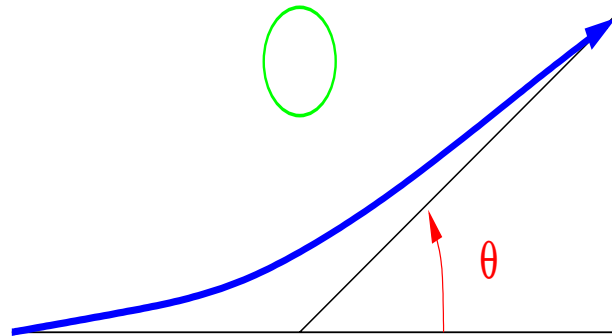


# Simulation of Multiple Coulomb scattering in GEANT4

## Single Coulomb scattering

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

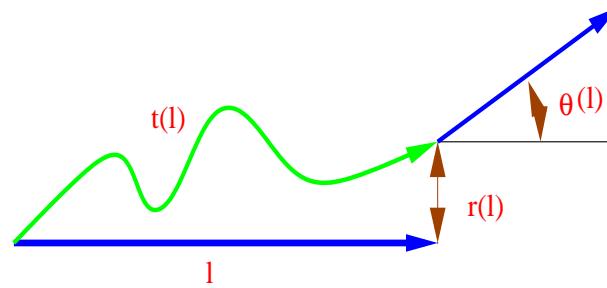


The cross section is given by the Rutherford formula

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

## 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

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

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

This formula of  $\theta_0$  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  $\theta_0$  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 :

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

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) :  $t \iff l$   
 $t \implies l : F(l, t, \lambda)$   
 $l \implies t : G(t, l, \lambda)$
- scattering angle distribution:  $f(\cos\theta, t, \lambda)$
- lateral displacement :  $R(t, \lambda)$ .

## Physics input of the model

first transport mean free path :

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

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 :  $(1 - \cos\chi) \implies (1 - P_i(\cos\chi))$ , (i-th Legendre polynomial).

Instead of using the cross section directly the model uses  $\lambda$  and  $\lambda_2$  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  $t/\lambda$  and  $t/\lambda_2$  variables.

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

1. selection of step length  $\Leftarrow$  physics processes + geometry  
(MSC performs the  $t \iff l$  transformations only)
2. transport to the initial direction : (not MSC business)
3. sample scattering angle  $\theta$
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)  
 $t = \min(t_{proc1}, t_{proc2}, \dots, t_{procn})$
2. do the  $t \rightarrow l$  transformation  $F(l, t, \lambda) \implies l_{phys}$   
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  
 $G(t, l_{step}, \lambda) \implies t_{step}$   
done by `AlongStepDoIt()` of MSC

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

Distribution with the theoretical mean values.

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

where

$$l_0 = \langle l \rangle + d (t - \langle l \rangle) \quad (4)$$

where  $\langle l \rangle$  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 theoretical mean value for  $l$

$$k = \frac{2 \langle l \rangle - t}{l_0 - \langle l \rangle} \quad (5)$$

The geometrical path length  $\Rightarrow$  true path length transformation is performed using the mean values

$$t = \langle t \rangle = -\lambda * \log \left( 1 - \frac{l}{\lambda} \right) \quad (6)$$

This transformation 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  $\theta$  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,  $f_3 = \text{const}$ ).

**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.

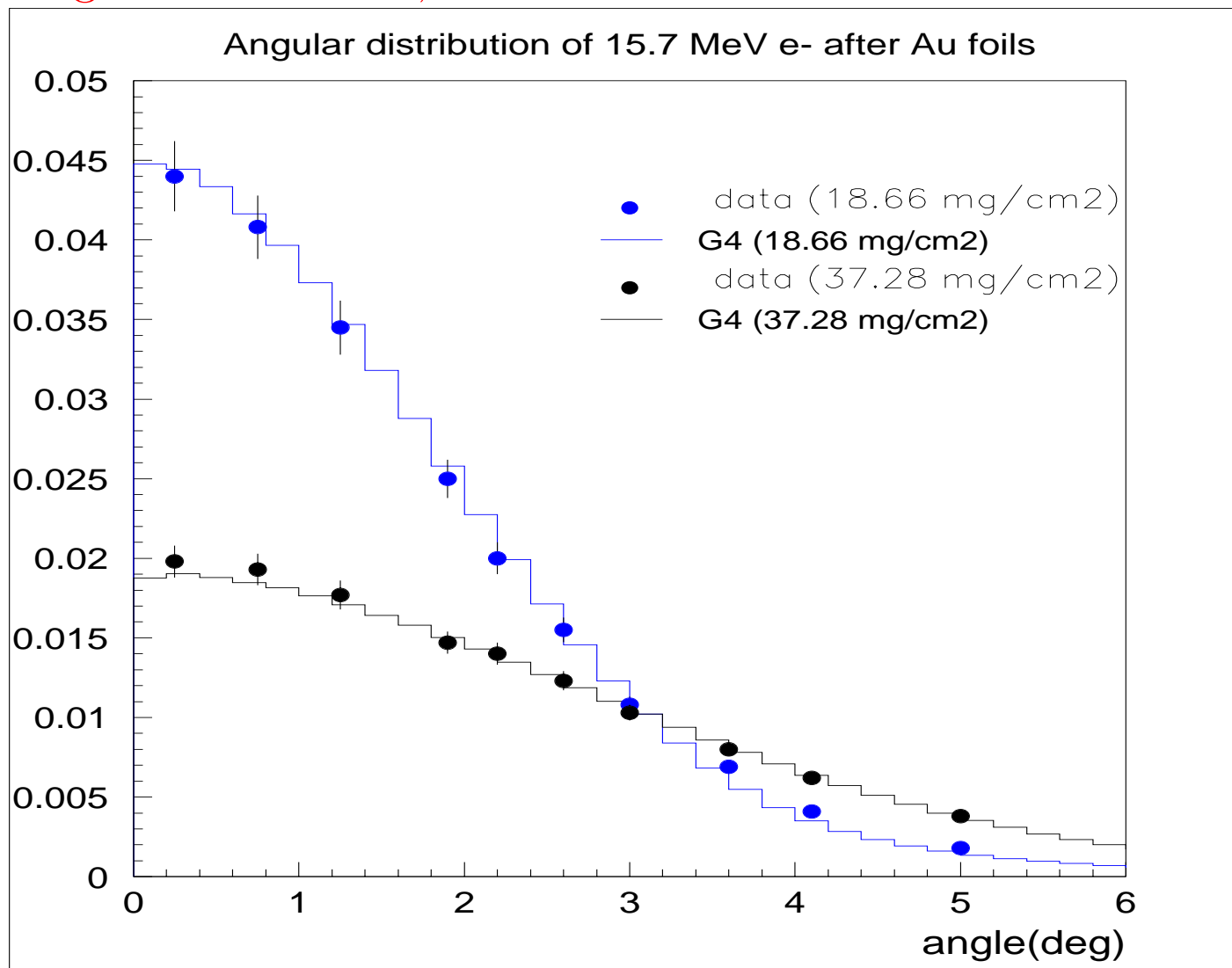
note: this step is executed only if the particle is 'far' from the boundary of the volume.

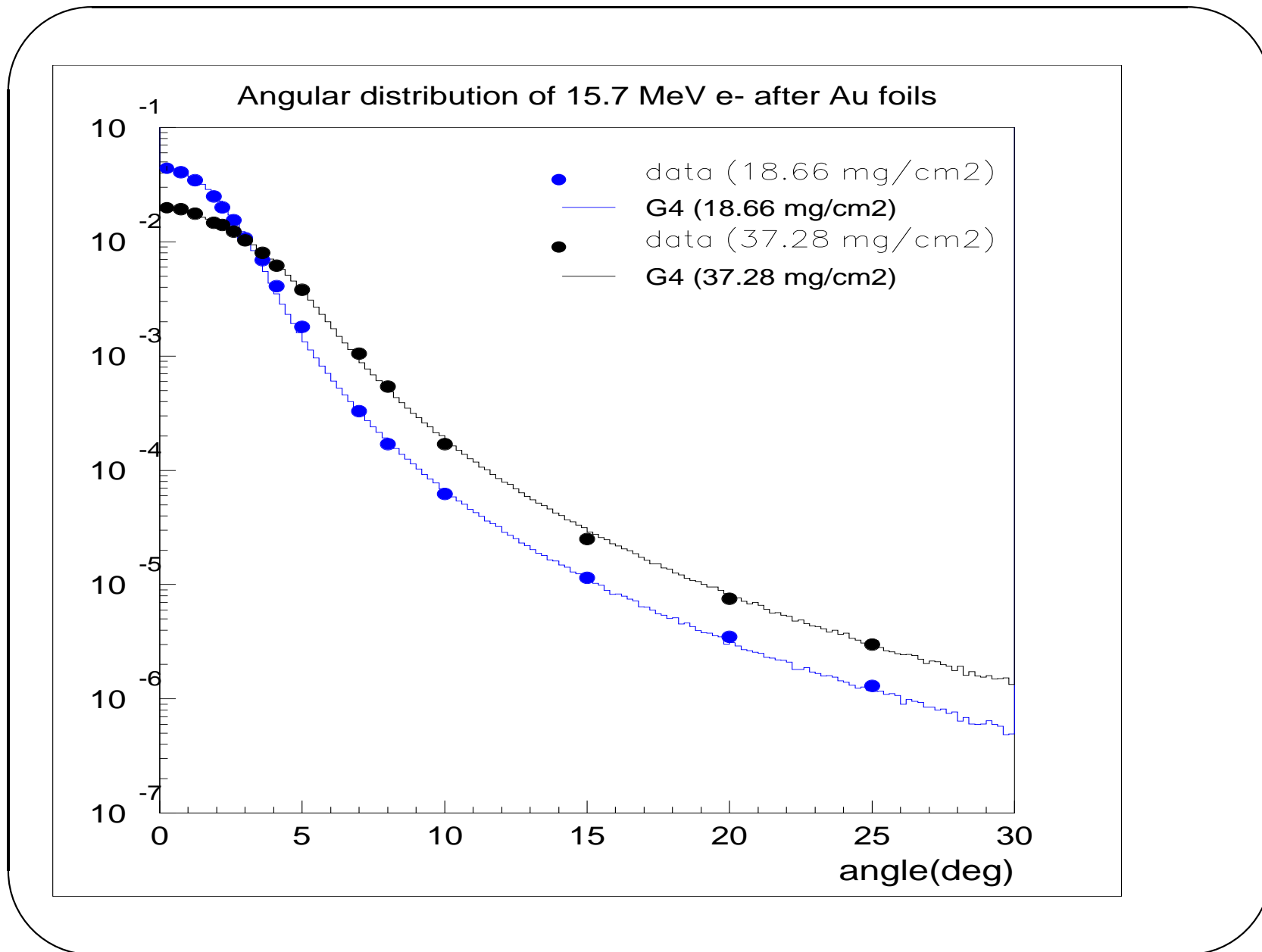
MSC is a `ContinuousDiscreteProcess`, until now we have seen `AlongStepGetPhysicalInteractionLength()` `AlongStepDoIt()` `PostStepDoIt()`.

