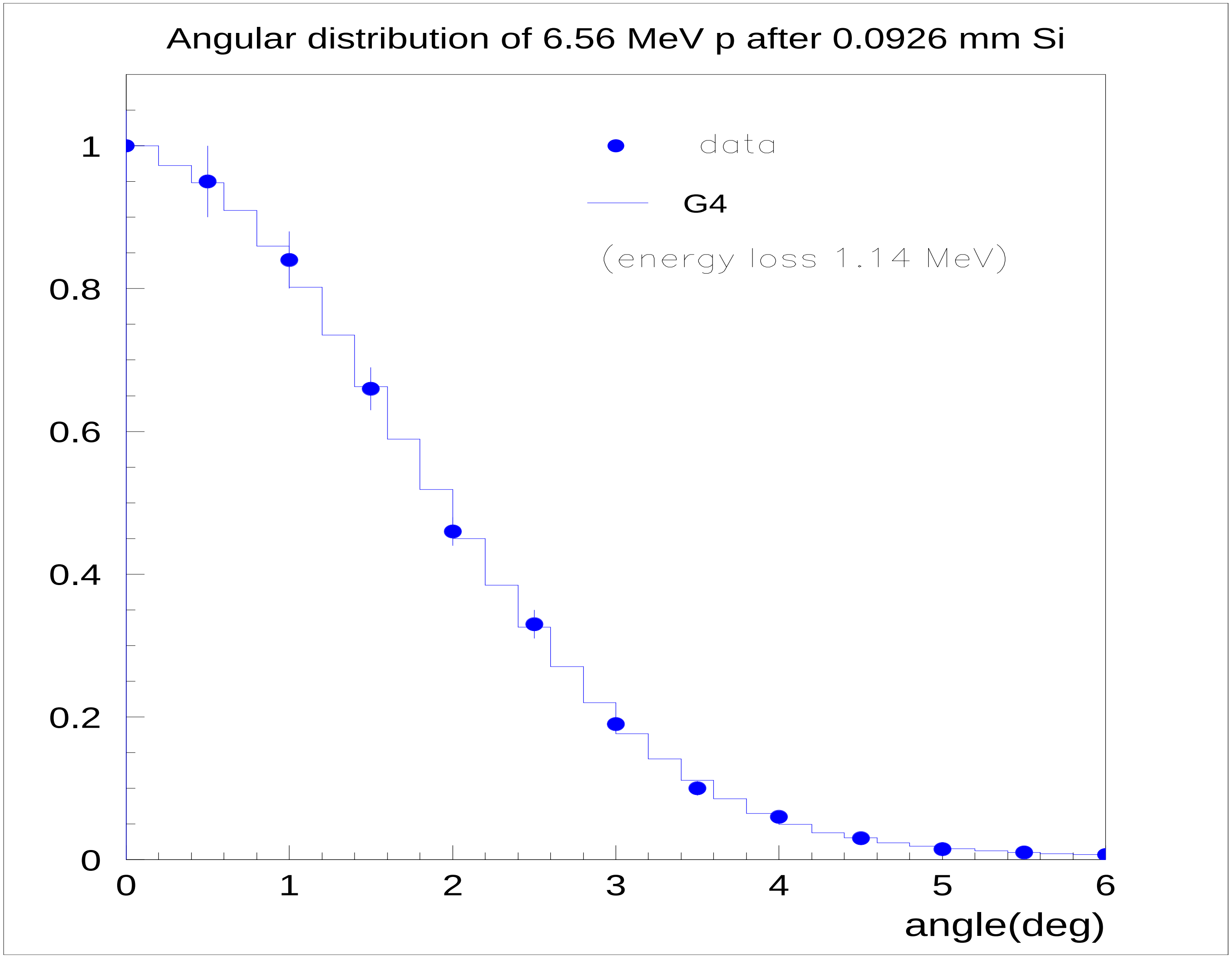
Simulation results $\Longleftrightarrow$ data, the ultimate test of the reliability of MC simulations

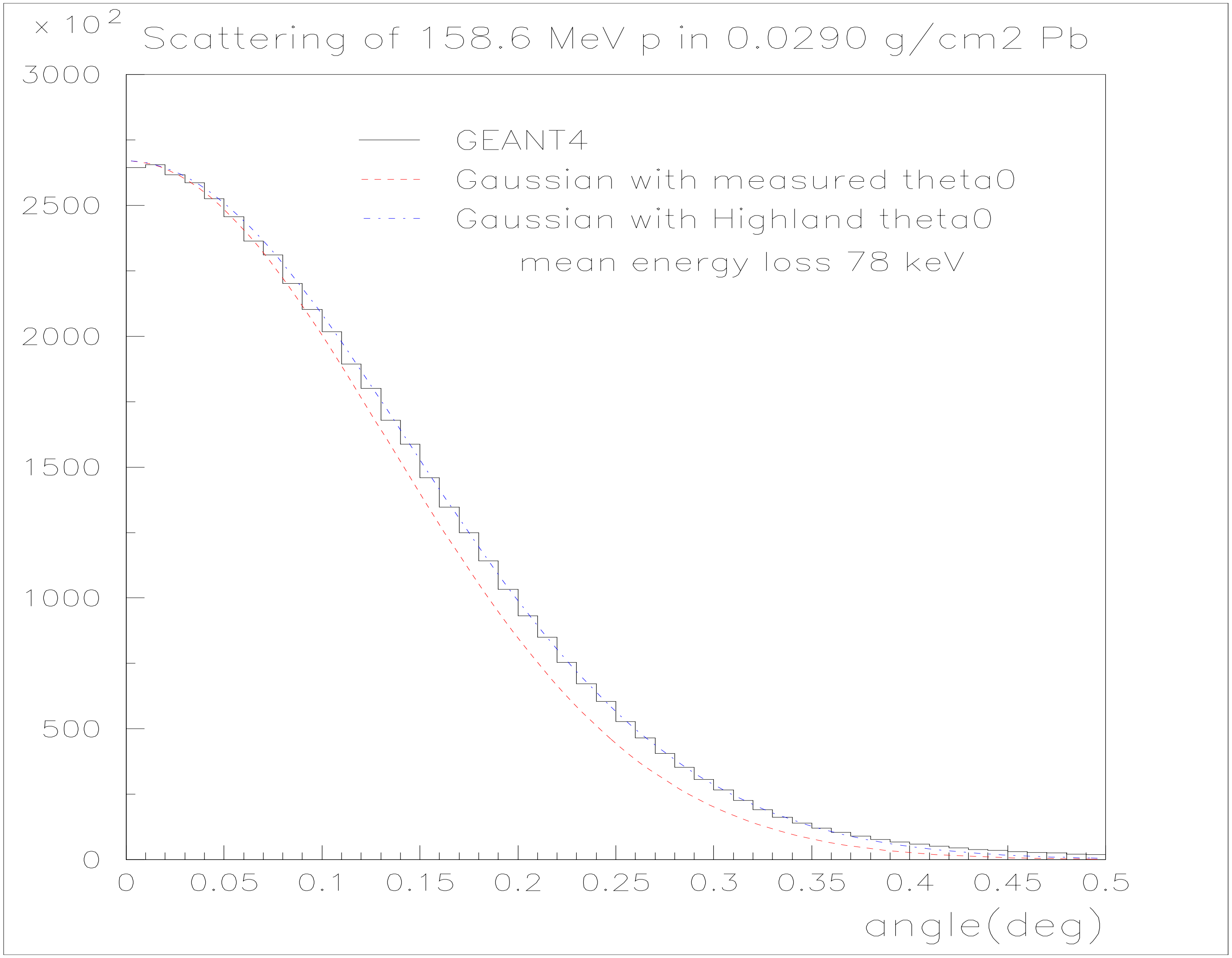
- scattering angle distributions
- energy deposit distribution in detectors
- transmission of charged particles (c_{tr}, θ and T_{tr} distr.)
- backscattering of charged particles (c_b, θ and T_b distr.)
- .....

