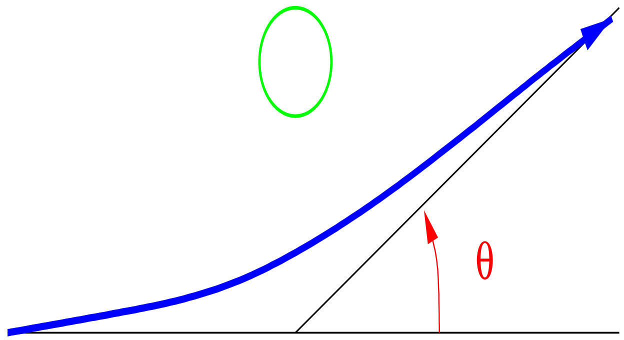
Multiple Coulomb Scattering in GEANT4

Summary:

The Multiple Scattering (MSC) model used in the simulation toolkit GEANT4 will be presented. After a short introduction of the MSC process and its simulation the model will be described. We present the path length correction and angle distribution computation in detail and desribe the implementation of the model in the framework of GEANT4. At the end of the talk a number of simulation - exp.data comparison will be presented to demonstrate of the capabilities of the simulation algorithm.

Single Coulomb scattering

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

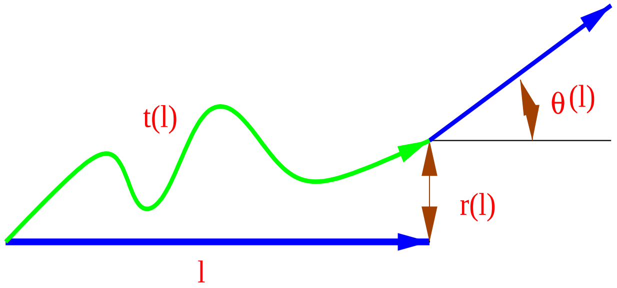


The cross section is given by the Rutherford formula

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

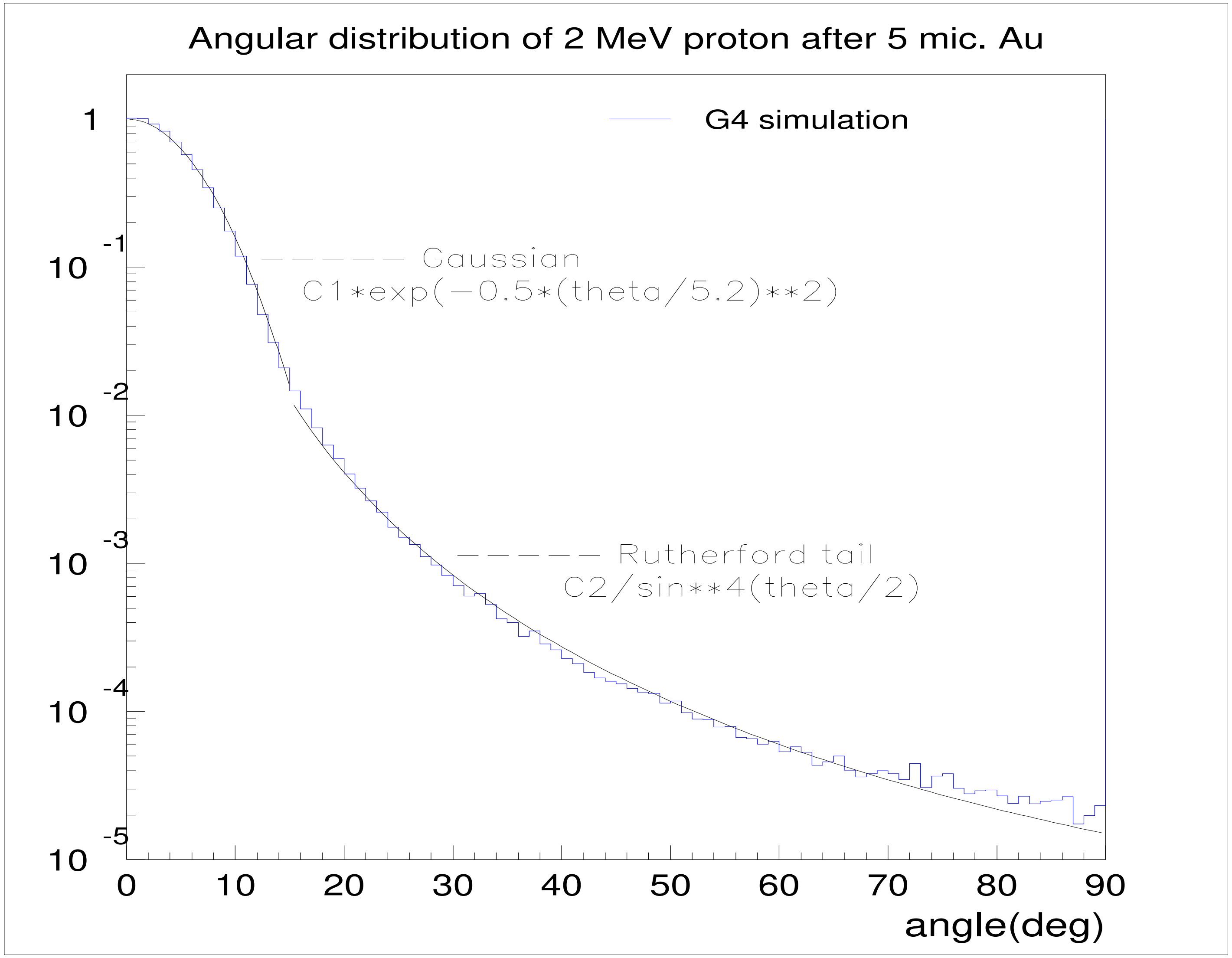
Multiple Coulomb scattering

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]

Illustration (Rutherford scattering)



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],[Lynch91]).