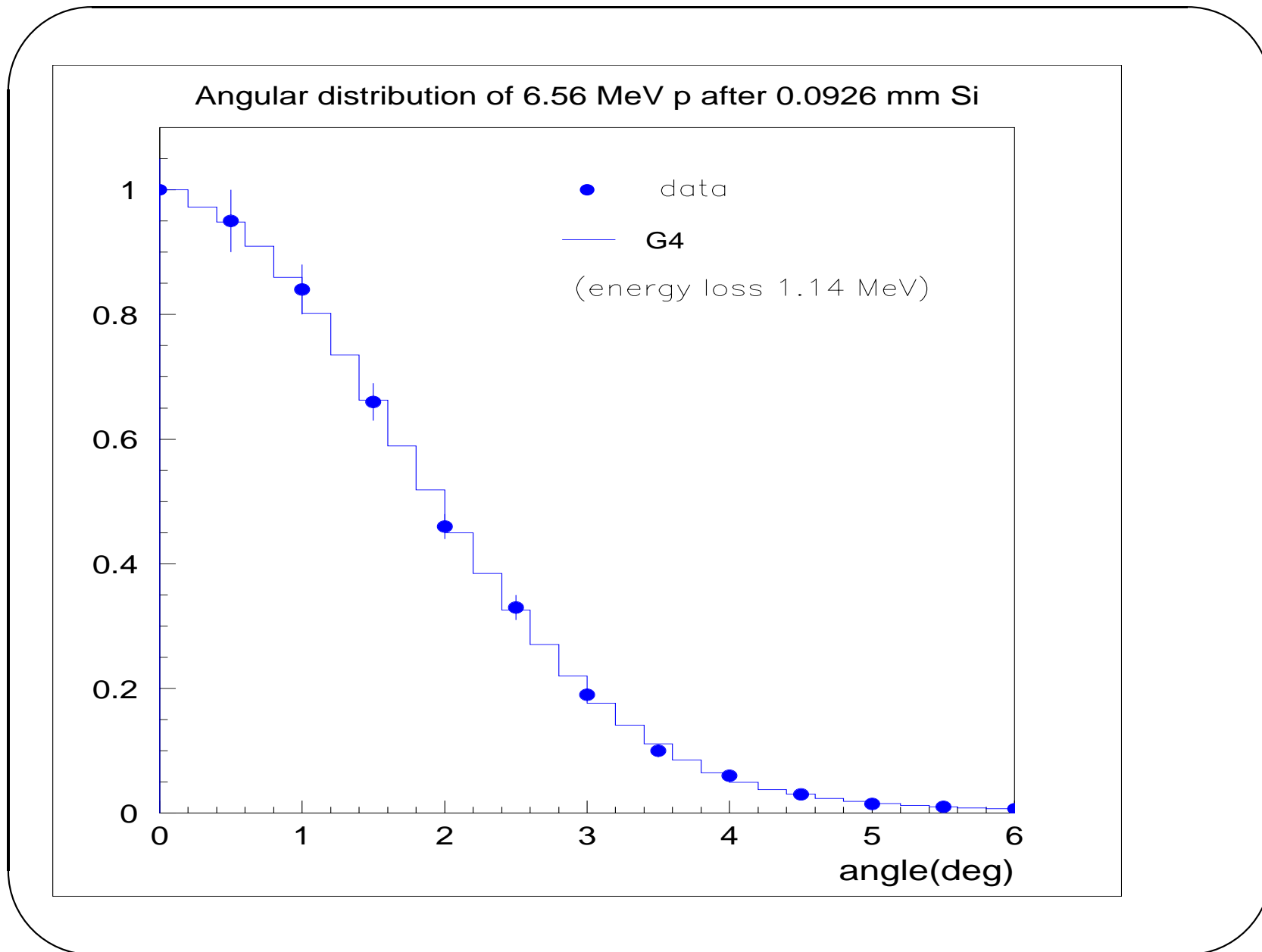
What is the task for `PostStepGetPhysicalInteractionLength()` ?  
It sets only a `ForceFlag` in order to ensure that `PostStepDoIt()` is called at every step.

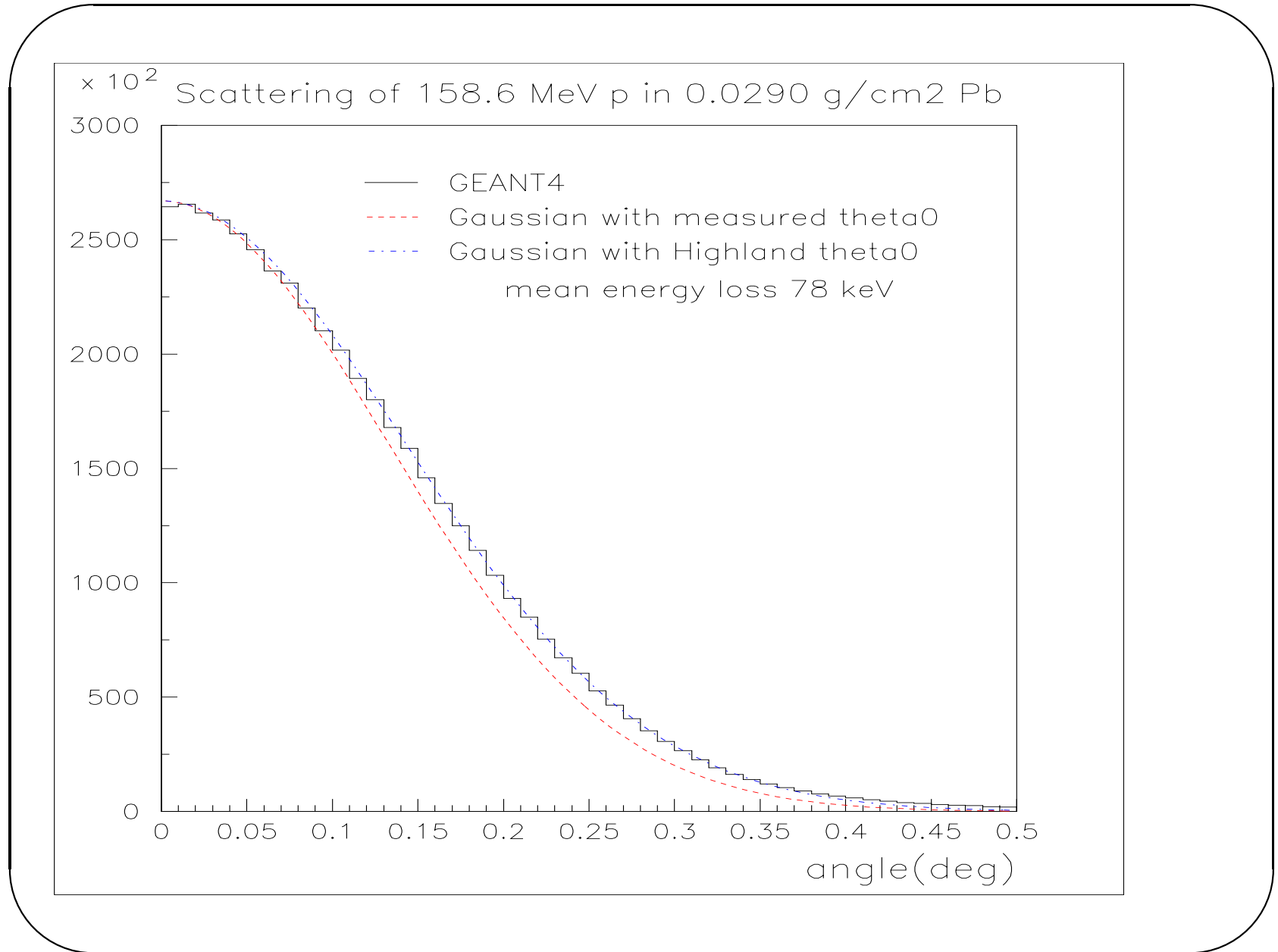
Simulation results  $\iff$  data, the ultimate test of the reliability of MC simulations

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

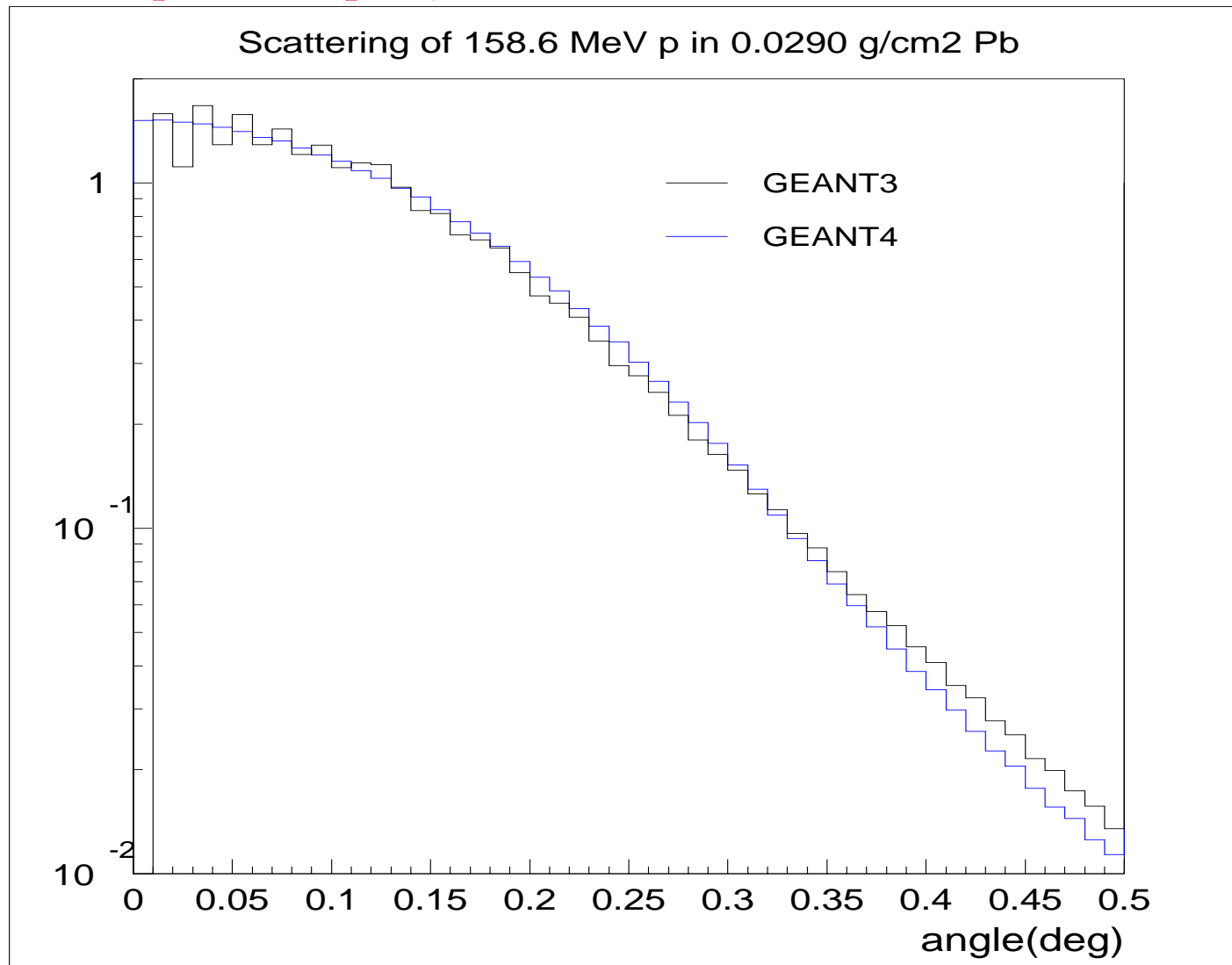
Angle distributions, Geant4  $\iff$  data