Angle distributions, Geant4 $\Longleftrightarrow$ data

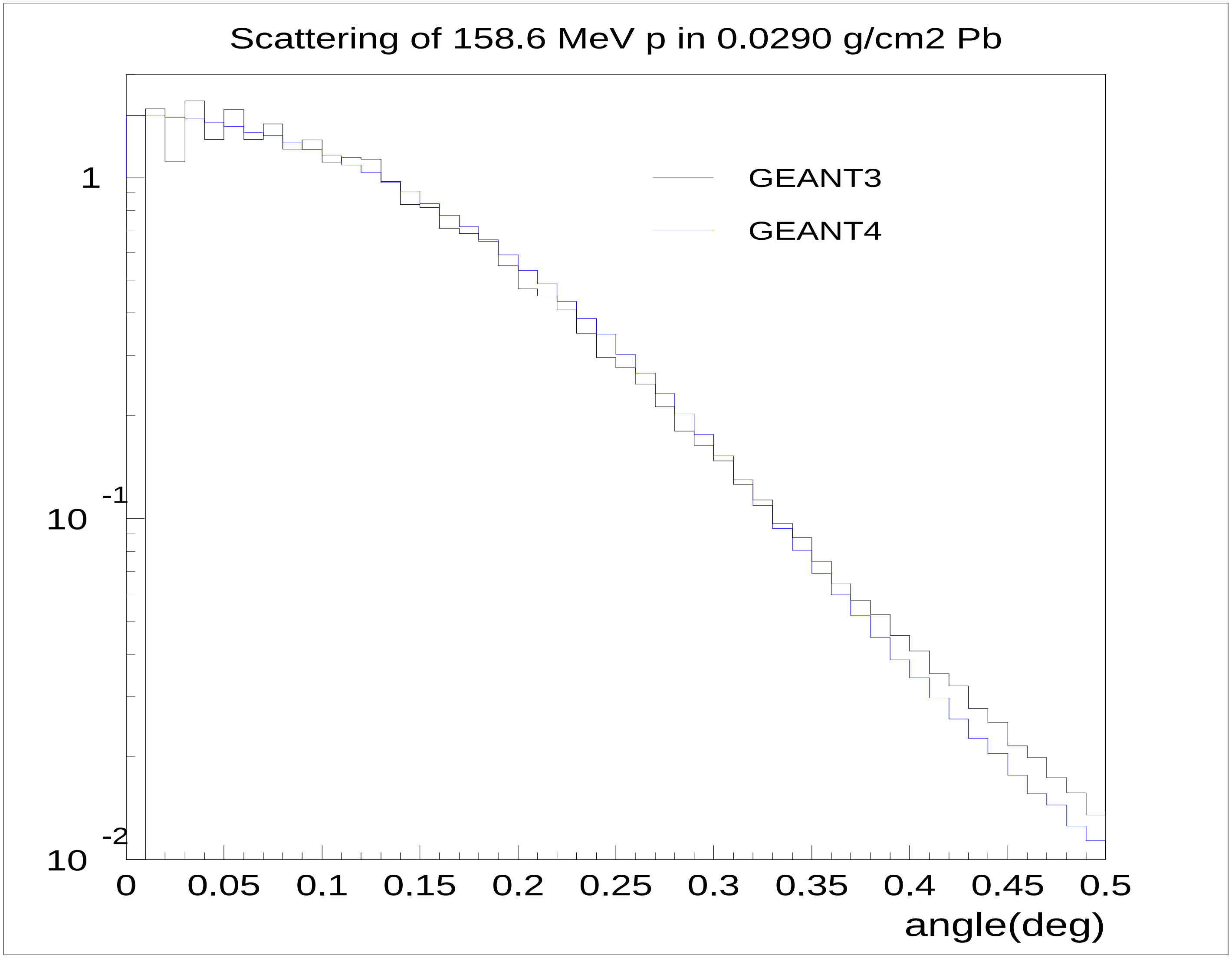



Angular distribution of 15.7 MeV e- after Au foils
data (18.66 mg/cm2)
G4 (18.66 mg/cm2)
data (37.28 mg/cm2)
G4 (37.28 mg/cm2)
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
10^-7
0
5
10
15
20
25
30
angle(deg)

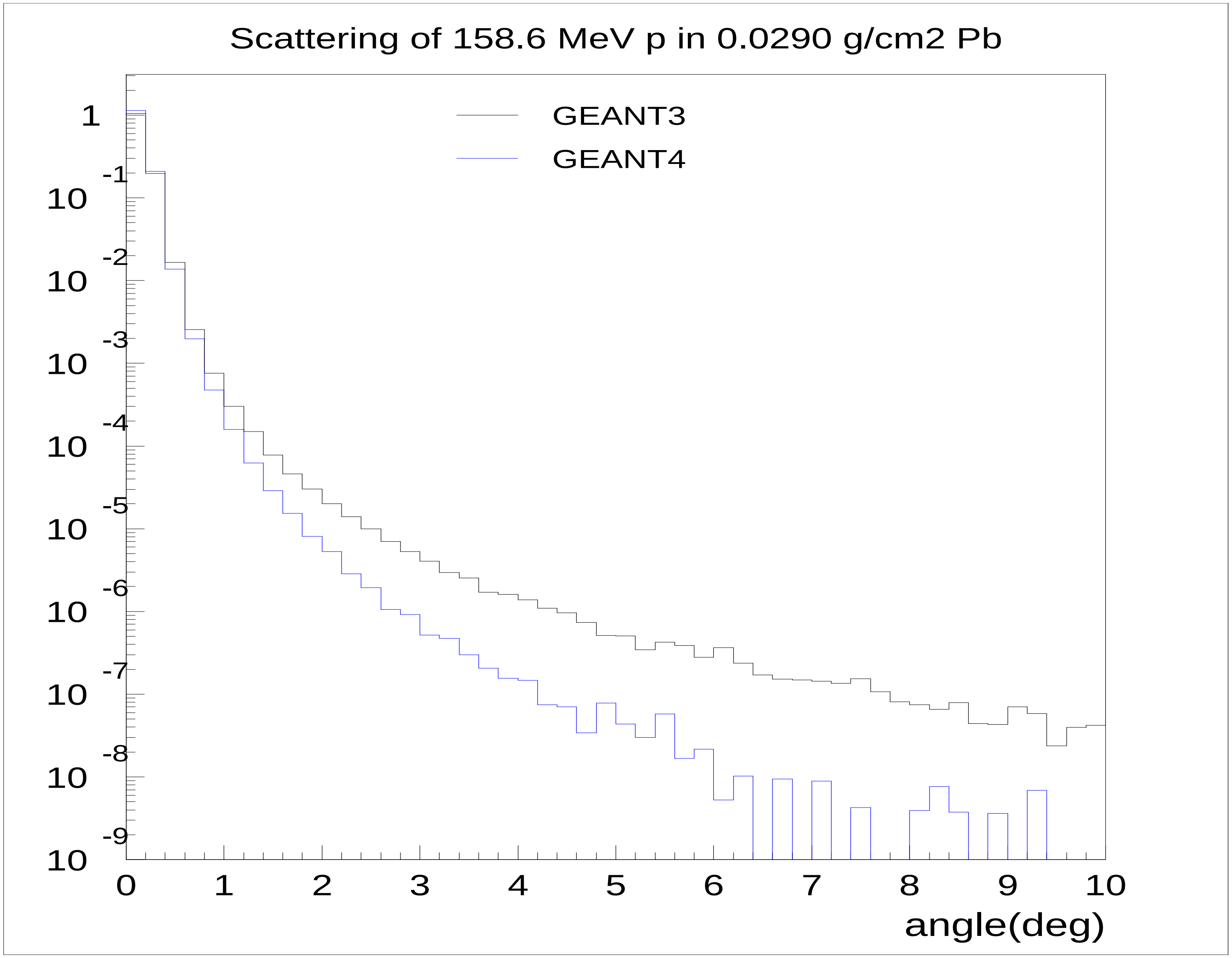

Angular distribution of 6.56 MeV p after 0.0926 mm Si
data
G4
(energy loss 1.14 MeV)
1
0.8
0.6
0.4
0.2
0
0
1
2
3
4
5
6
angle(deg)

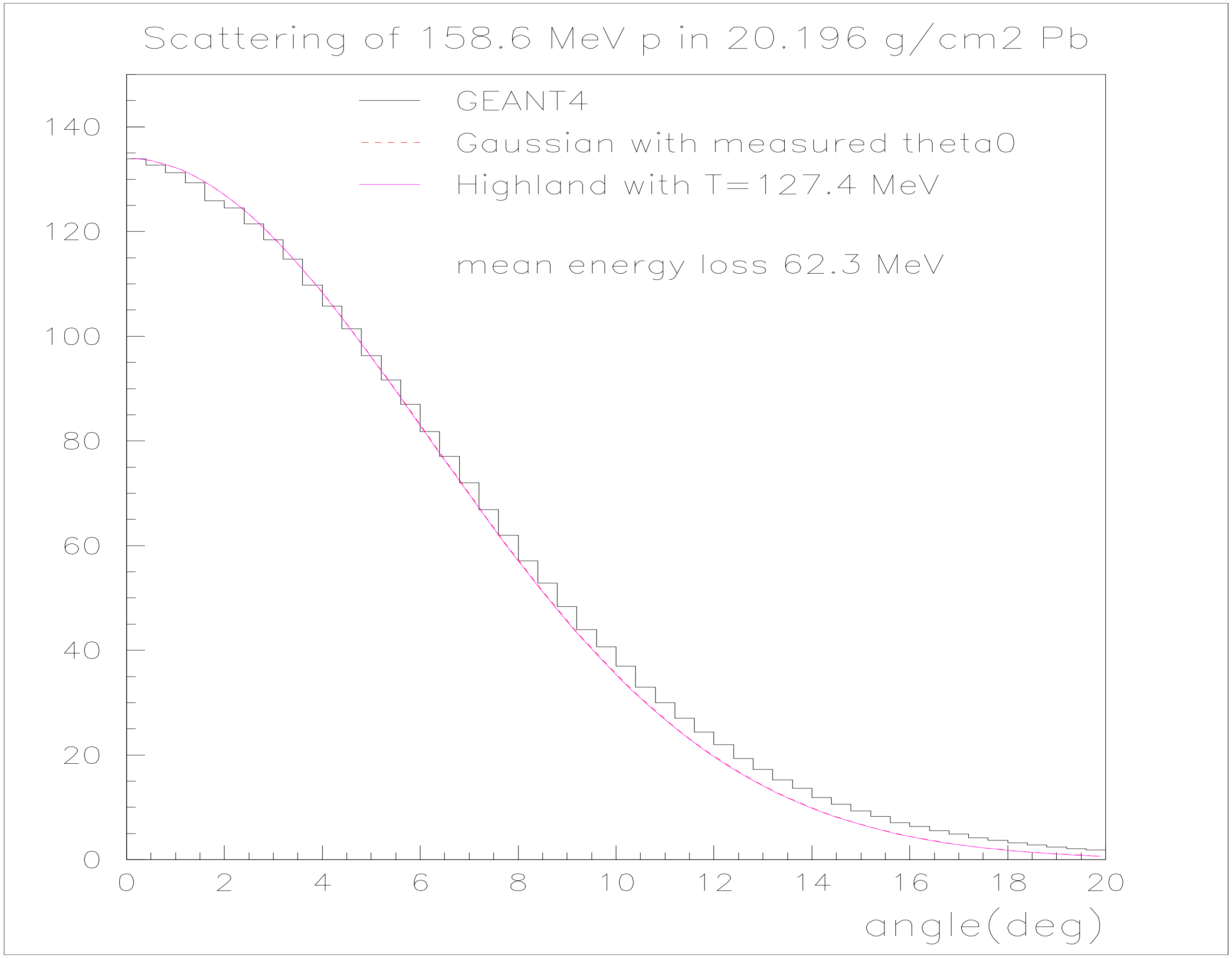

× 10^2
Scattering of 158.6 MeV p in 0.0290 g/cm2 Pb
3000
2500
2000
1500
1000
500
0
GEANT4
Gaussian with measured theta0
Gaussian with Highland theta0
mean energy loss 78 keV
0 0.05 0.1 0.15 0.2 0.25 0.3 0.35 0.4 0.45 0.5
angle(deg)