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.

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

Physics input of the model

first transport mean free path :

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

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.

Model functions - 1. transformation $t \Longrightarrow l$:

$$F(t, \lambda) = C u^{\xi} (1 - u) \tag{3}$$

where $u = l/t$ $0 \leq u \leq 1$, C is a normalization constant . From the theory we have

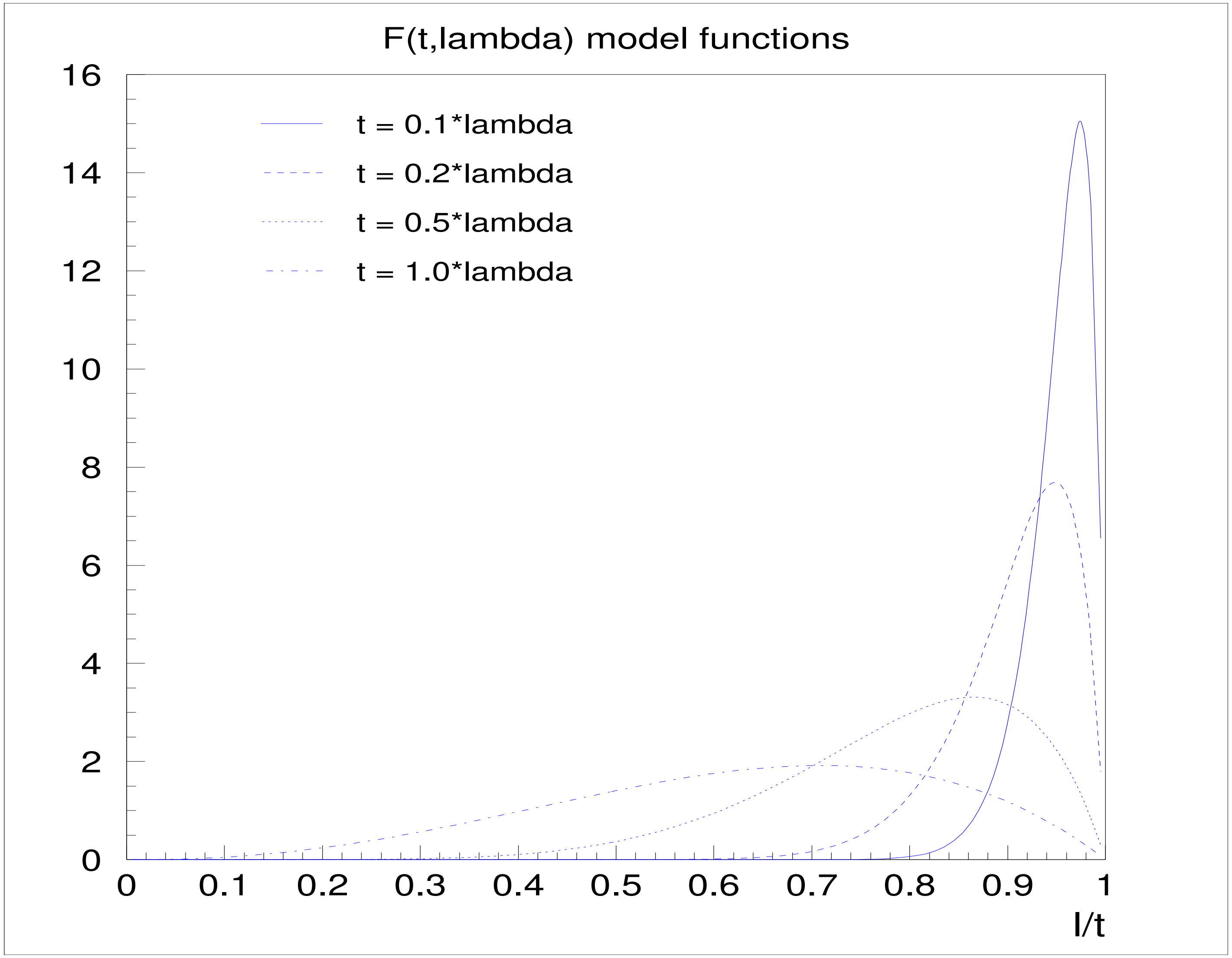
$$< l >= \lambda(1 - e^{t/\lambda}) \tag{4}$$

Eqs. 3 and 4 can be used to compute ξ:

$$\xi = \frac{3 < l > -t}{t - < l >} \tag{5}$$

The function is shown in the next slide for diff. t values.