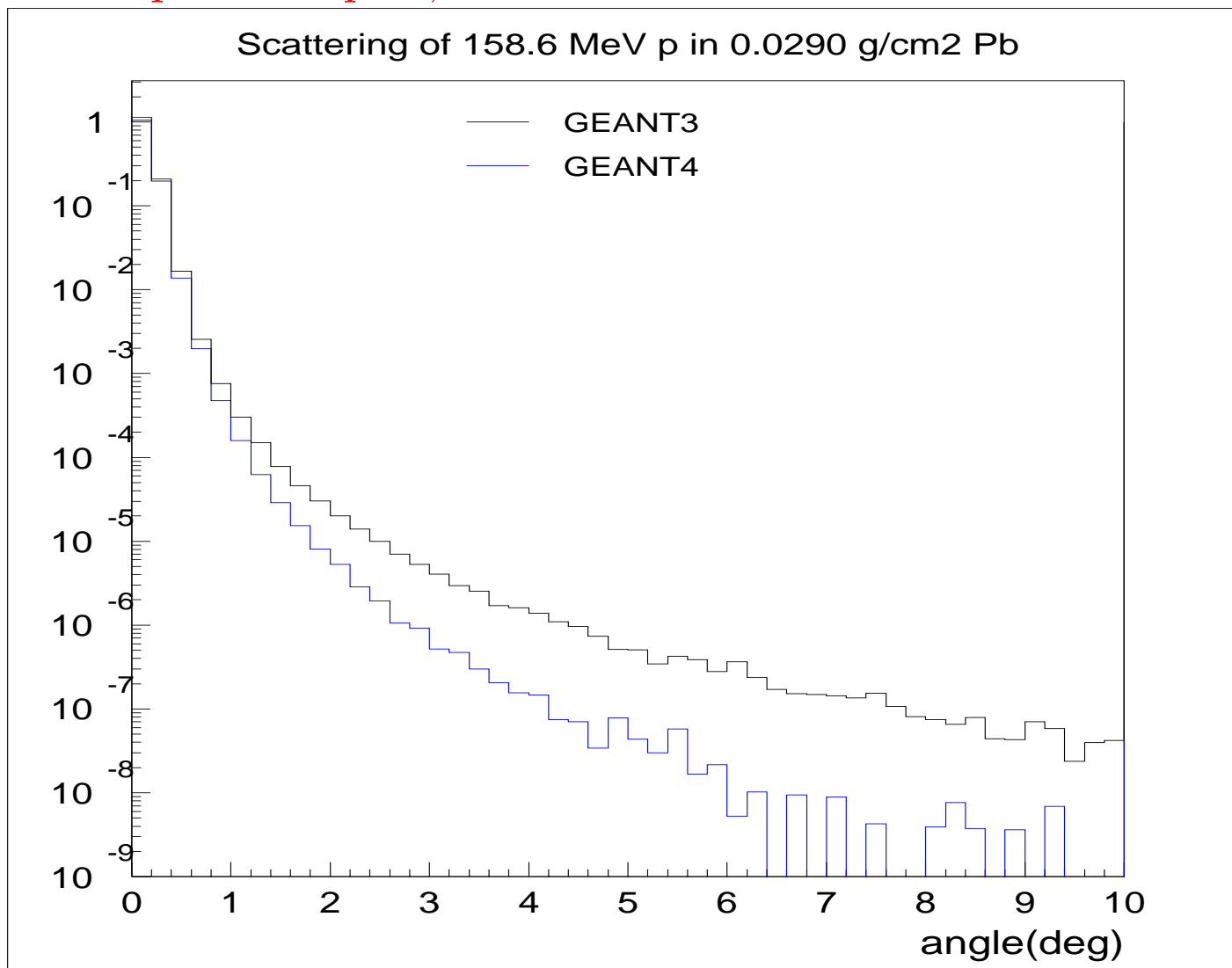


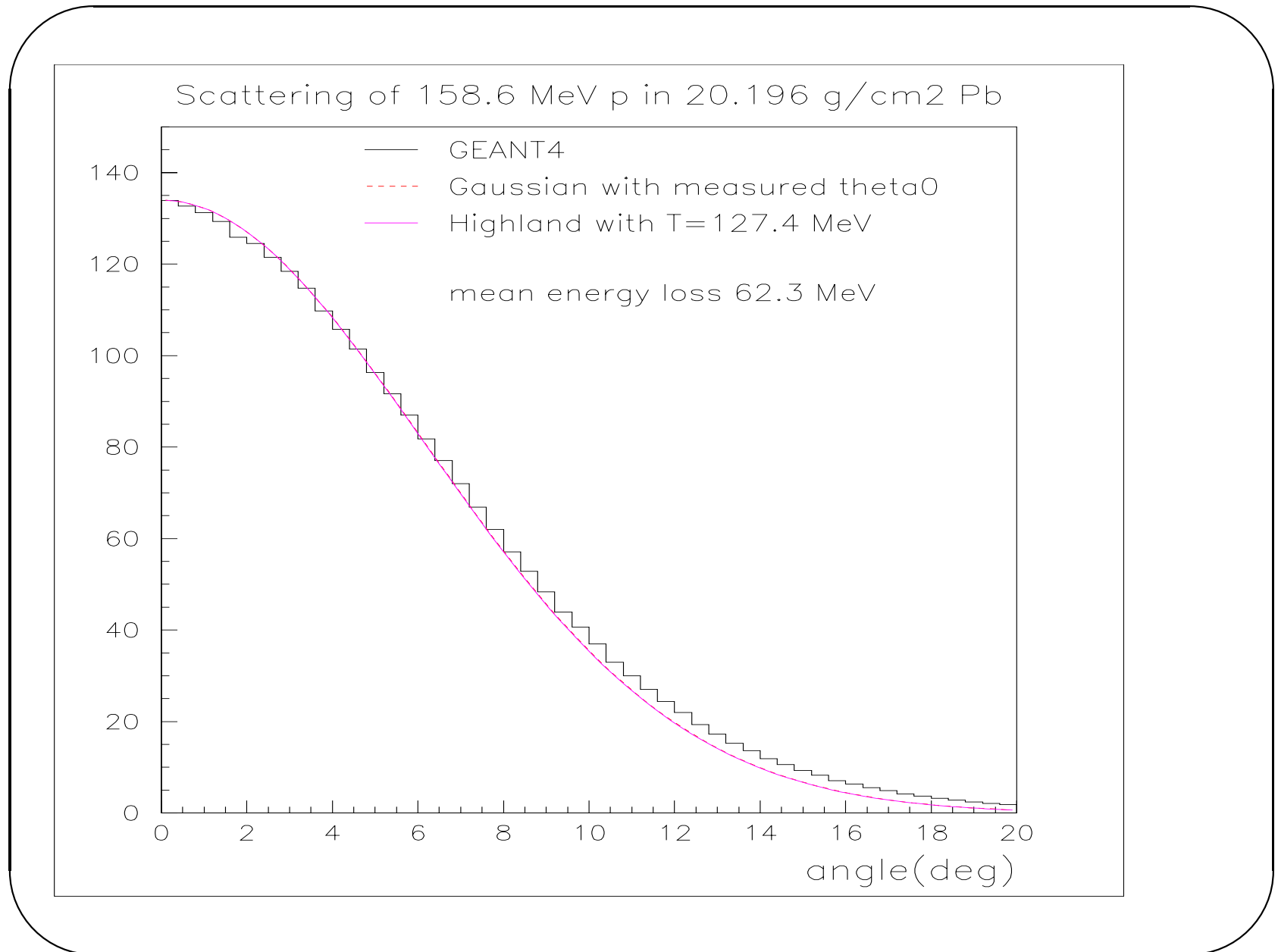


as the previous plot, but GEANT4  $\iff$  GEANT3

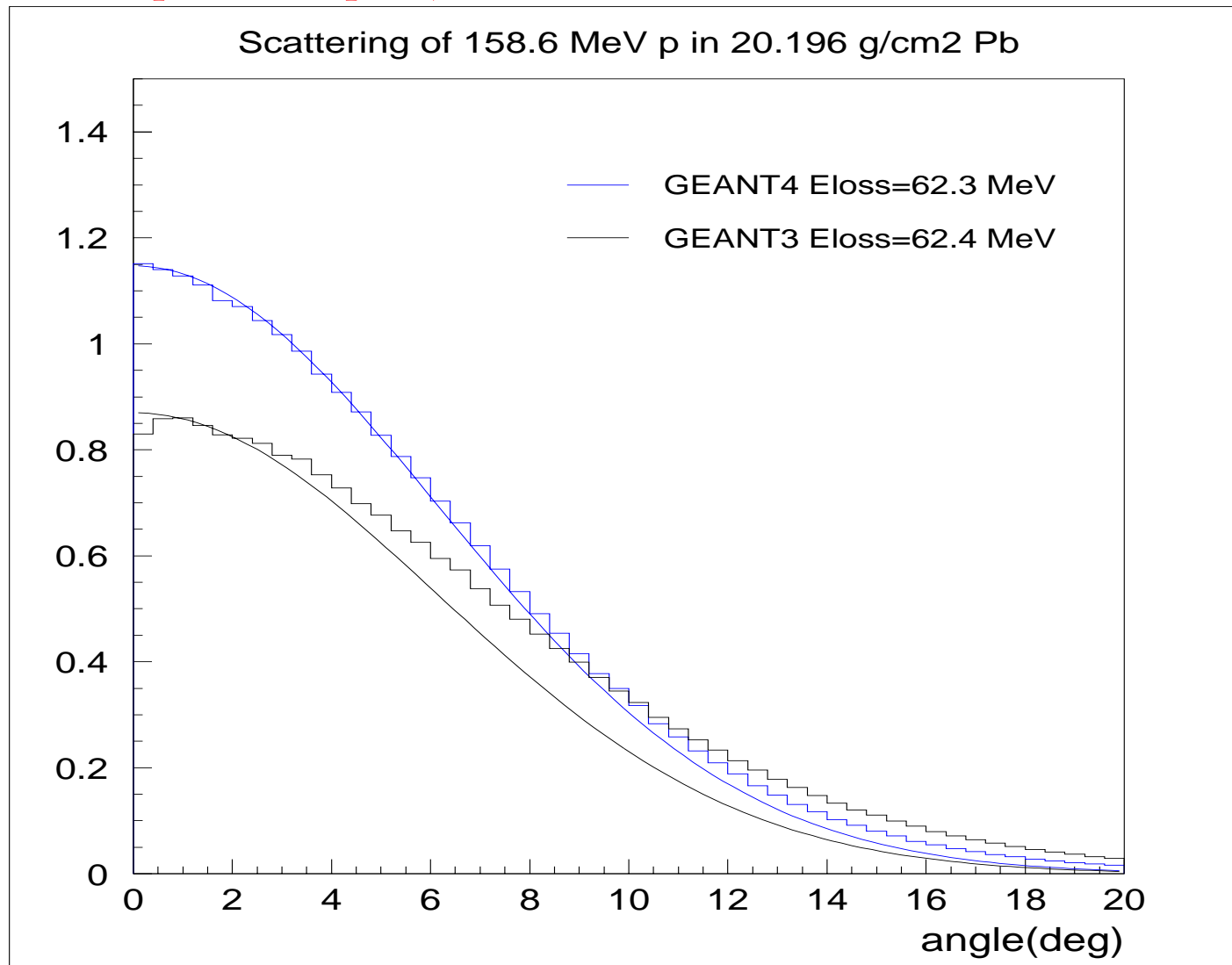


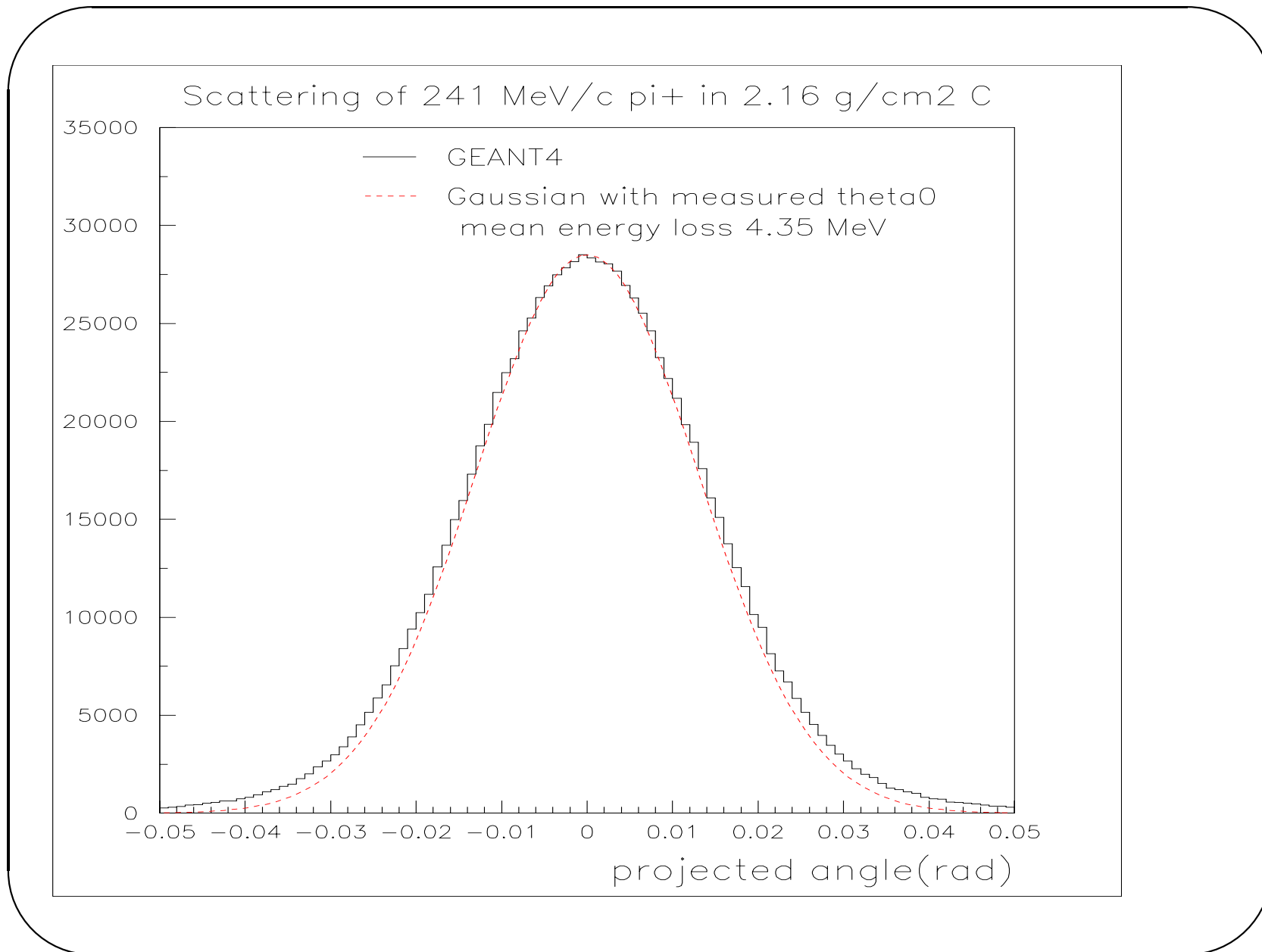