as the previous plot, but GEANT4 $\Longleftrightarrow$ GEANT3

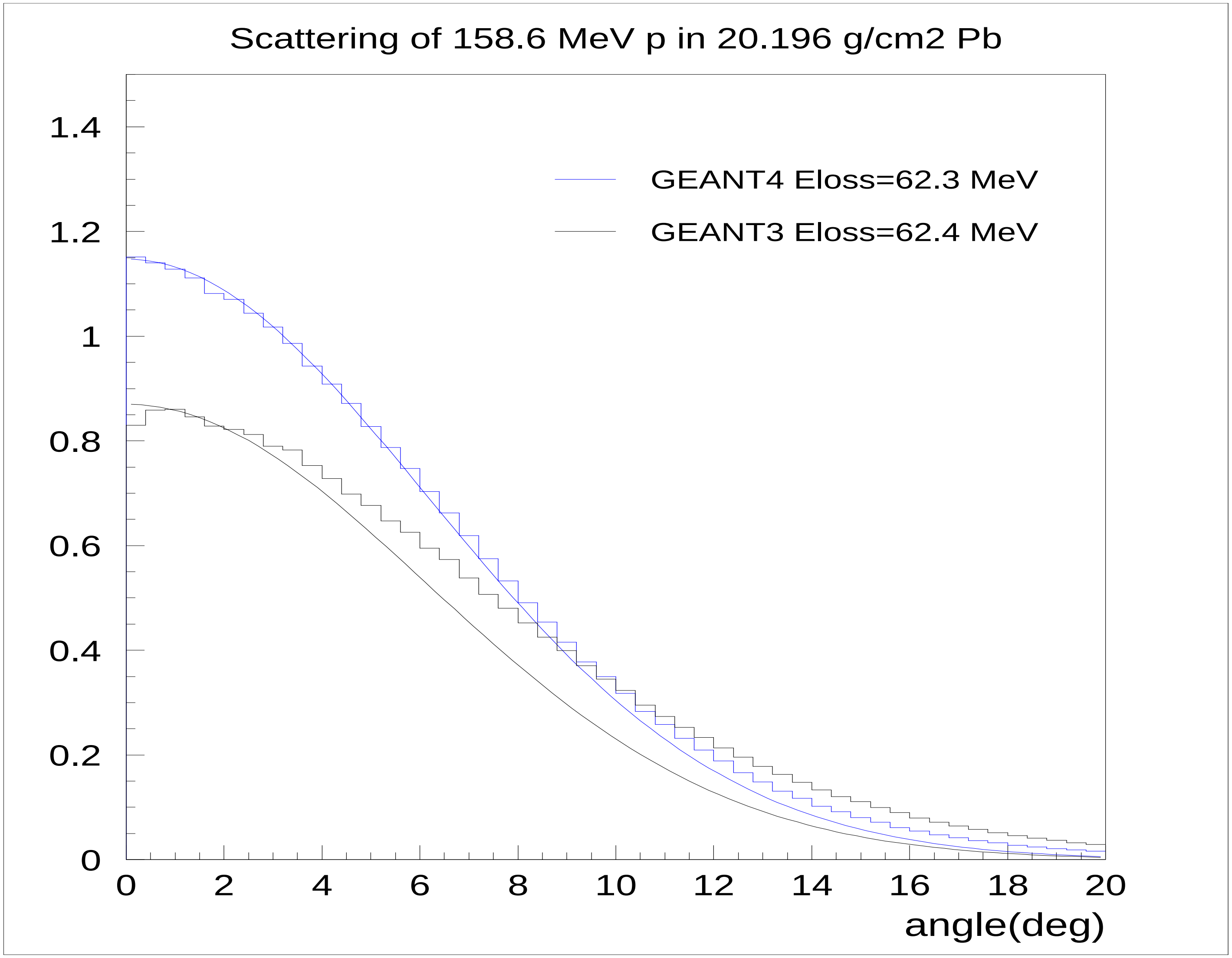


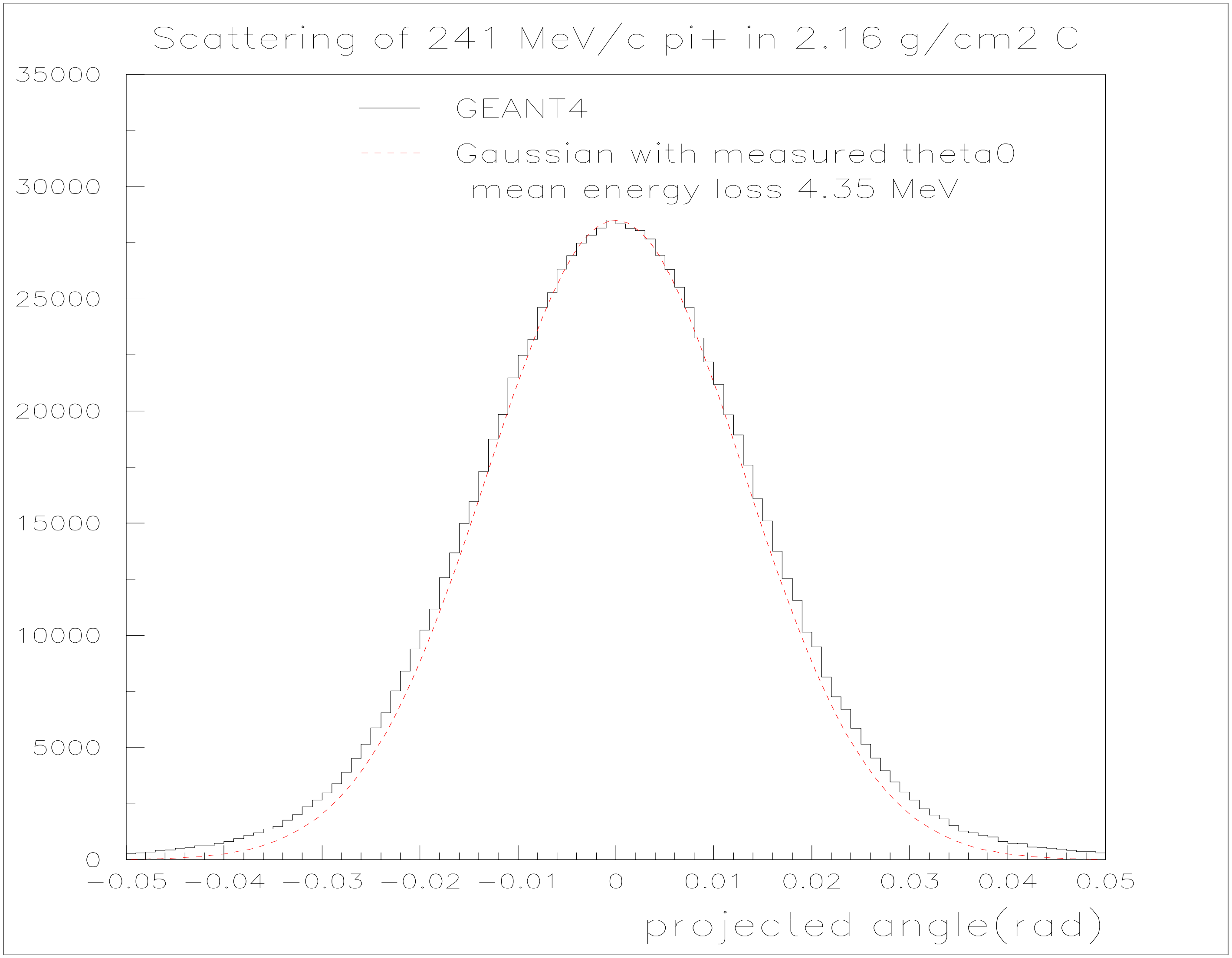
as the previous plot, but GEANT4 $\Longleftrightarrow$ GEANT3 with tails