Illustration: $F(t, \lambda)$



Model functions - 2. Angle distribution : θ is sampled from the model distribution $f(x,t,\lambda)$ $(x = cos\theta)$.

$$f(x,t) = q * \{p * f_1(x,t,\lambda) + (1-p) * f_2(x,t,\lambda)\} + (1-q) * f_3(x,t,\lambda) \tag{6}$$

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

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

$$f_1(x,t,\lambda) = C_1 * e^{-a(1-x)} \qquad x \in [x_0,\ 1] \tag{7}$$

$$f_2(x,t,\lambda) = C_2 \frac{1.}{(b-x)^2} \qquad x \in [-1,\ x0] \tag{8}$$

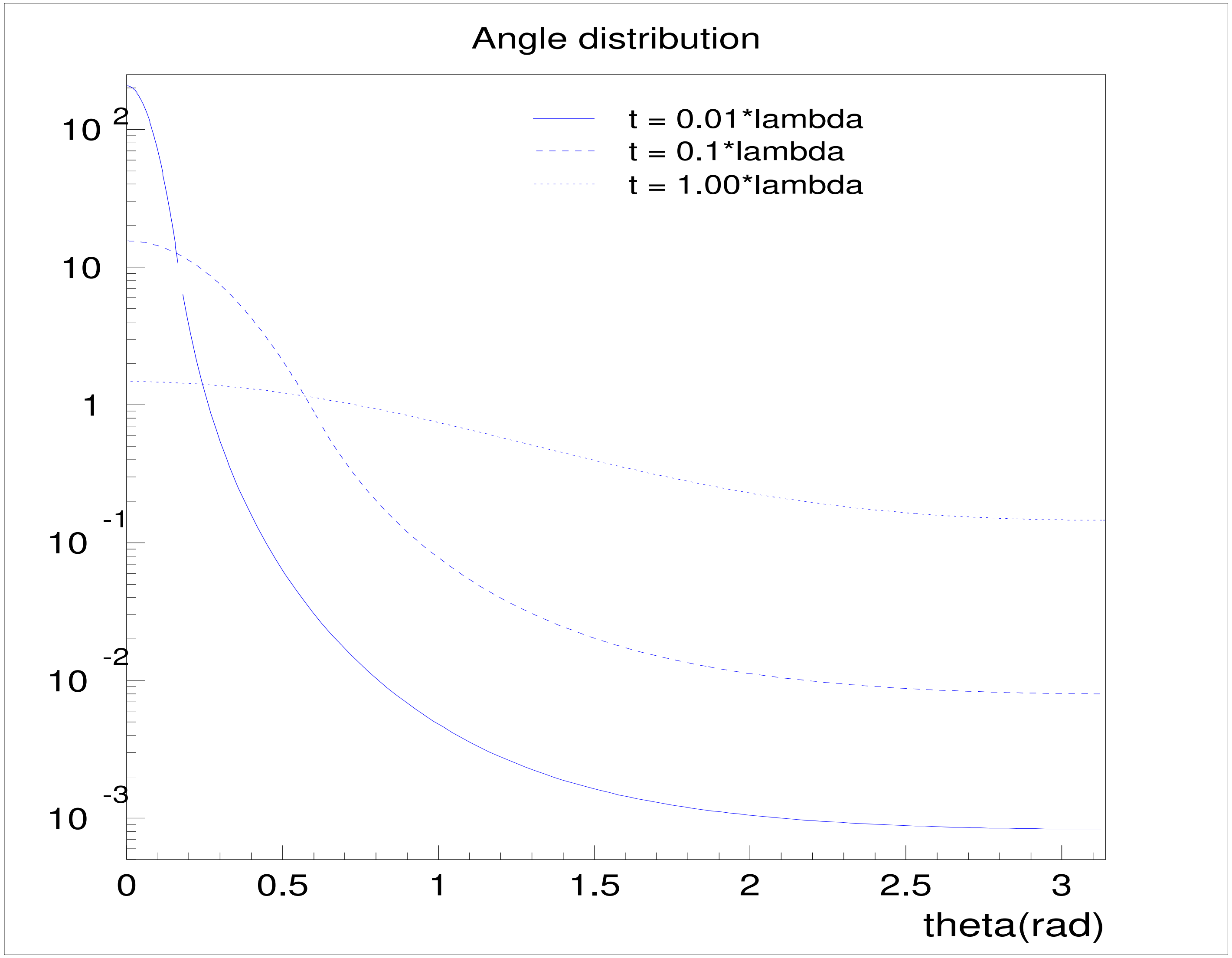
$$f_3(x,t,\lambda) = \frac{1}{2} \qquad x \in [-1,\ 1] \tag{9}$$

a, b, x_0 and the weigths p, q are parameters of the model. The parameters determined from the conditions:

- $f(x,t)$ should be continuous at $x = x_0$
- 1st derivative of $f(x,t)$ should be continuous at $x = x_0$
- the mean value of x should agree with the value given by theory

$\Longrightarrow$ there are 2 independent parameters only:
We have chosen the parameterization $a = a(t/\lambda) = a(\tau)$ and $x_0 = 1 - 3/a$. The form of the function $a(\tau)$ has been determined from the requirement that the variance of $f(x,t)$ should agree with the theory. It is worth to note that $f_1 \approx$ Gaussian for small angle, f_2 has a Rutherford tail.

Illustration: $f(cos\theta, t)$



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

STEP 3, performed by PostStepDoIt() of MSC

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

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().