as the previous plot, but GEANT4  $\iff$  GEANT3 with tails

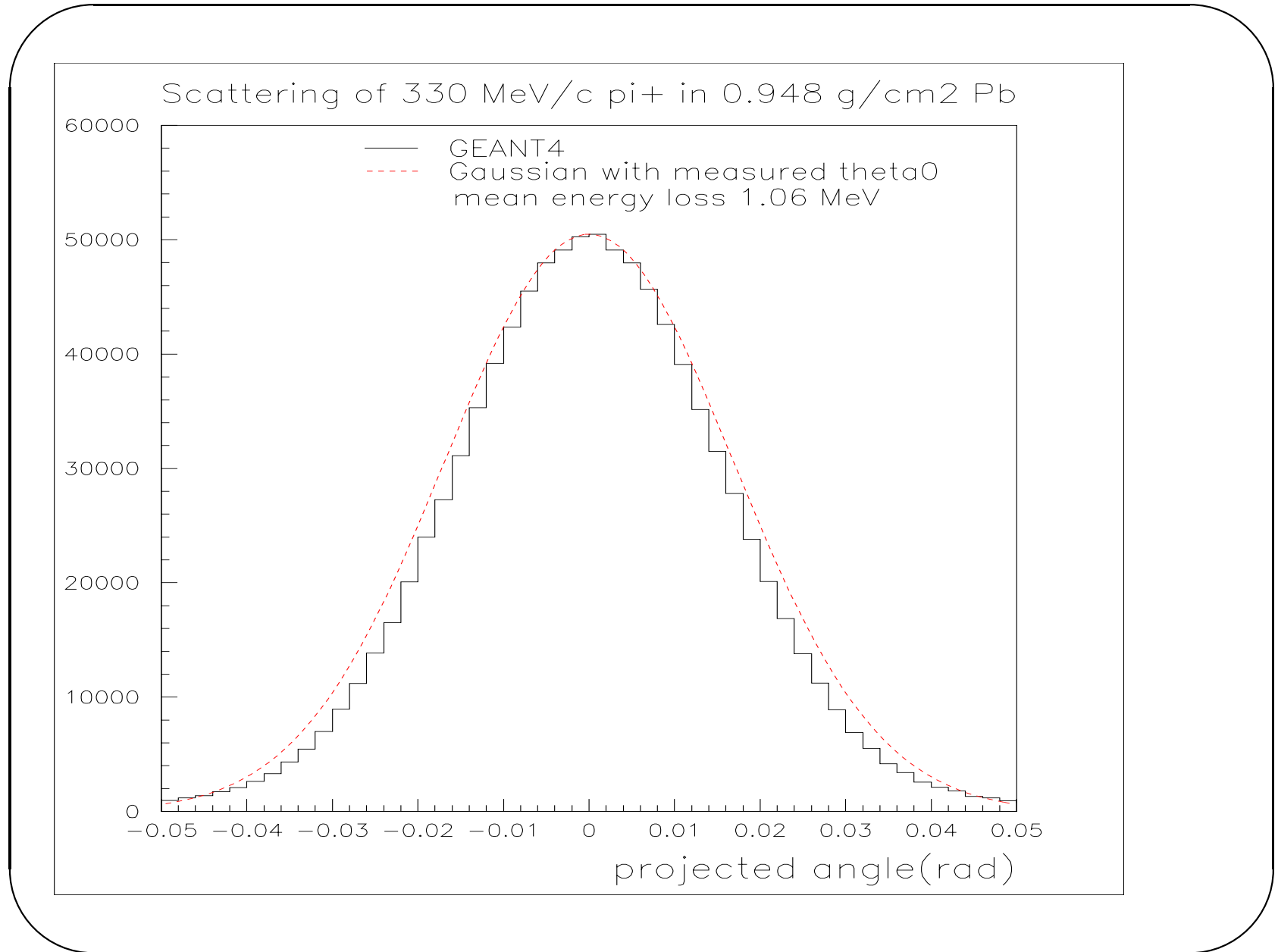




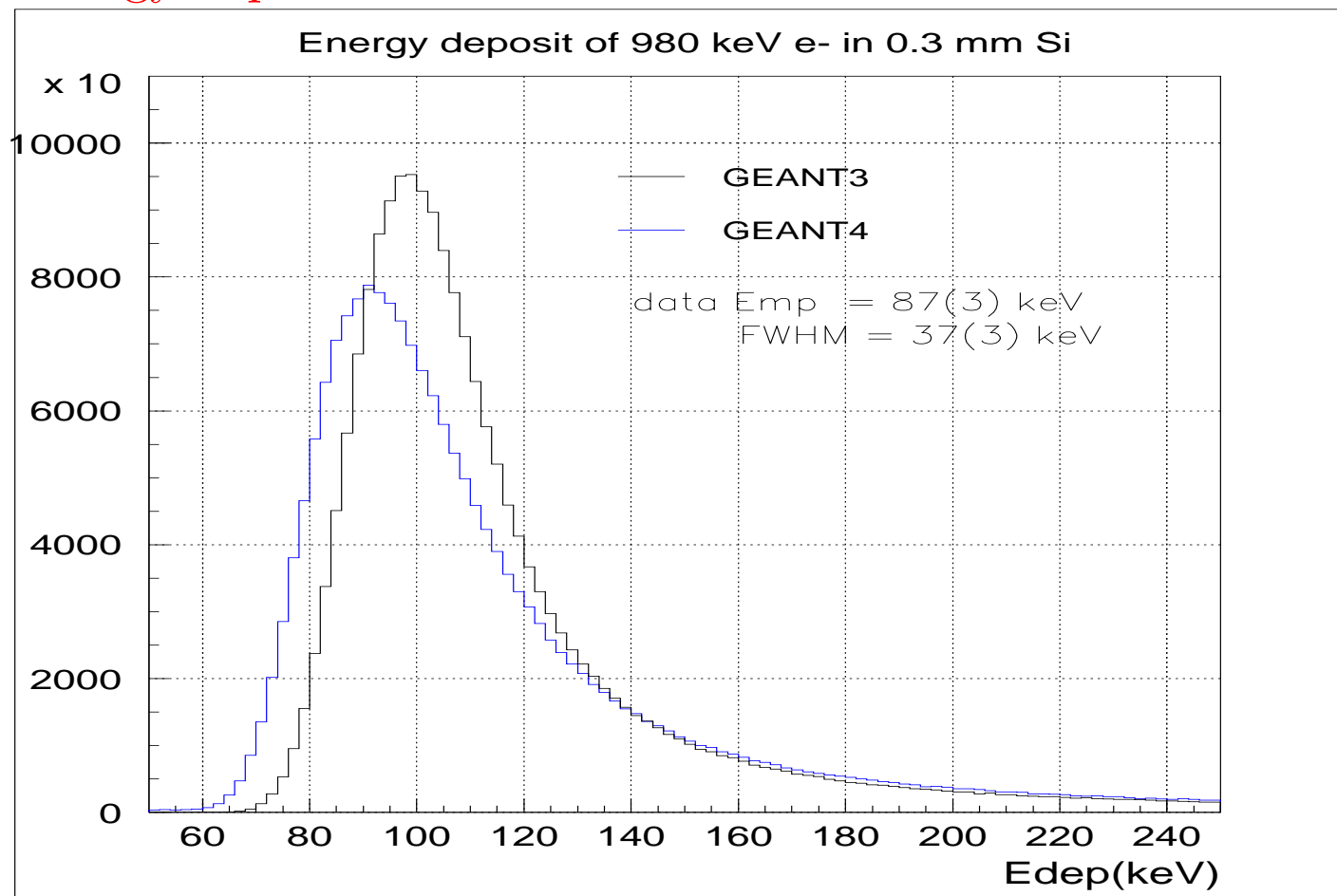
as the previous plot, but GEANT4  $\iff$  GEANT3