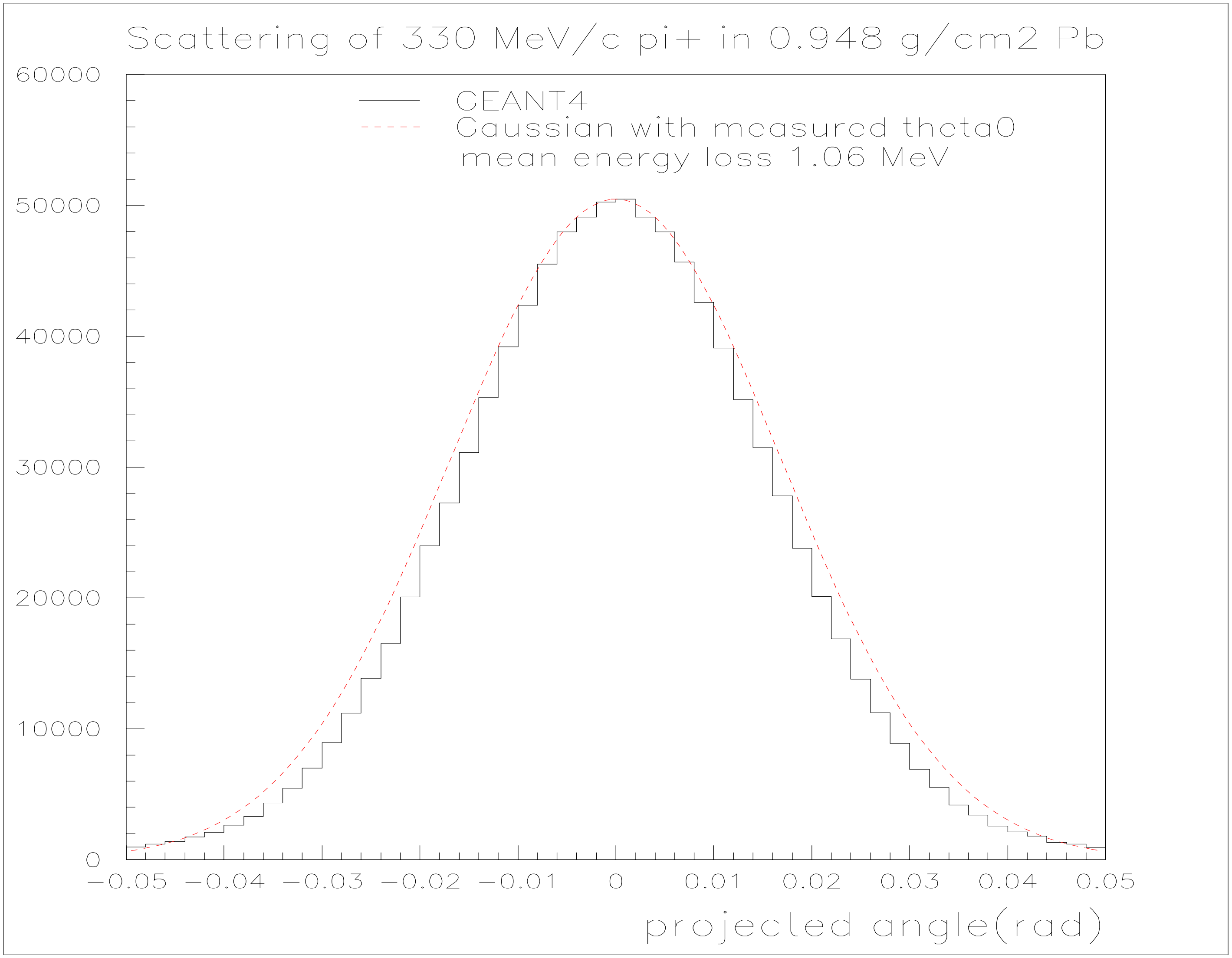



Scattering of 158.6 MeV p in 20.196 g/cm2 Pb
GEANT4
Gaussian with measured theta0
Highland with T=127.4 MeV
mean energy loss 62.3 MeV
0
20
40
60
80
100
120
140
0
2
4
6
8
10
12
14
16
18
20
angle(deg)

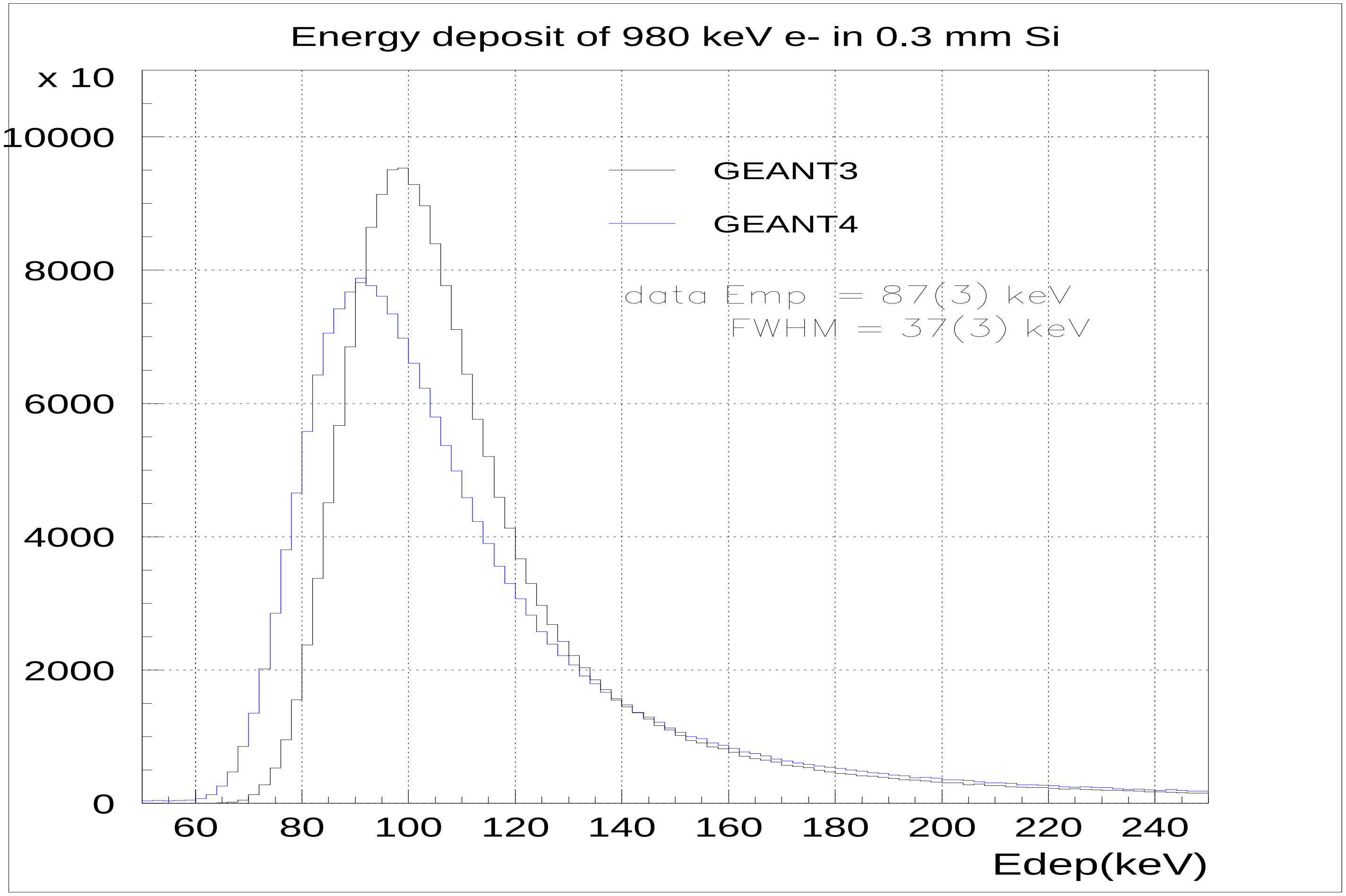
as the previous plot, but GEANT4 $\Longleftrightarrow$ GEANT3




Scattering of 241 MeV/c pi+ in 2.16 g/cm2 C
GEANT4
Gaussian with measured theta0
mean energy loss 4.35 MeV
35000
30000
25000
20000
15000
10000
5000
0
−0.05
−0.04
−0.03
−0.02
−0.01
0
0.01
0.02
0.03
0.04
0.05
projected angle(rad)

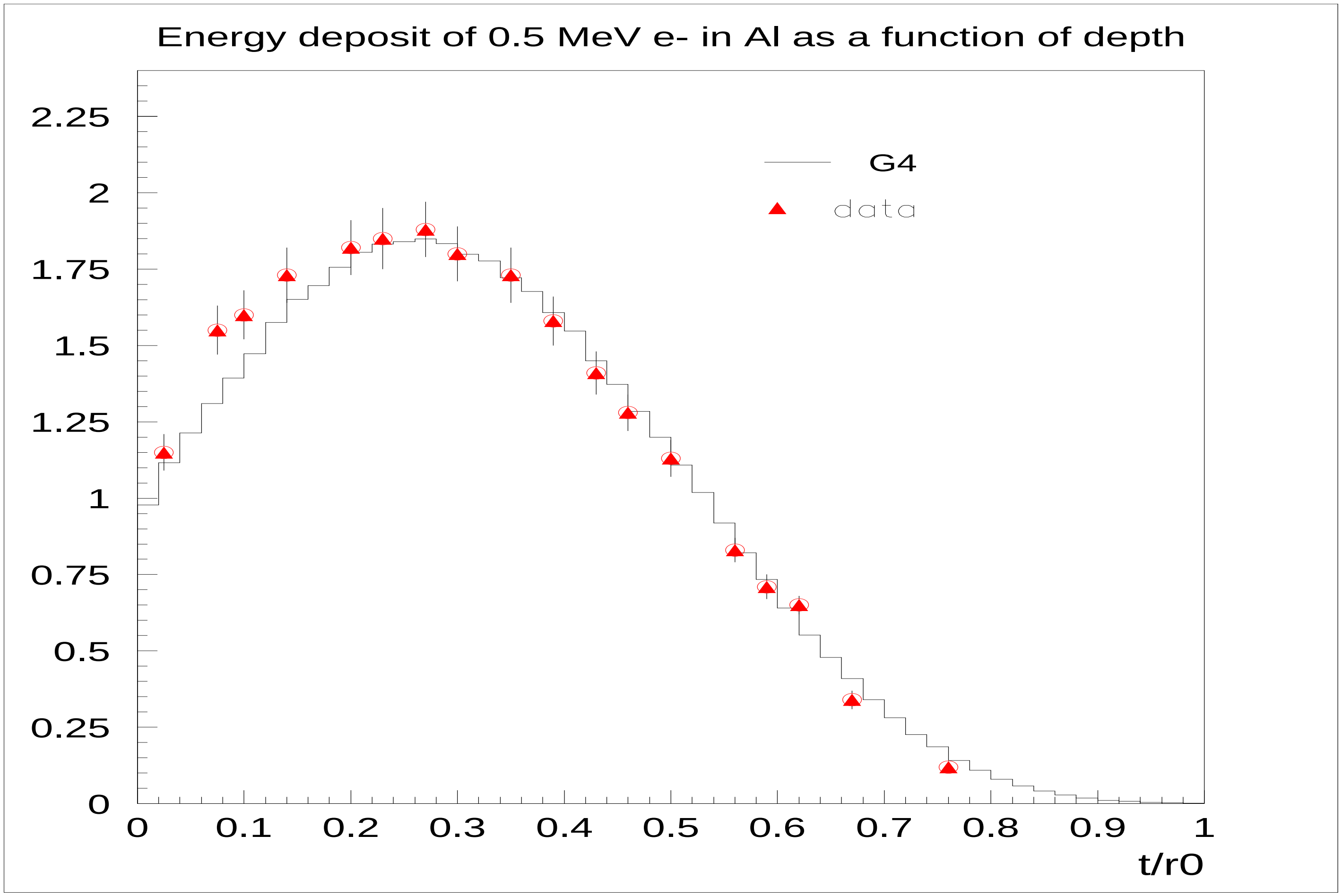

Scattering of 330 MeV/c pi+ in 0.948 g/cm2 Pb
GEANT4
Gaussian with measured theta0
mean energy loss 1.06 MeV
60000
50000
40000
30000
20000
10000
0
−0.05
−0.04
−0.03
−0.02
−0.01
0
0.01
0.02
0.03
0.04
0.05
projected angle(rad)