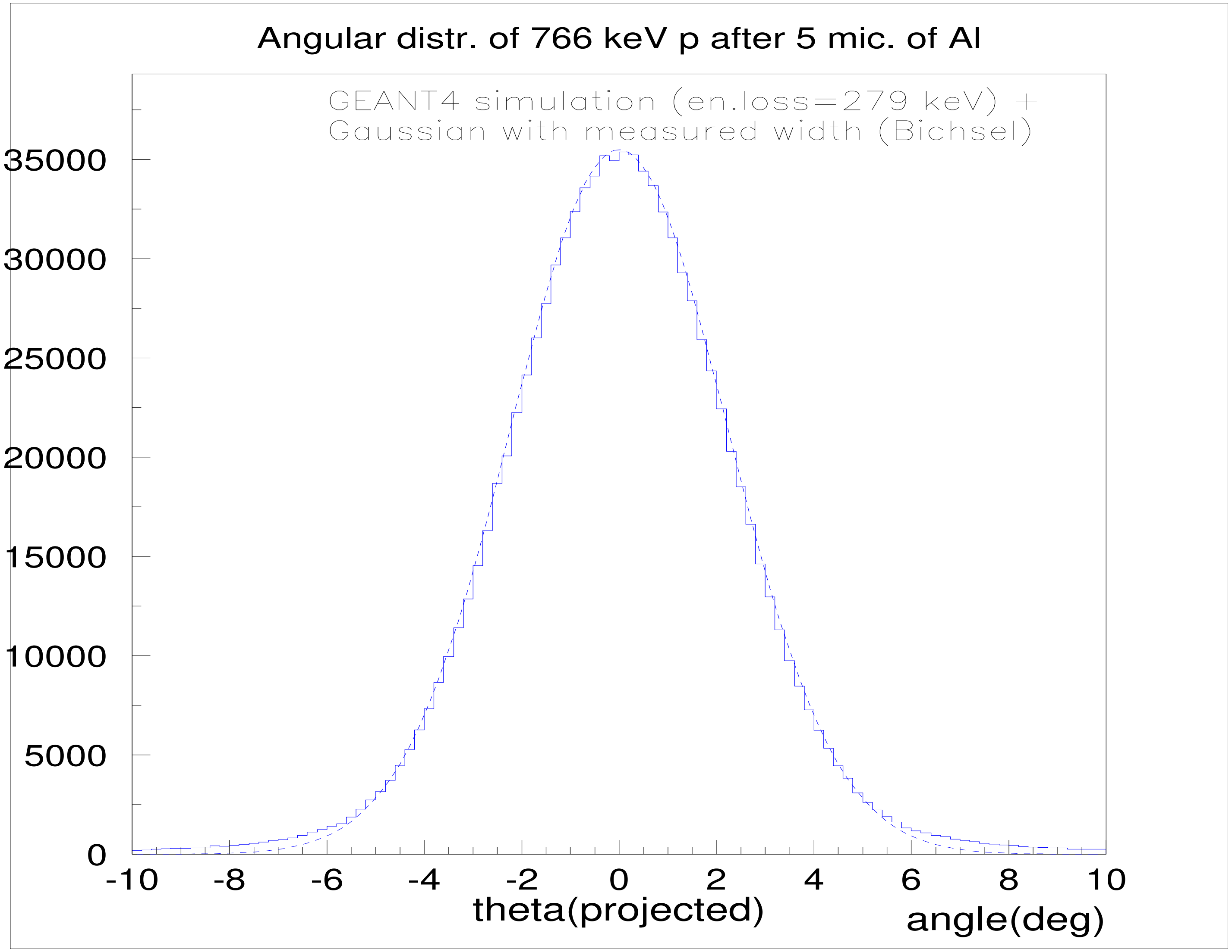
What is the task for PostStepGetPhysicalInteractionLength() ?

It sets only a ForceFlag in order to ensure that PostStepDoIt() is called at every step.