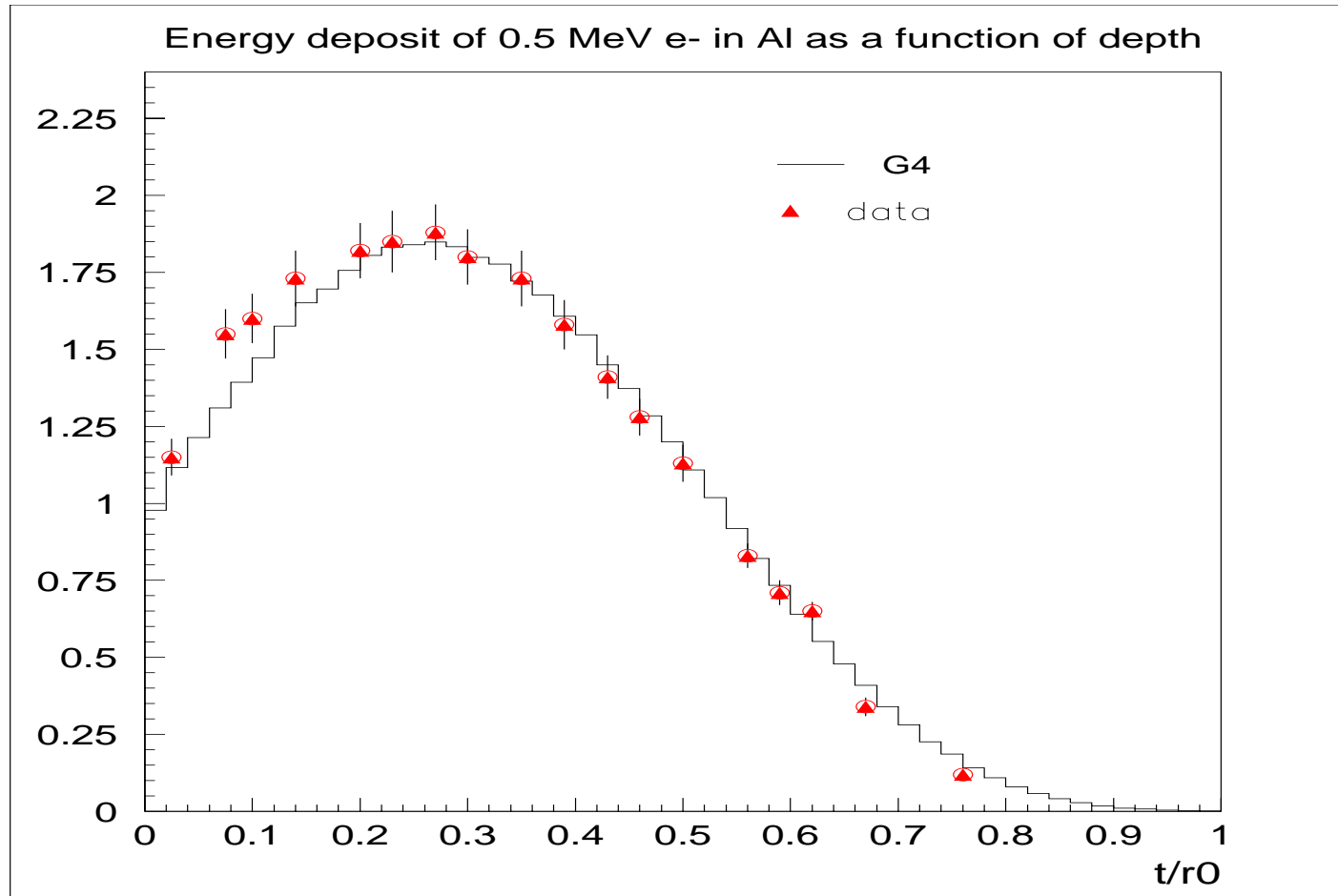


## Energy deposit distribution in Si detector



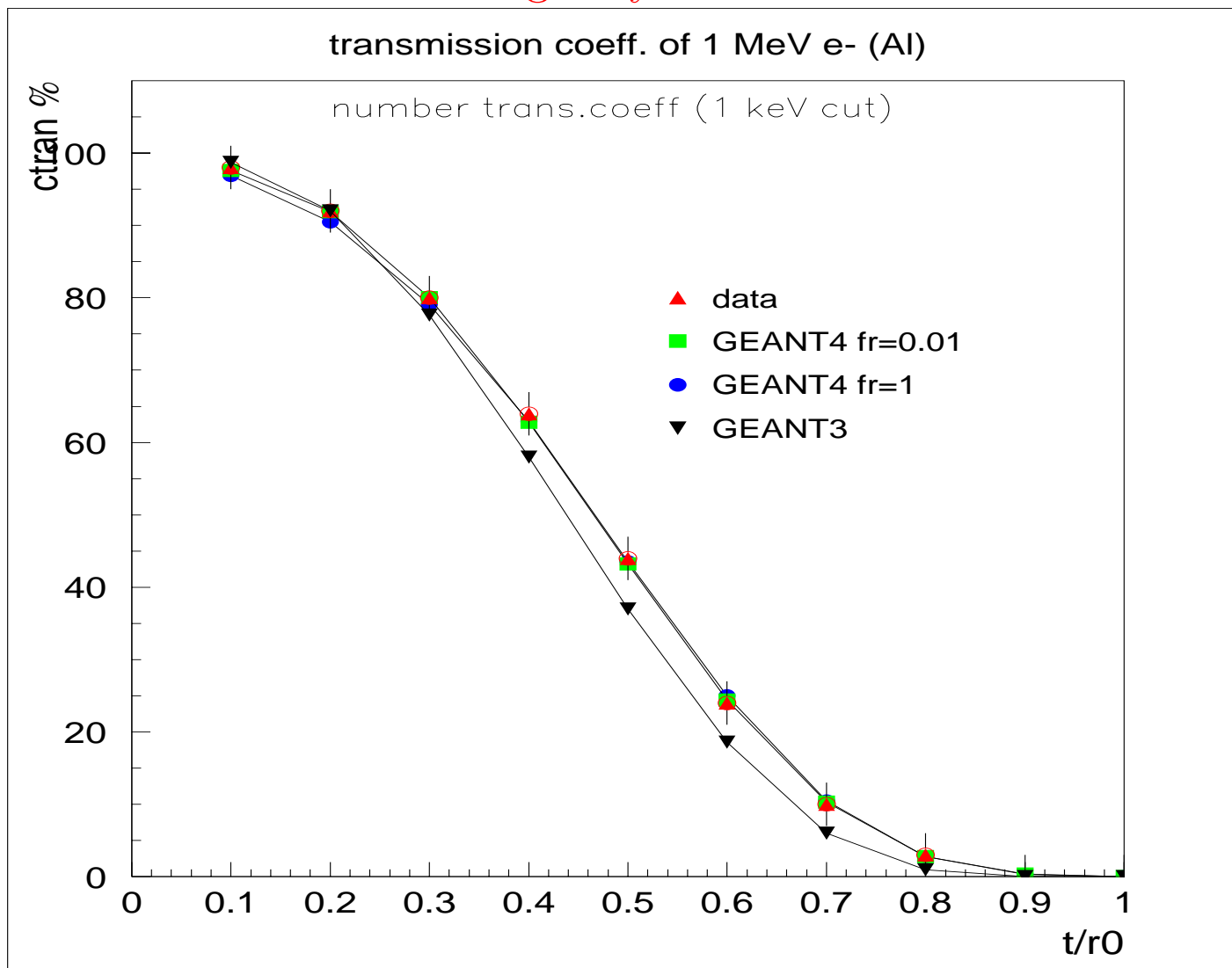
without MSC GEANT4 = GEANT3  $\implies$  difference comes from the different MSC simulation !