Energy deposit distribution in Si detector



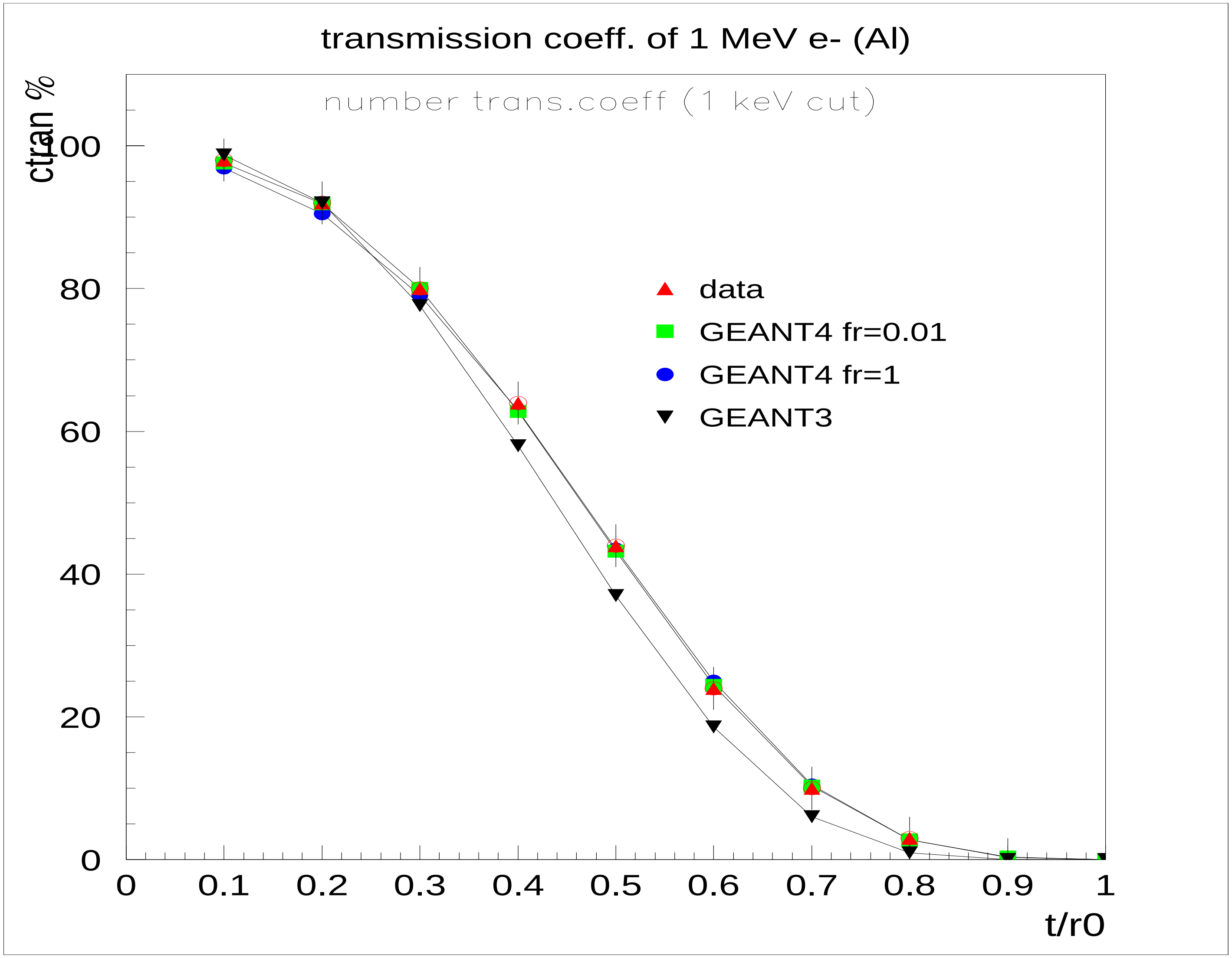
without MSC GEANT4 = GEANT3 $\Longrightarrow$ difference comes from the different MSC simulation !

Depth-dose distribution

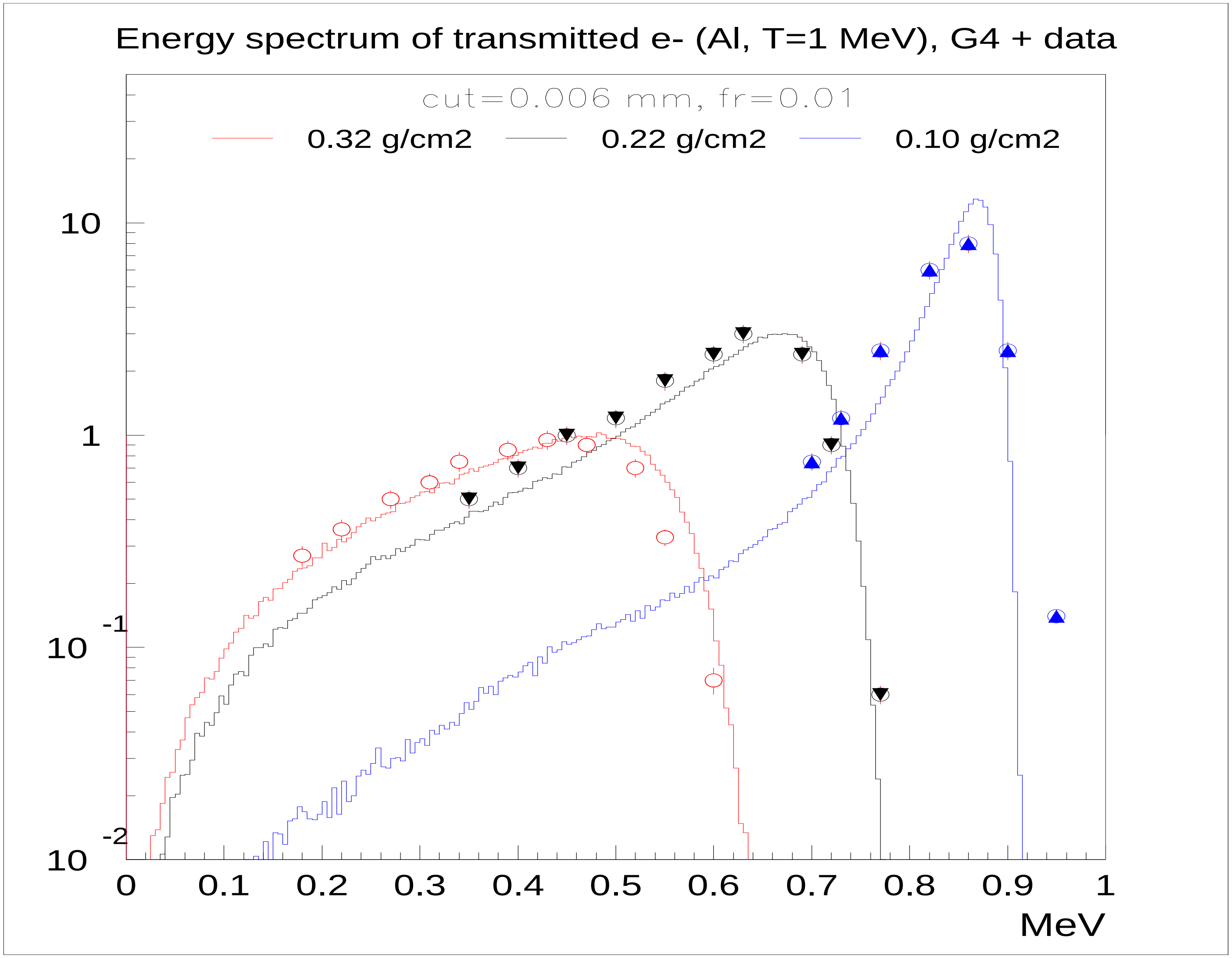


(error on data $\approx 5 - 10\%$).