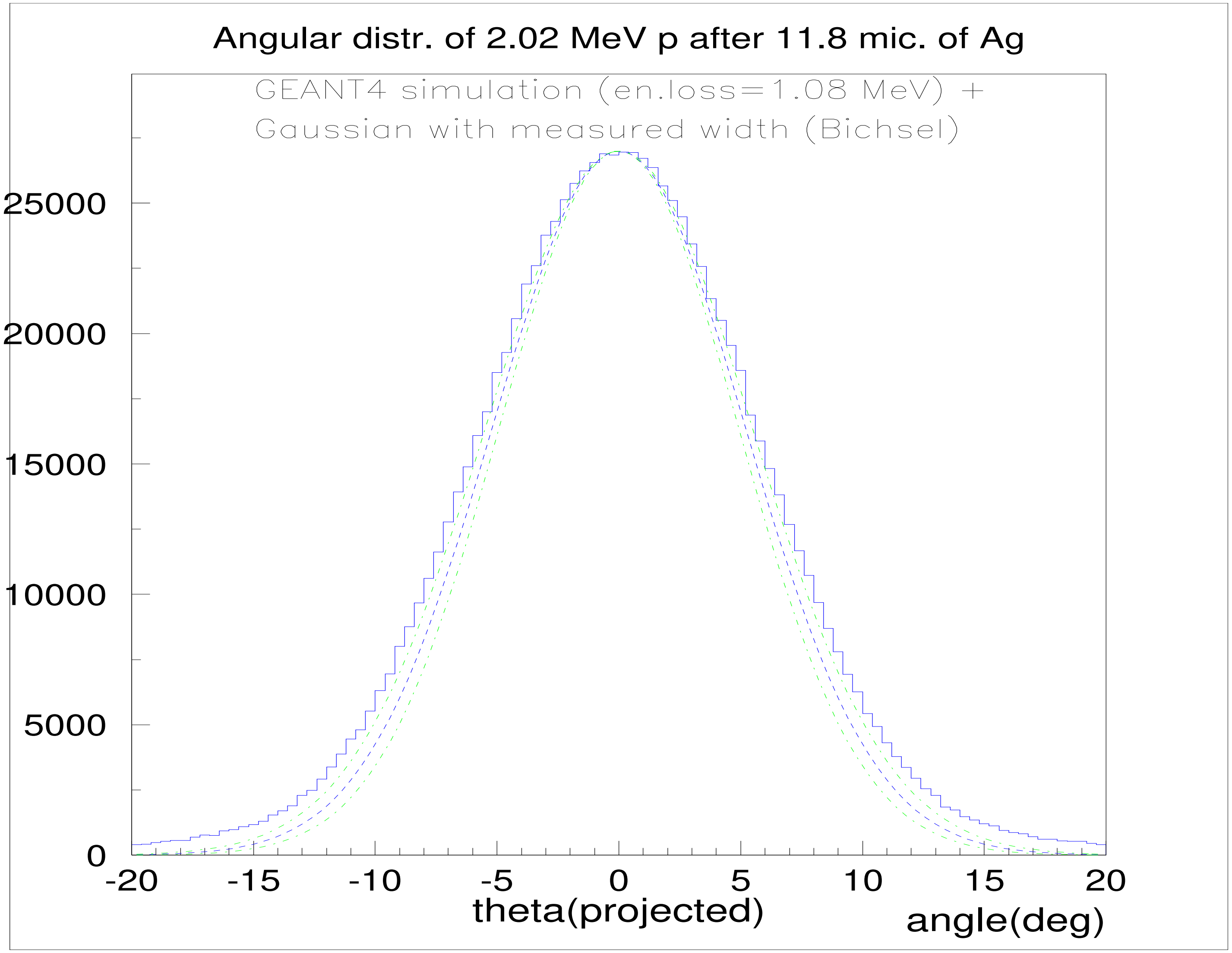
Simulation results $\Longleftrightarrow$ data, the ultimate test of the reliability of MC simulations

- 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.)
- .....

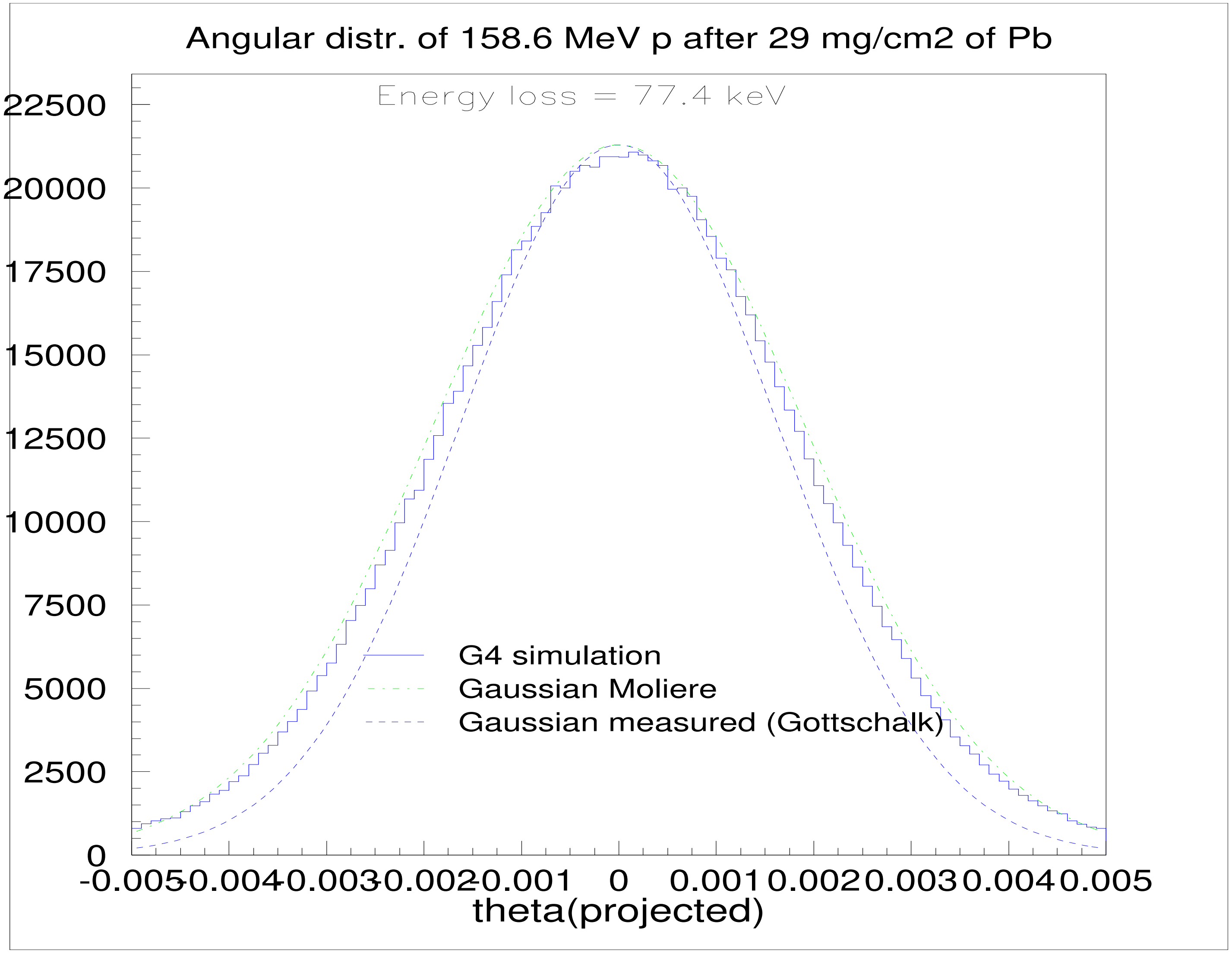
Angle distributions, low energy proton 1.