## Depth-dose distribution

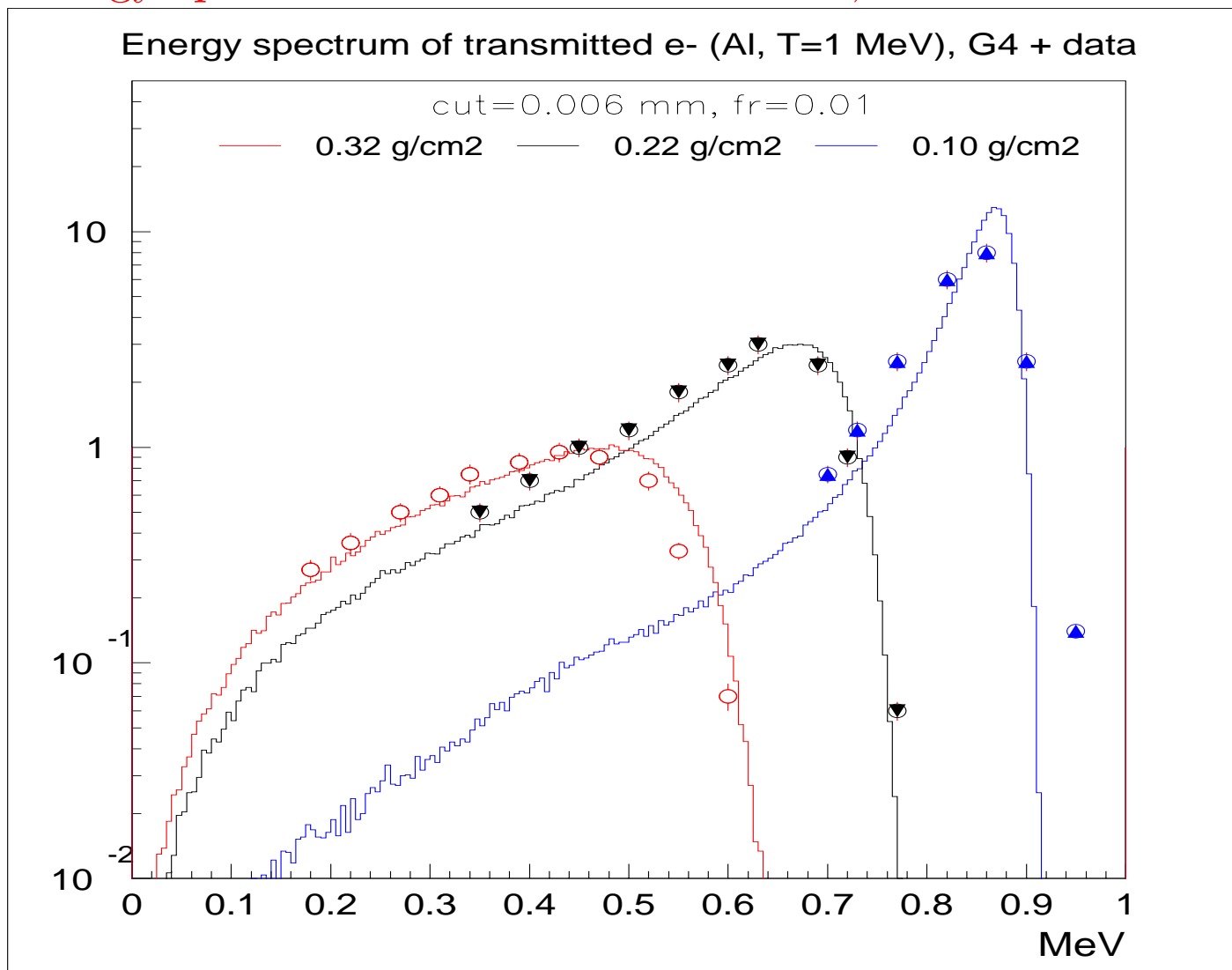


(error on data  $\approx 5 - 10\%$ ).

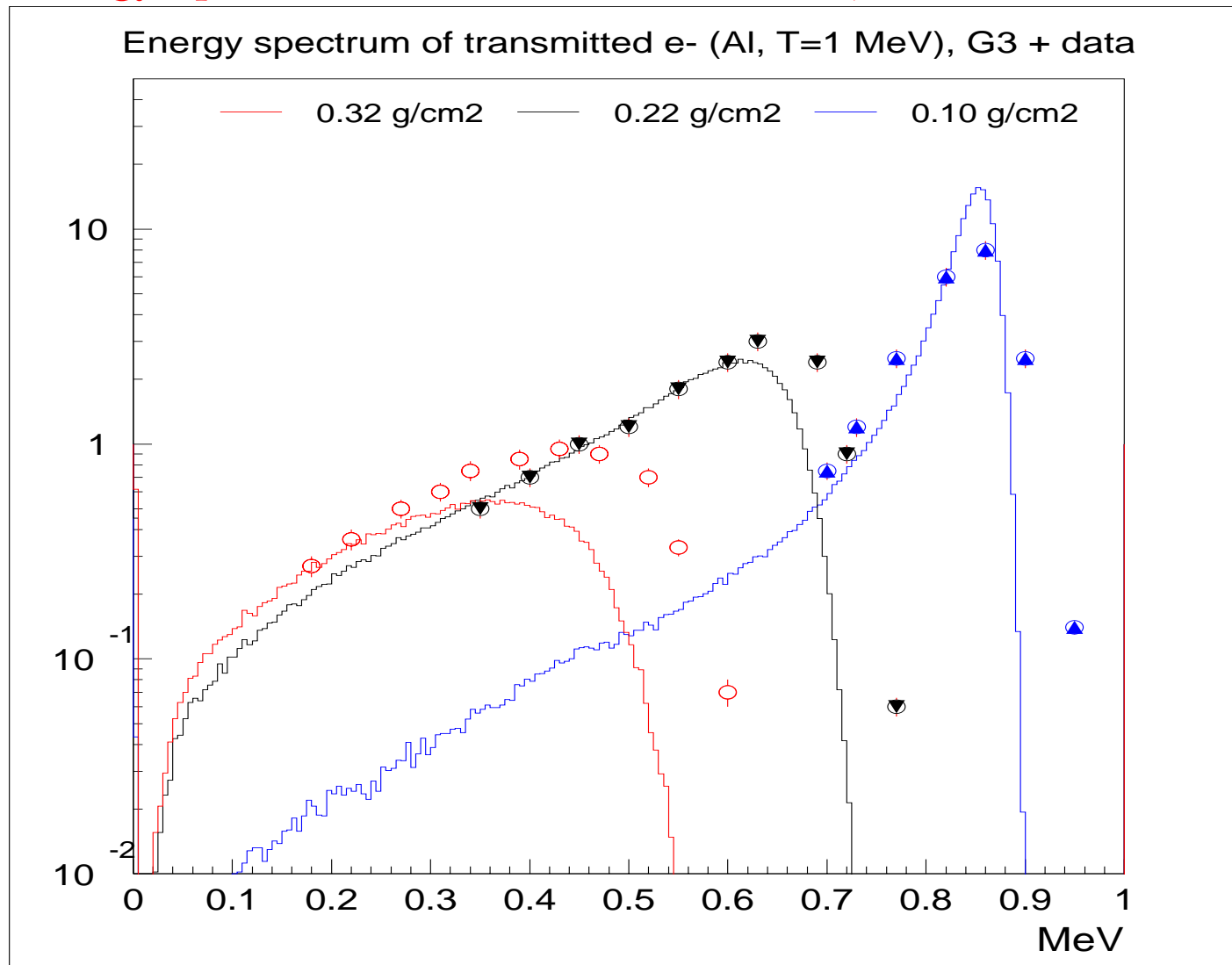
## Transmission of e- through layers



## 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 algorithm:  
limit the step in MSC when entering a volume . Algorithm:

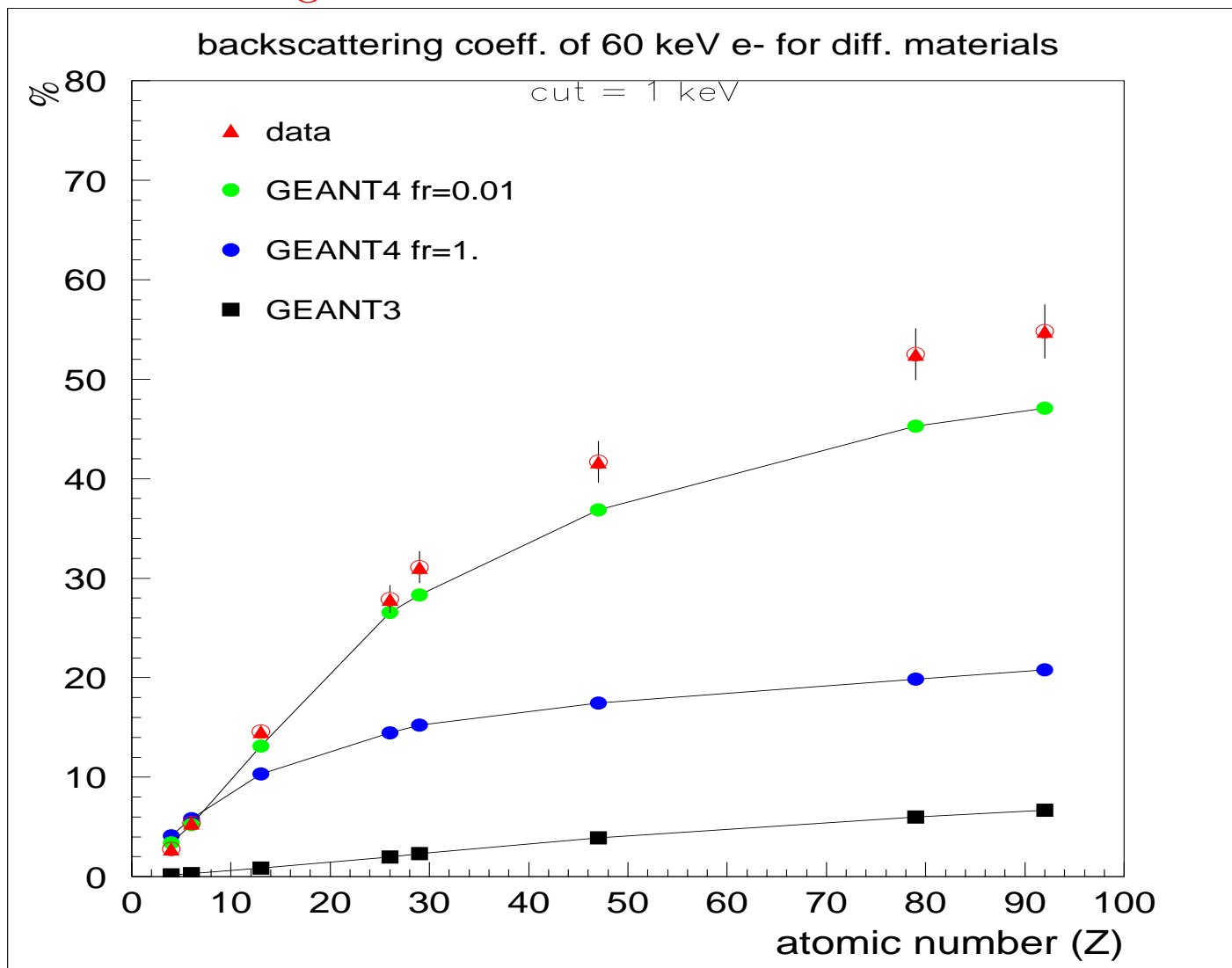
$$t_{lim} = fr * max(\lambda, range)$$

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

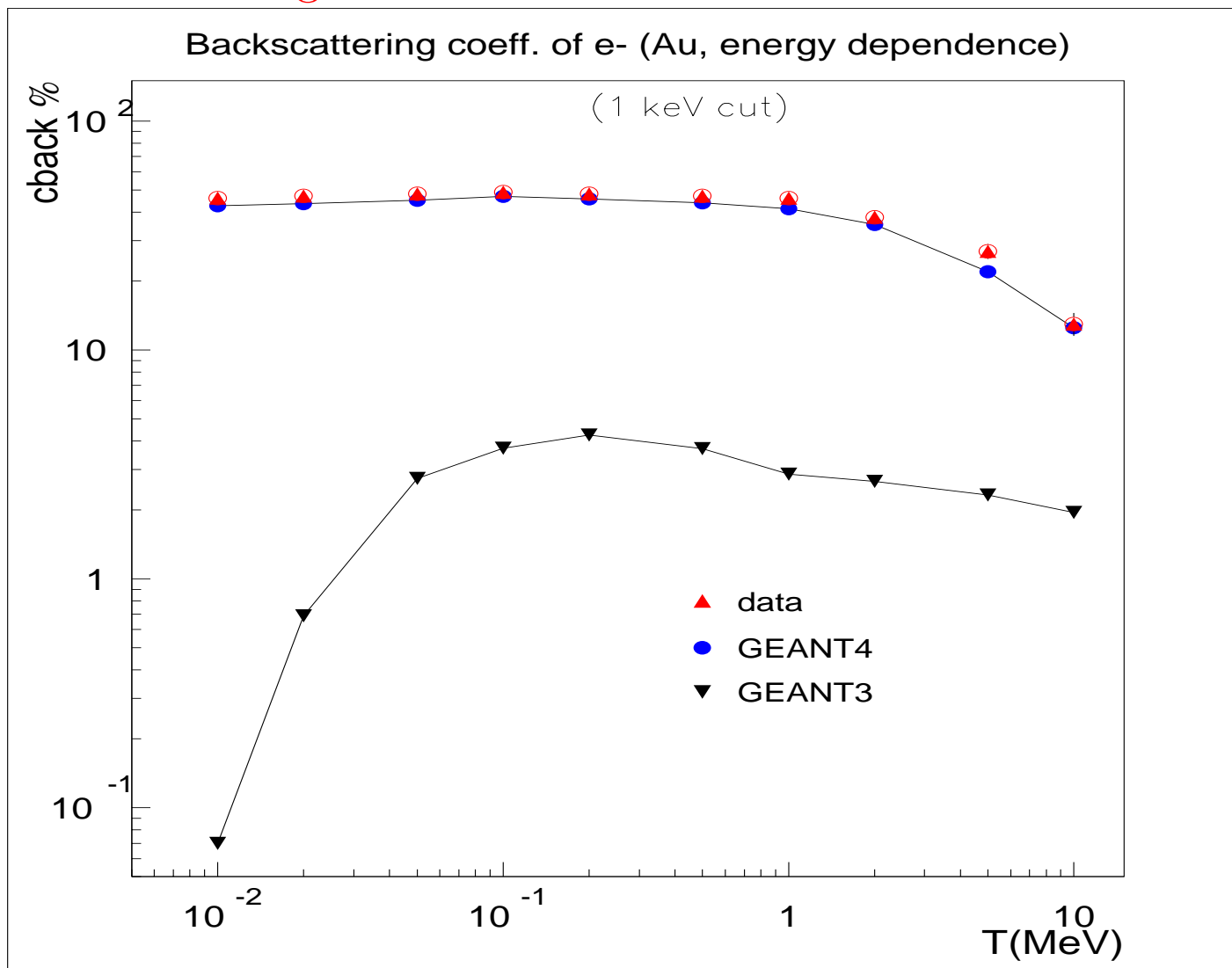
This is NOT the user limit, the step is limited only after entering a volume and the step limit energy and particle dependent !