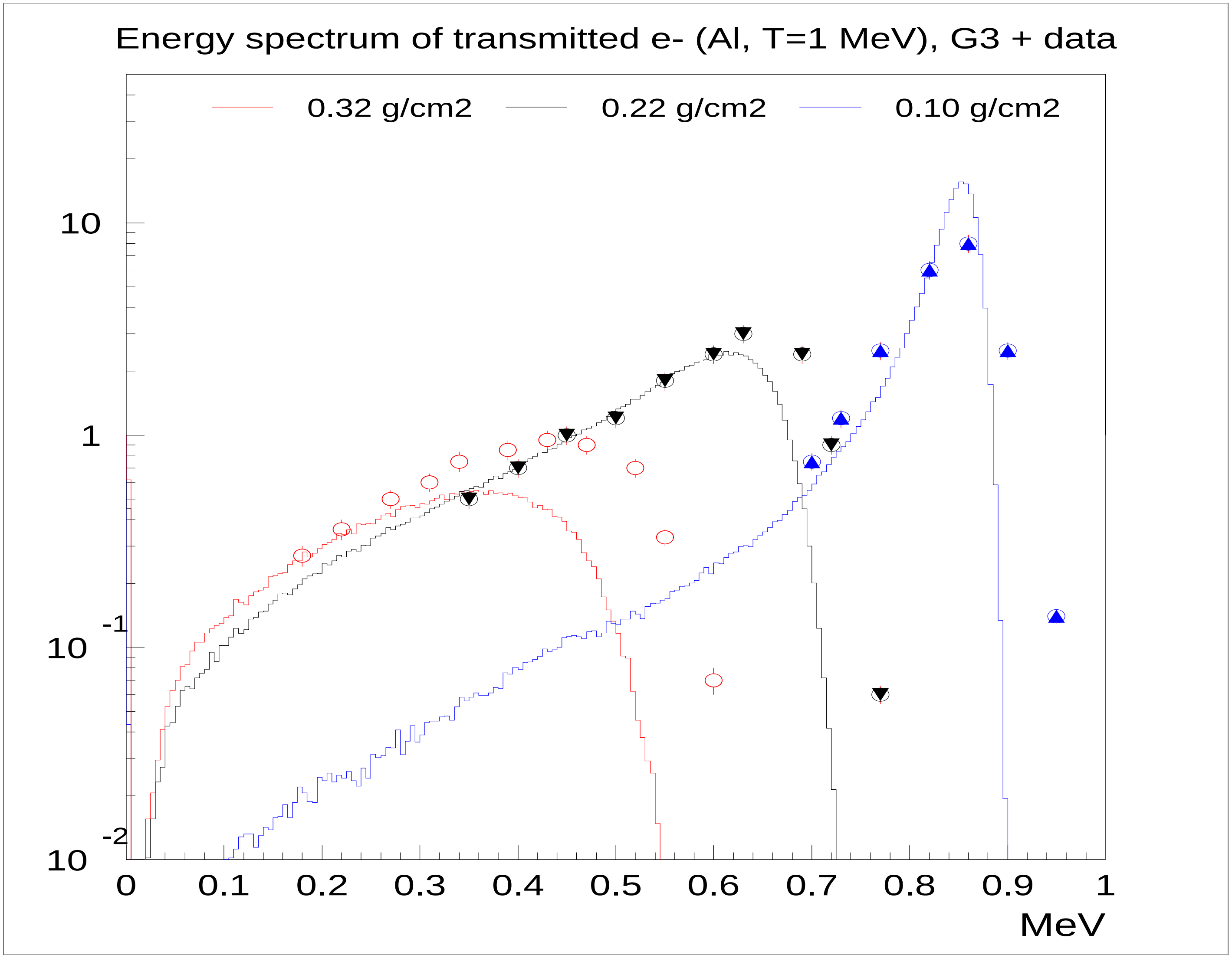
Transmission of e- through layers



Energy spectra of transmitted electrons, G4+data



Energy spectra of transmitted electrons, G3+data



Backscattering is a difficult problem for condensed simulations. One step to the good direction in the GEANT4 MSC algoritm: limit the step in MSC when entering a volume . Algorithm:

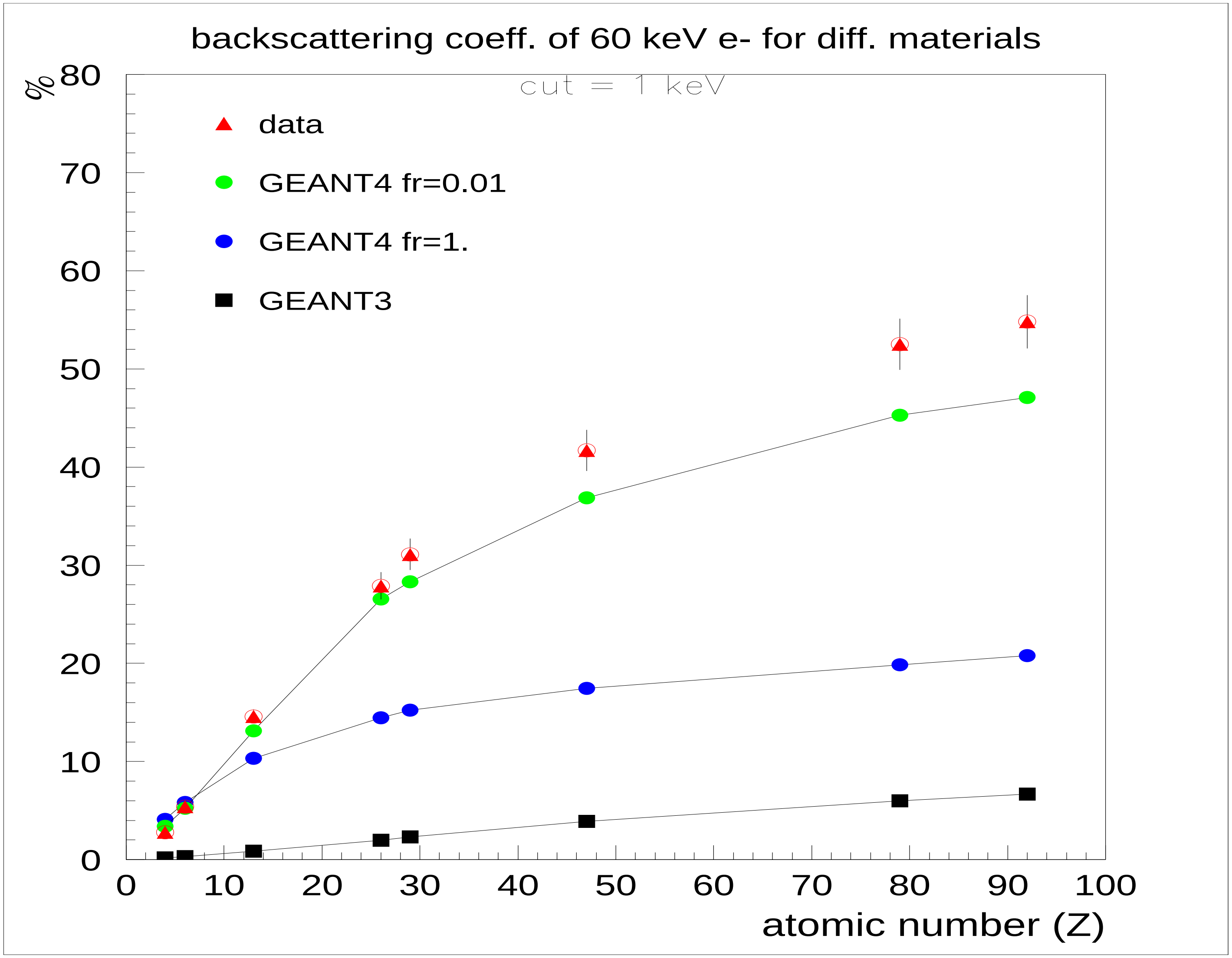
$t_{lim} = fr * max(\lambda, range)$

where $fr \in [0,\ 1]$.If $fr = 1$ there is no step restriction.

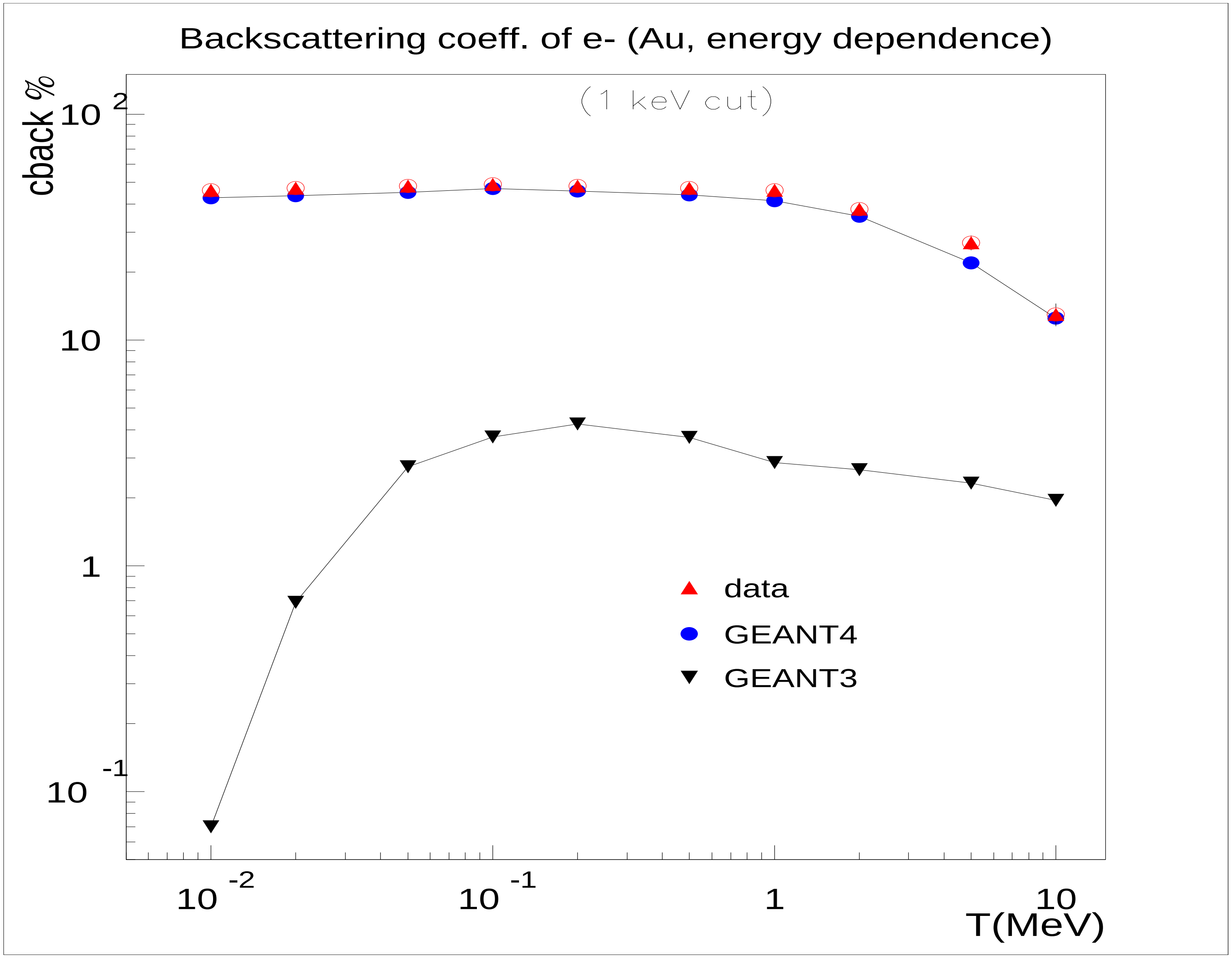
This is NOT the user limit, the step is limited only after entering a volume and the step limit energy and particle dependent !