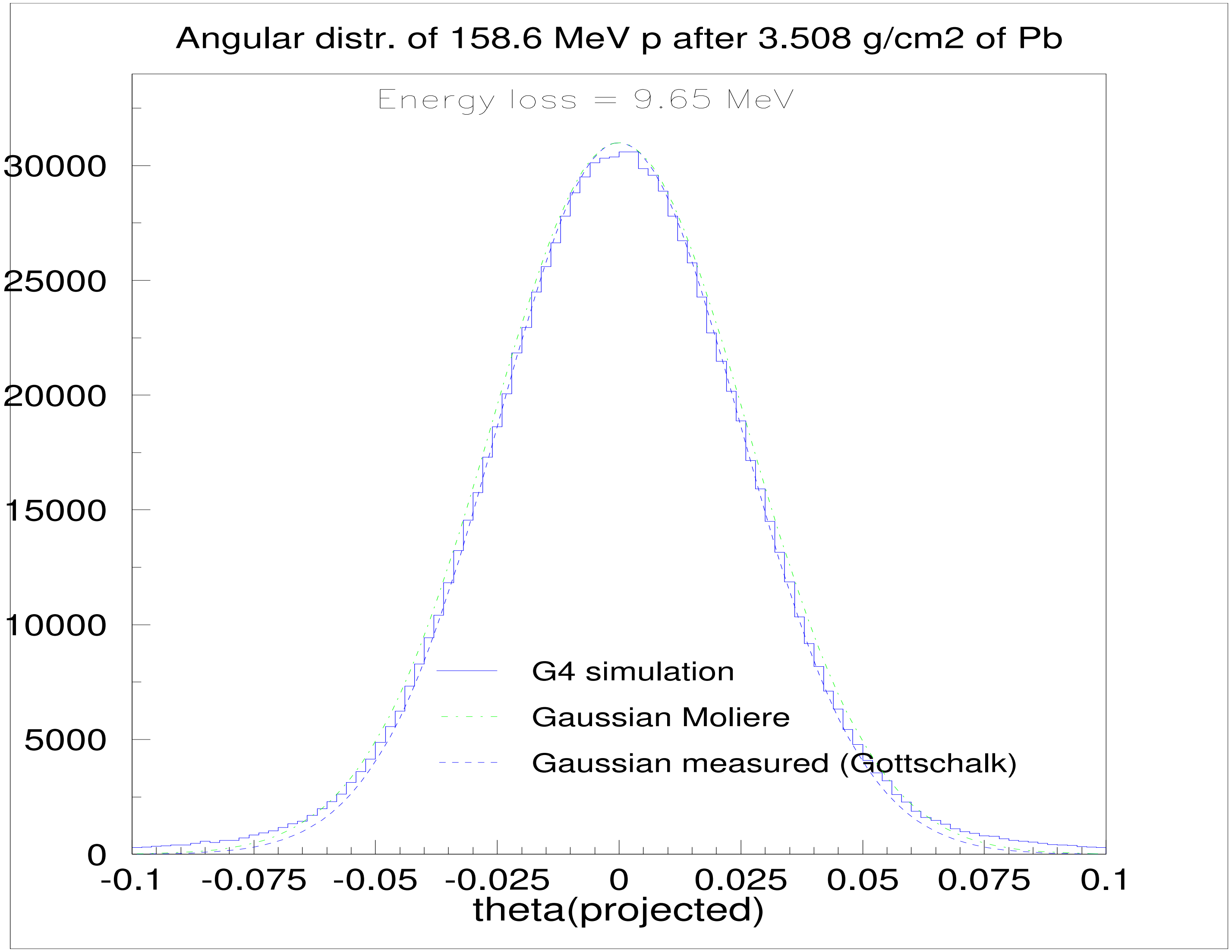
Angle distributions, low energy proton 2.