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

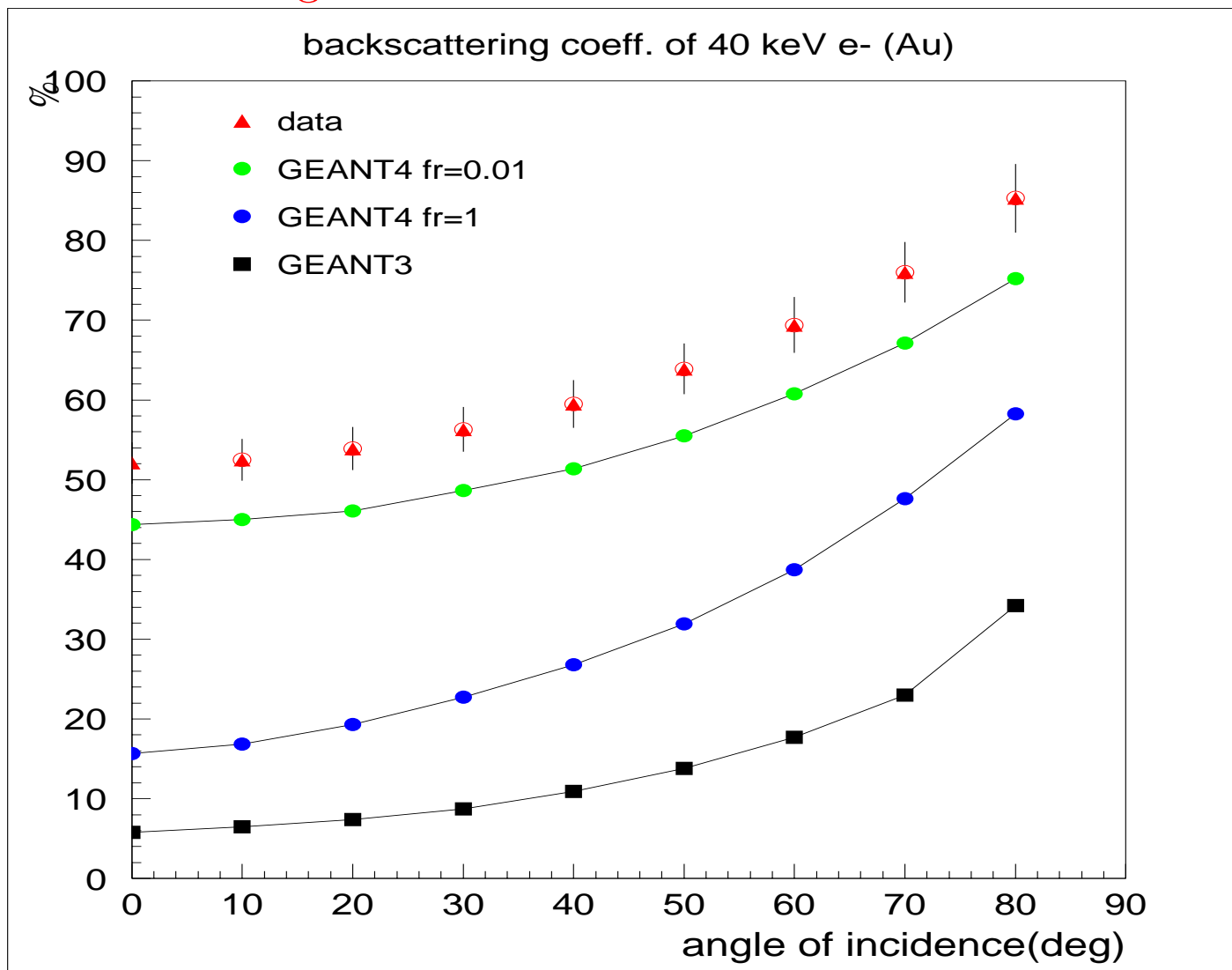
## Backscattering of e- G4+data+G3



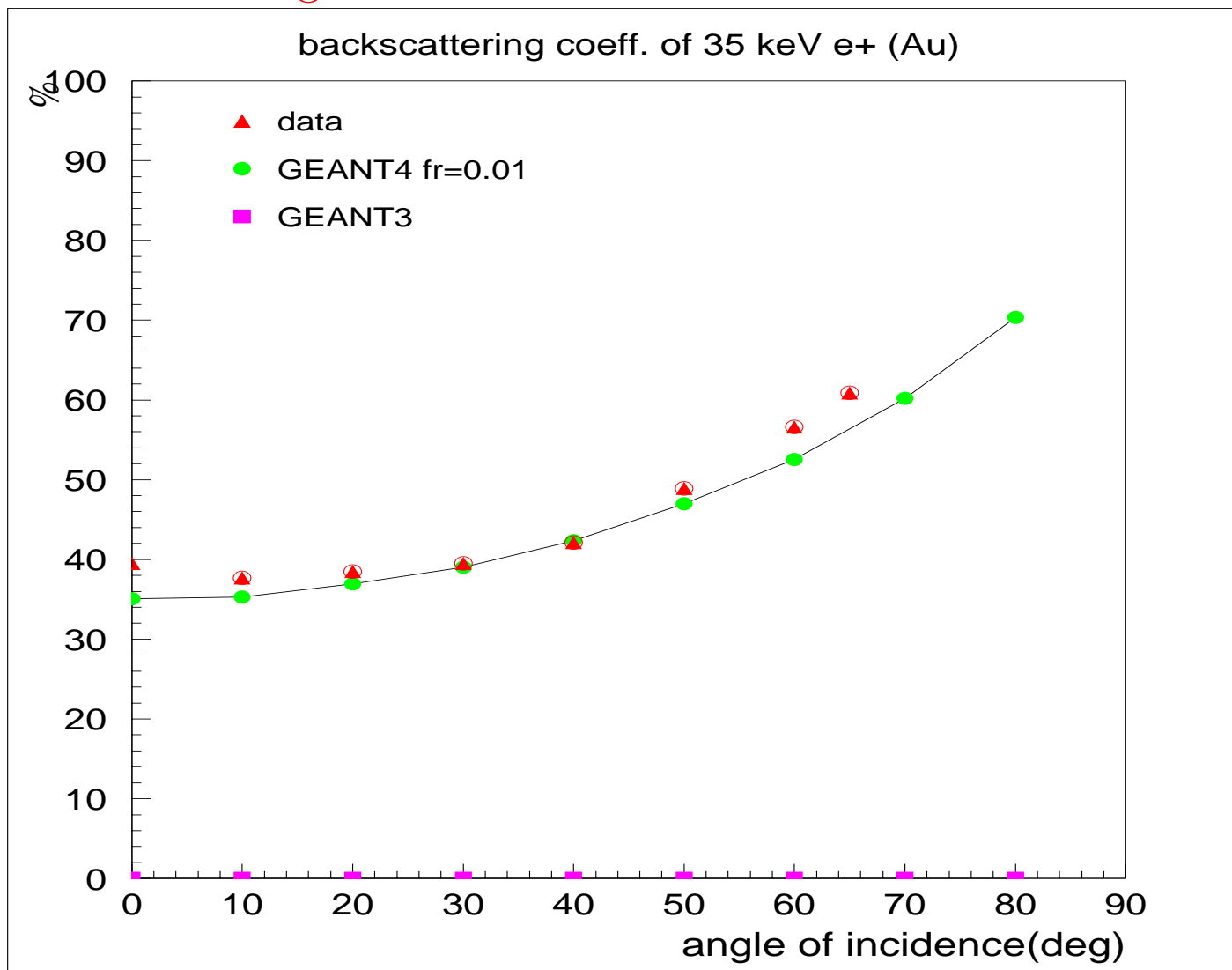
## Backscattering of e- G4+data+G3



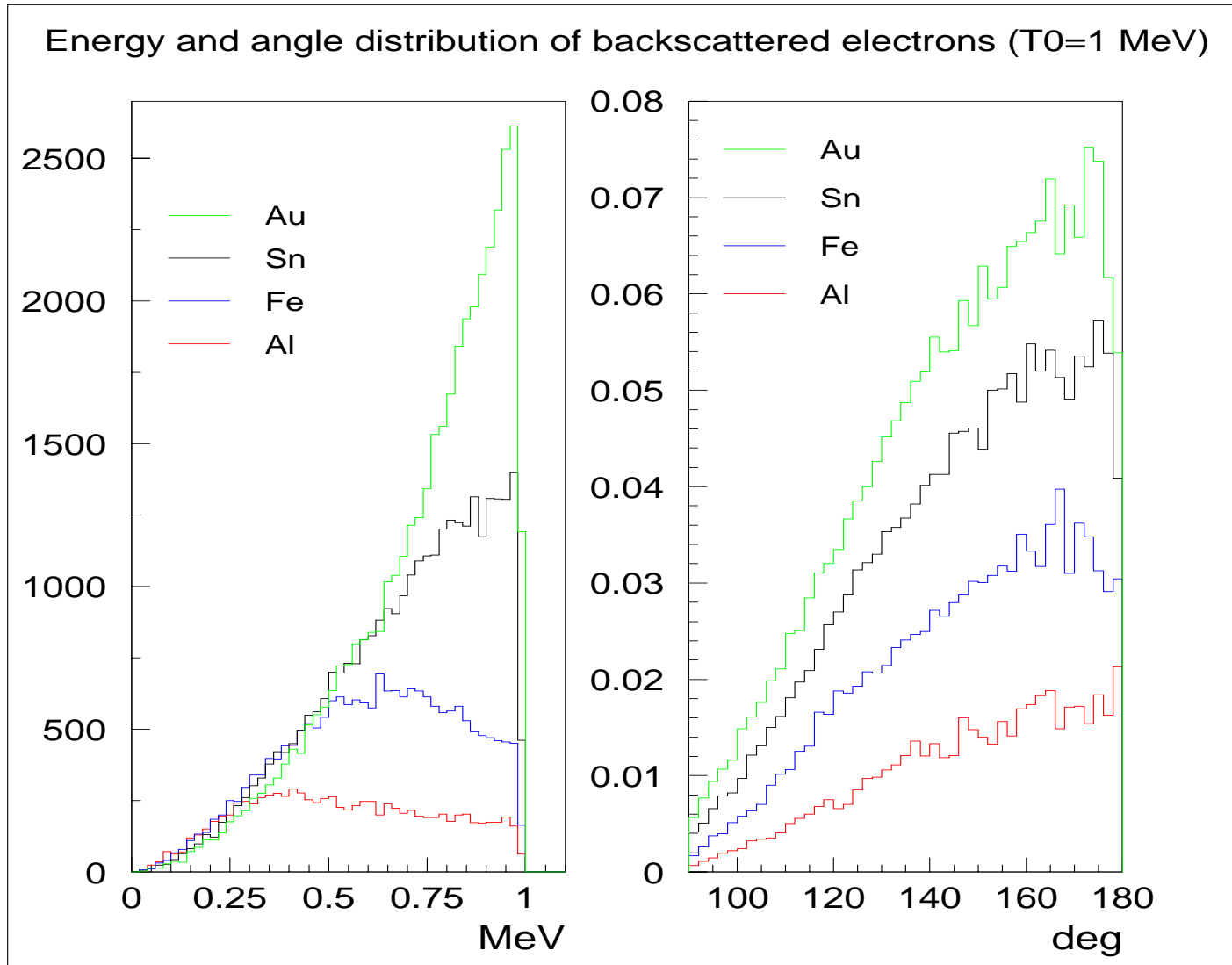
## Backscattering of e- G4+data+G3



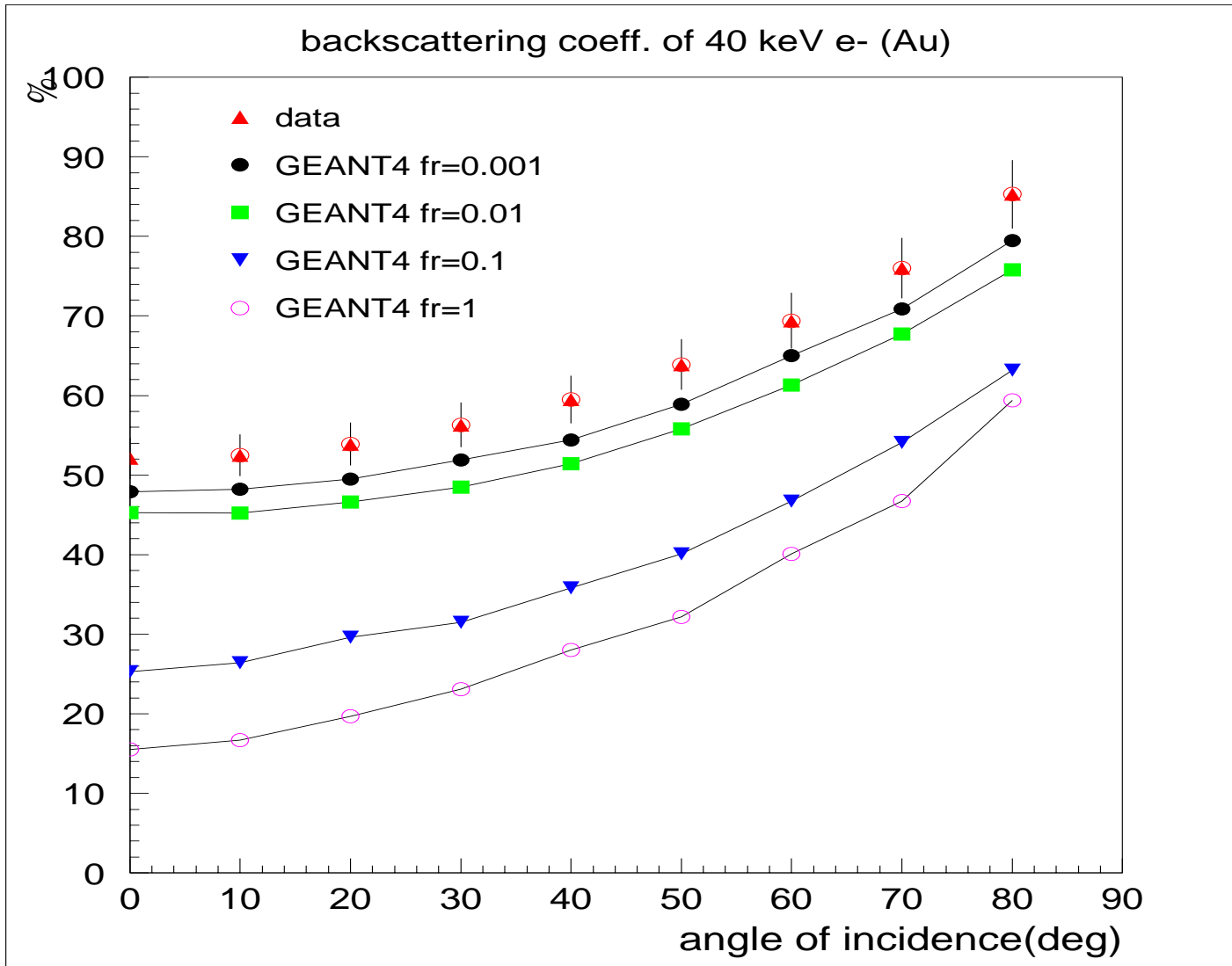
## Backscattering of e<sup>+</sup> G4+data+G3



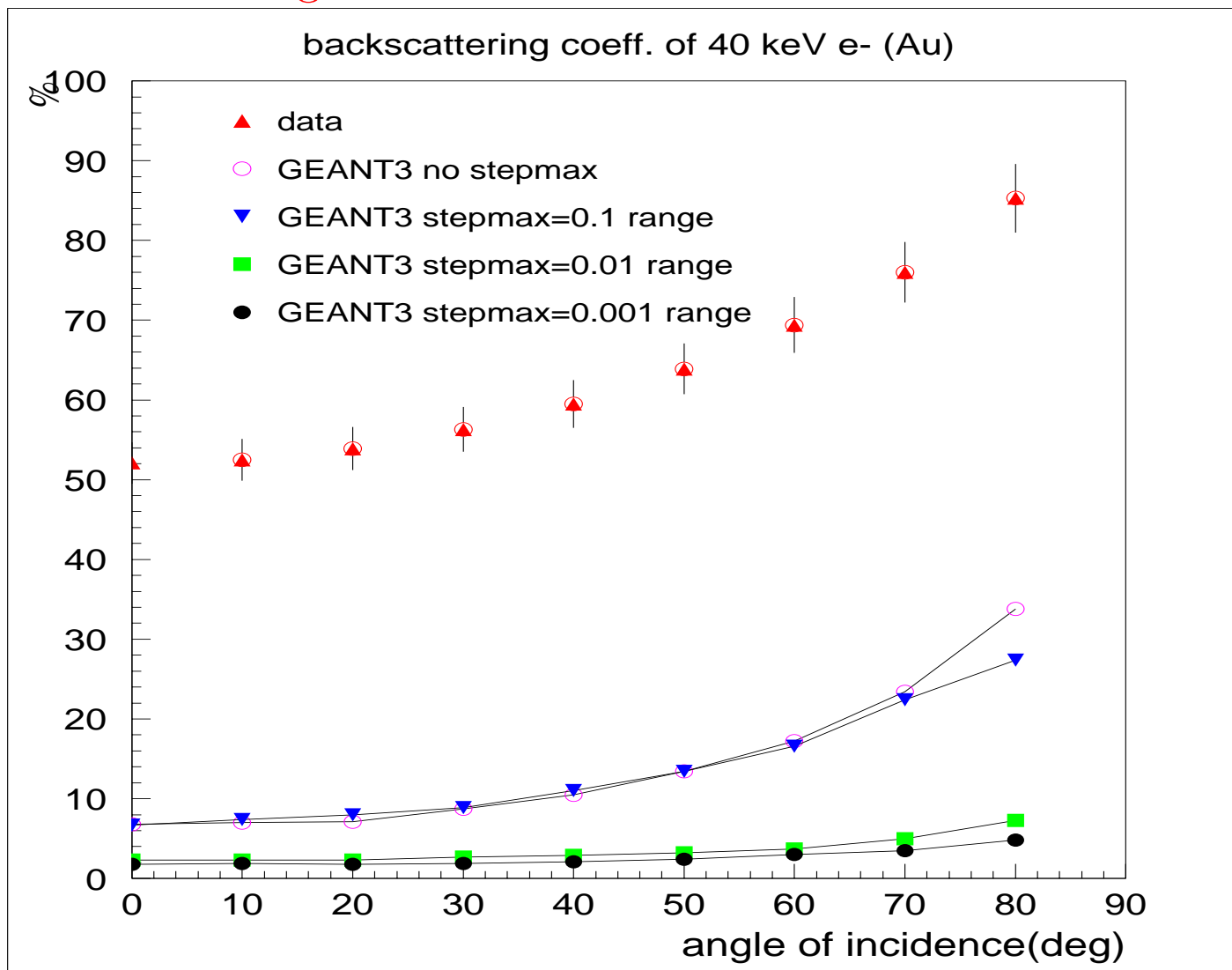
Backscattering of e- G4 simulation  $\approx$  exp.data not shown here



### Backscattering of e- G4+data



## Backscattering of e- G3+data



## References

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