(Limiting the step length at boundaries is not enough, to get good backscattering we need good angle distribution as well!)

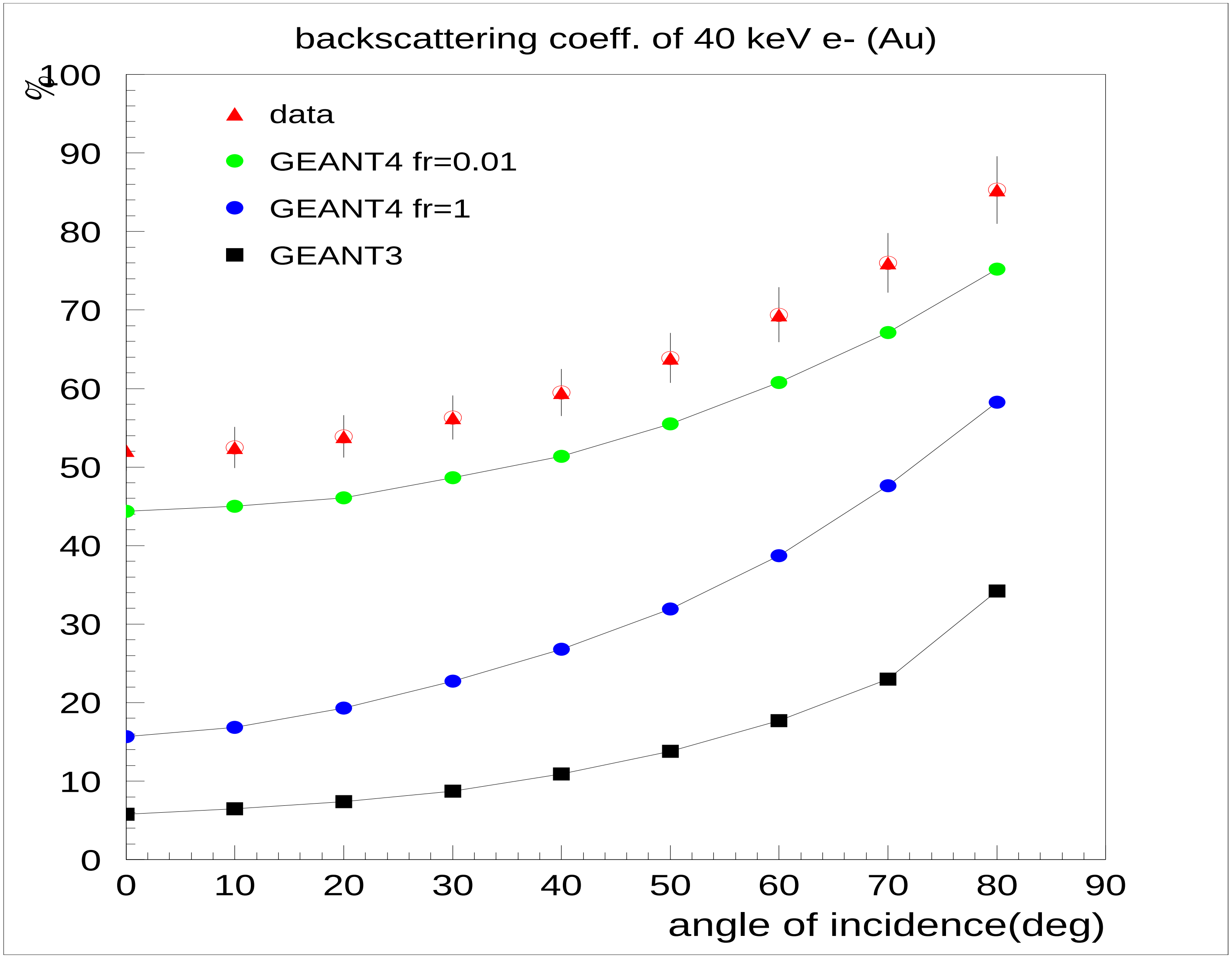
Backscattering of e- G4+data+G3



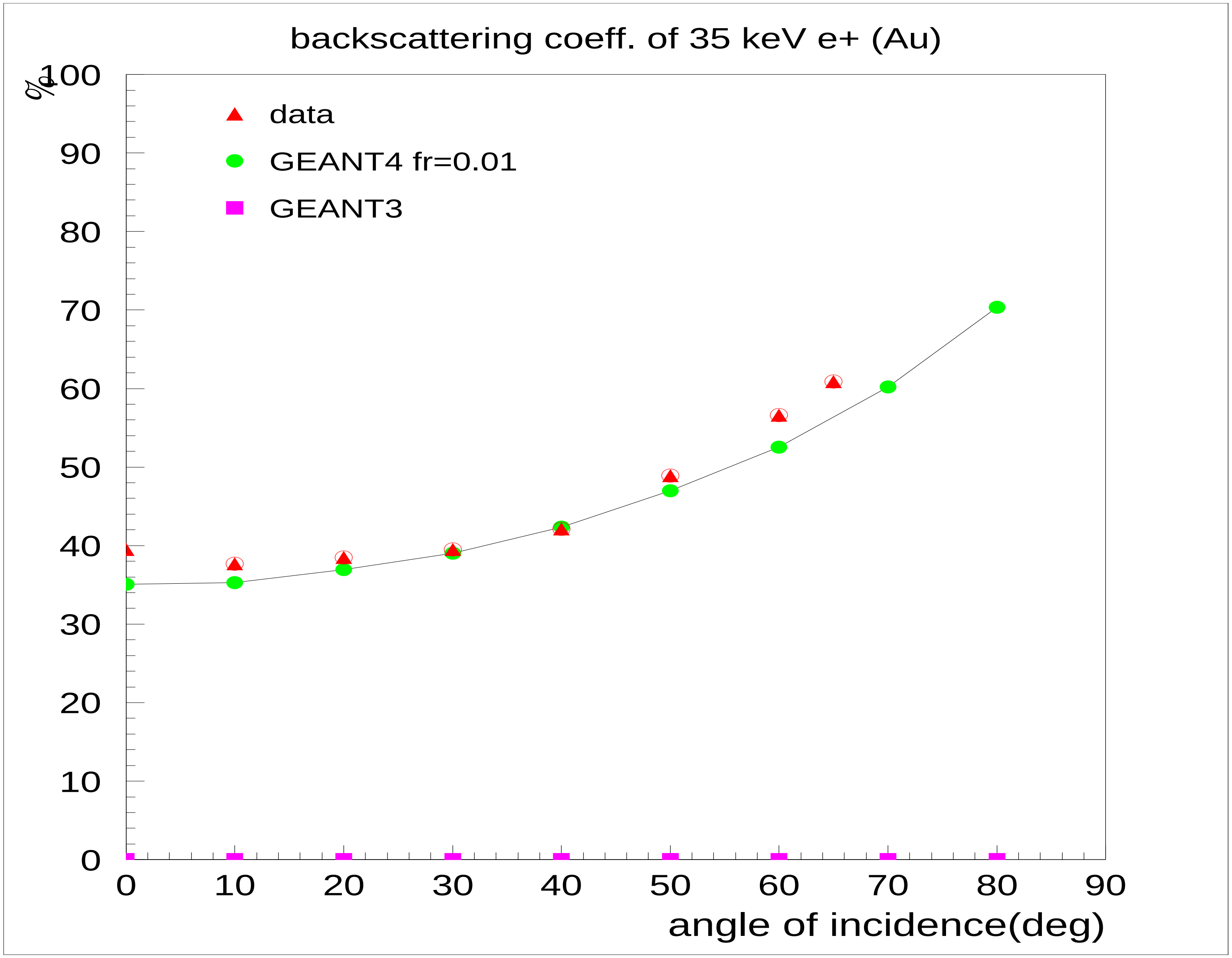
Backscattering of e- G4+data+G3



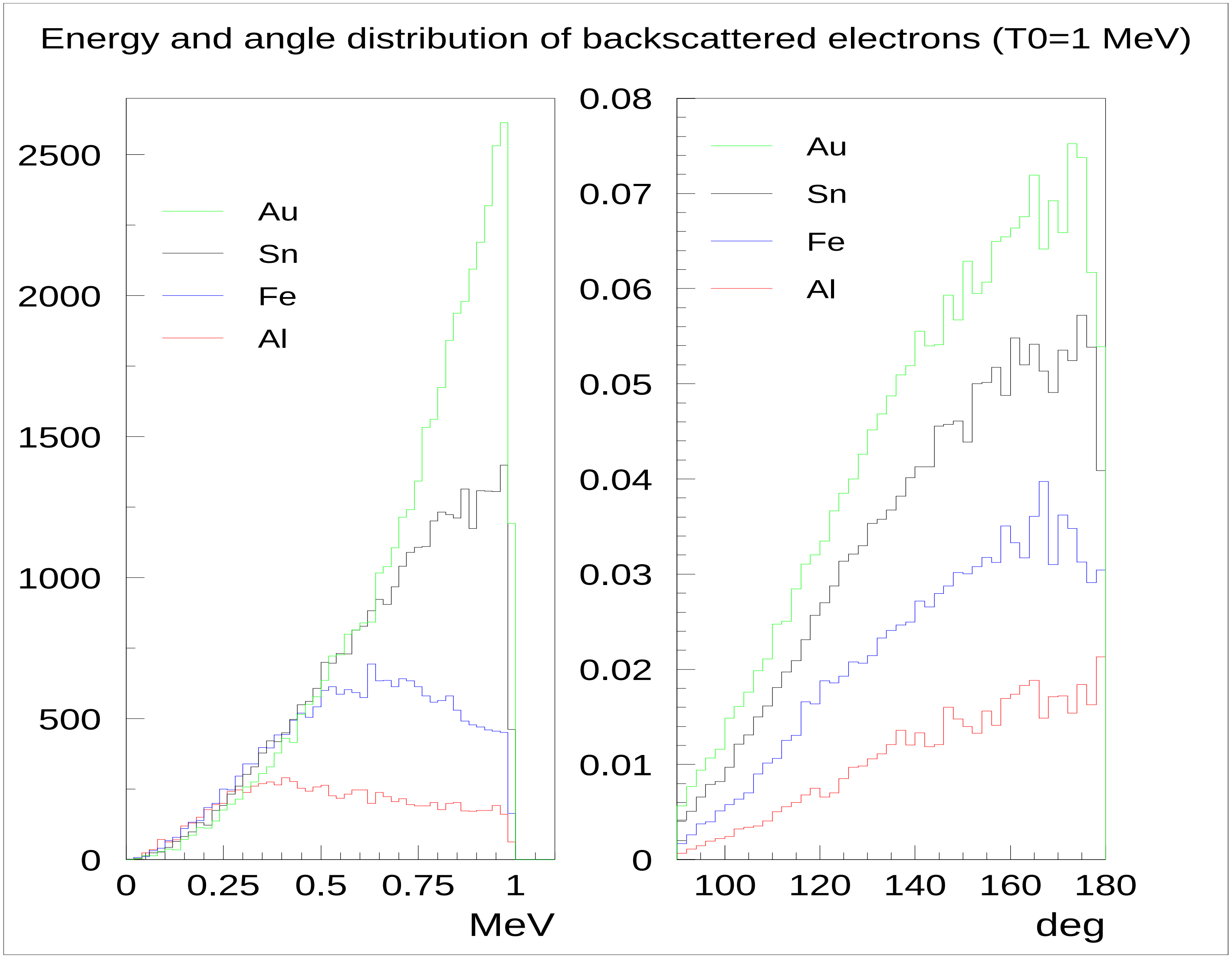