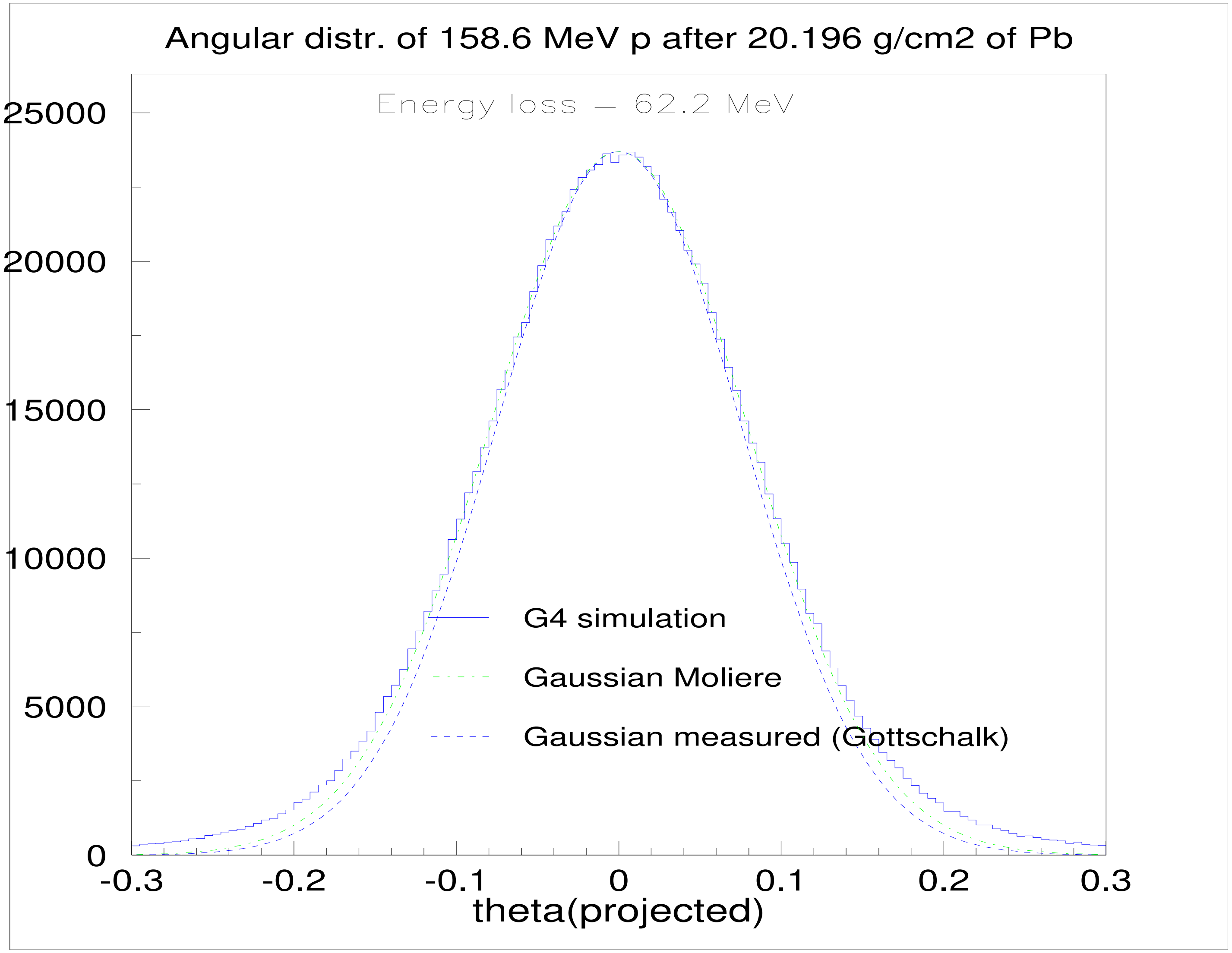
Angle distributions, 158.6 MeV p thin layer of Pb



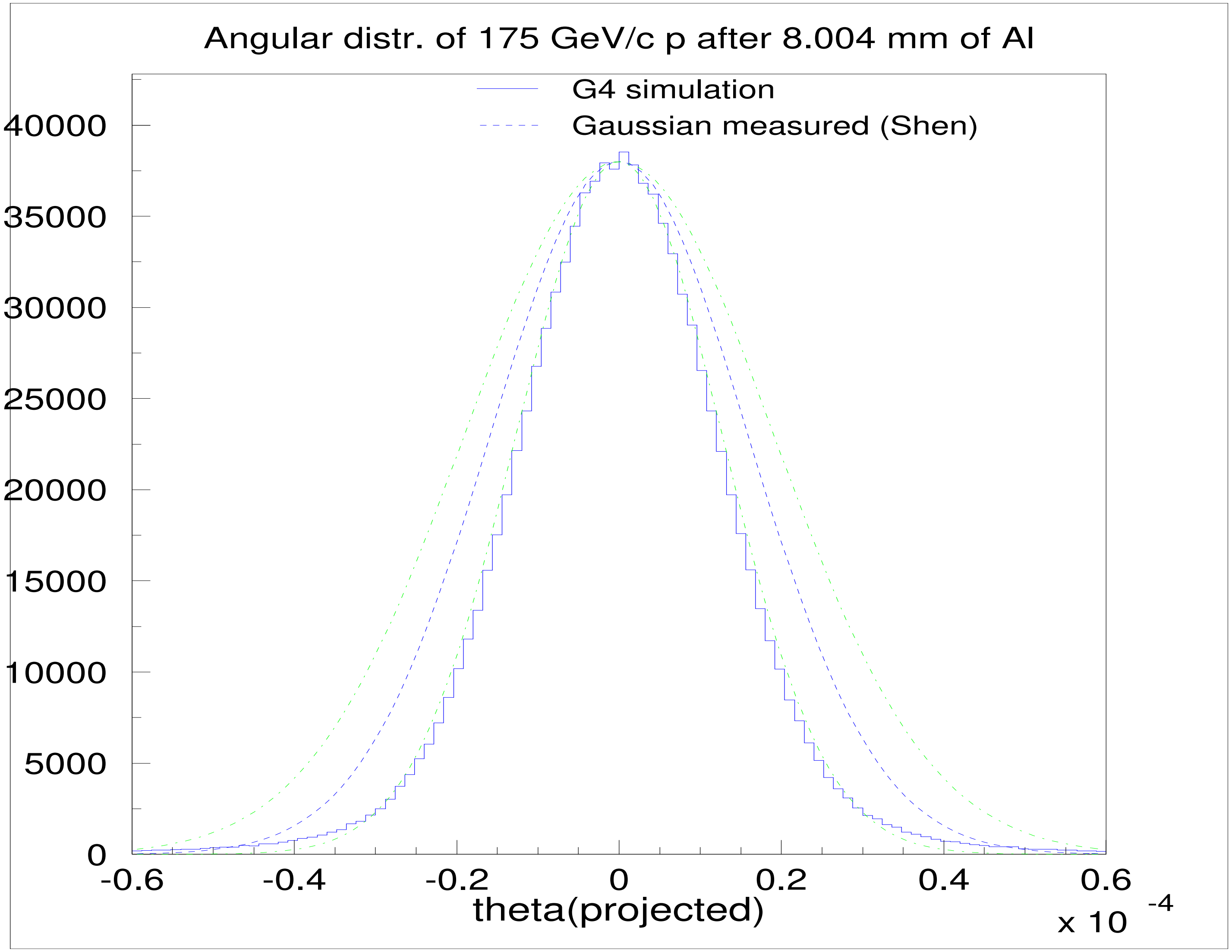
Angle distributions, 158.6 MeV p not so thin layer of Pb