Backscattering of e- G4+data+G3



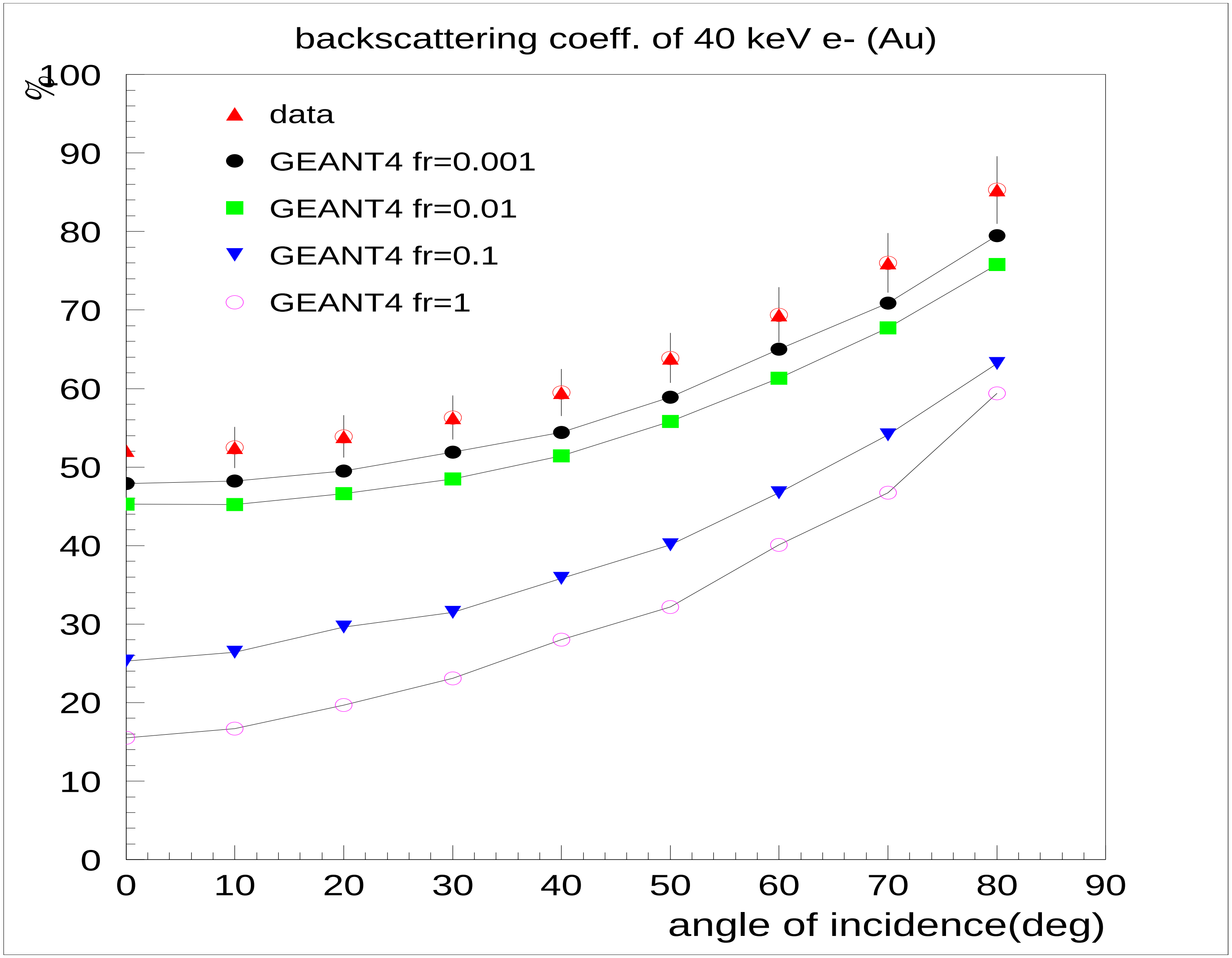
Backscattering of e+ G4+data+G3



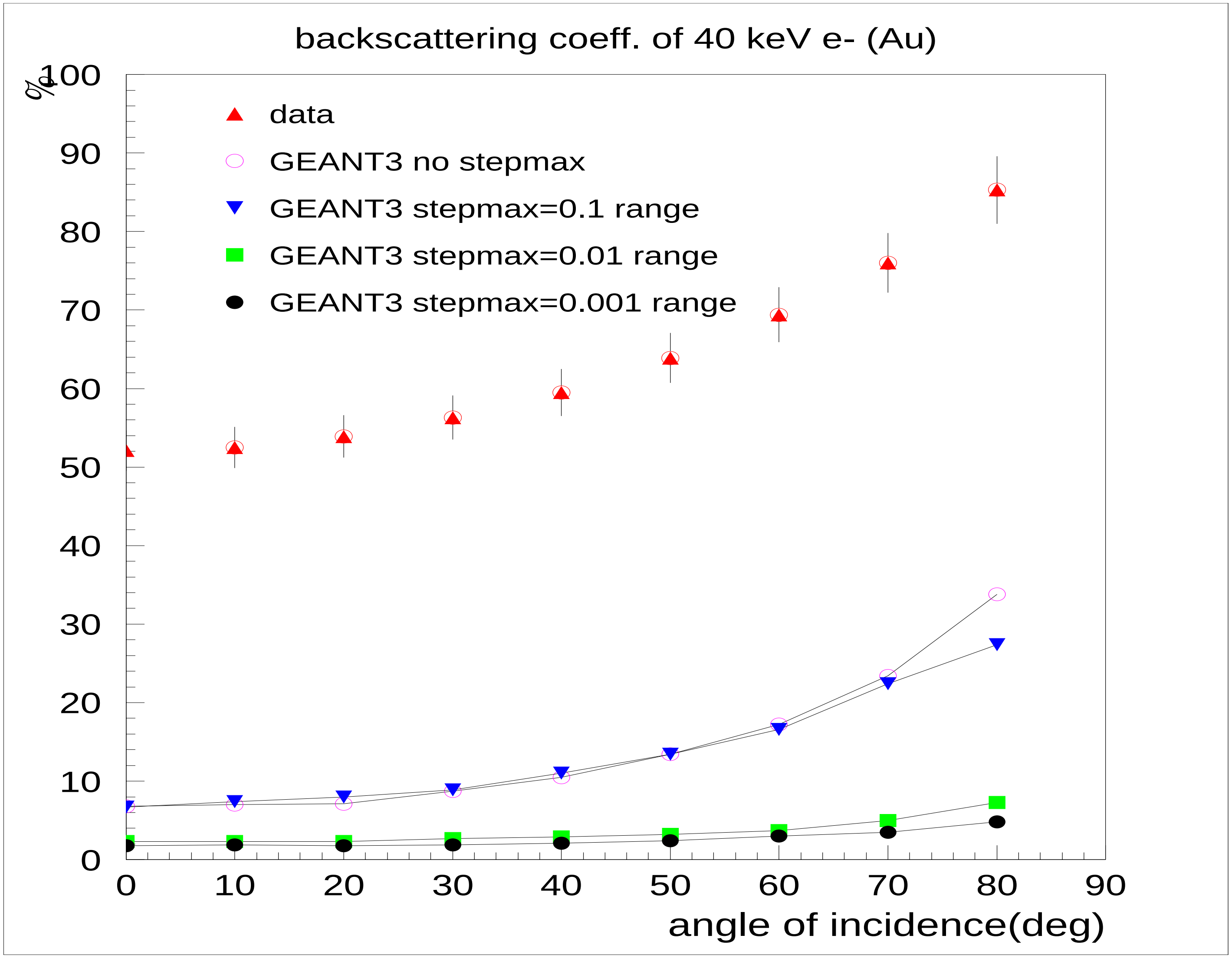
Backscattering of e- G4 simulation ≈ exp.data not shown here



Backscattering of e- G4+data



Backscattering of e- G3+data



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