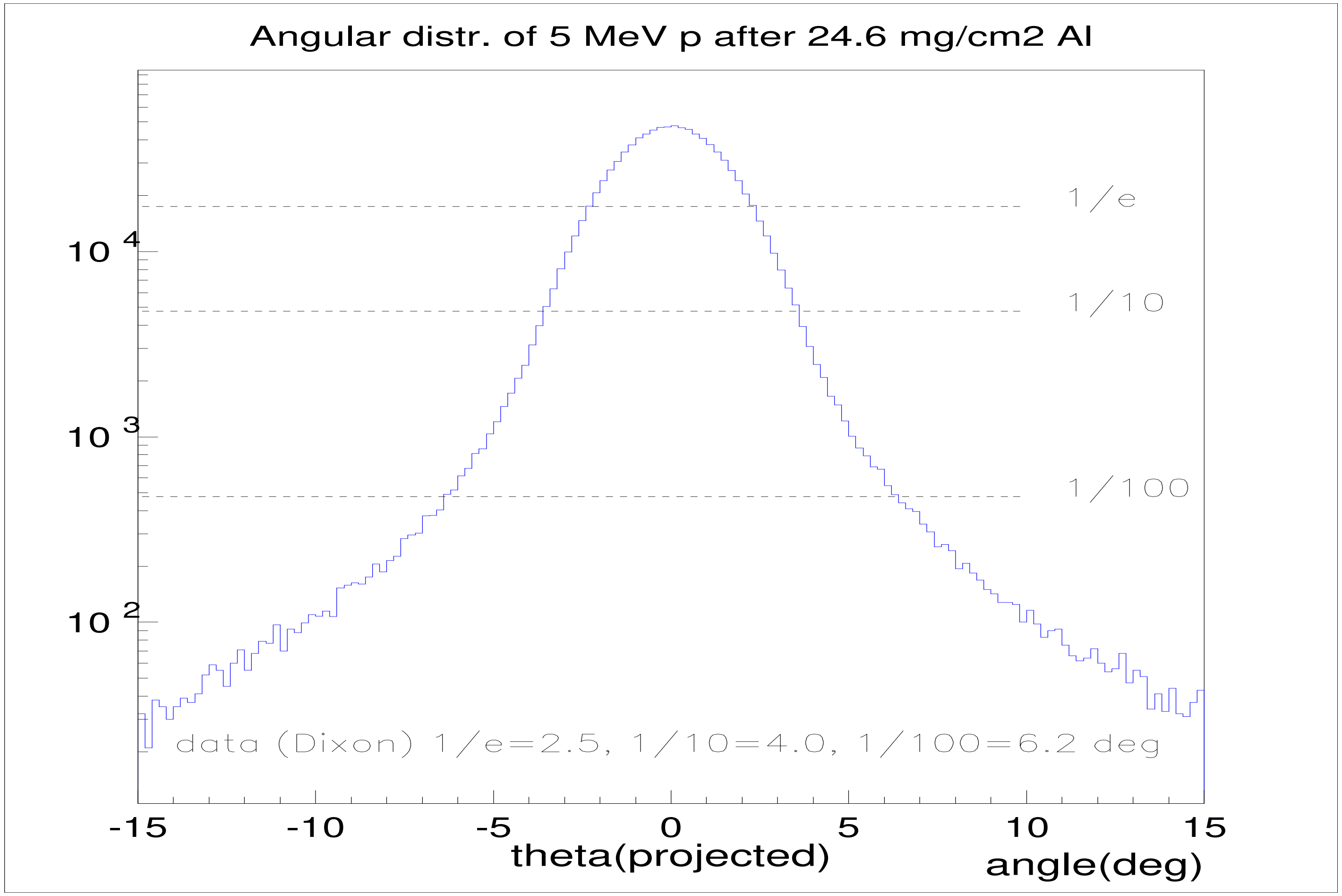
Angle distributions, 158.6 MeV p thick layer of Pb



Angle distributions, 175 GeV/c p 8 mm of Al

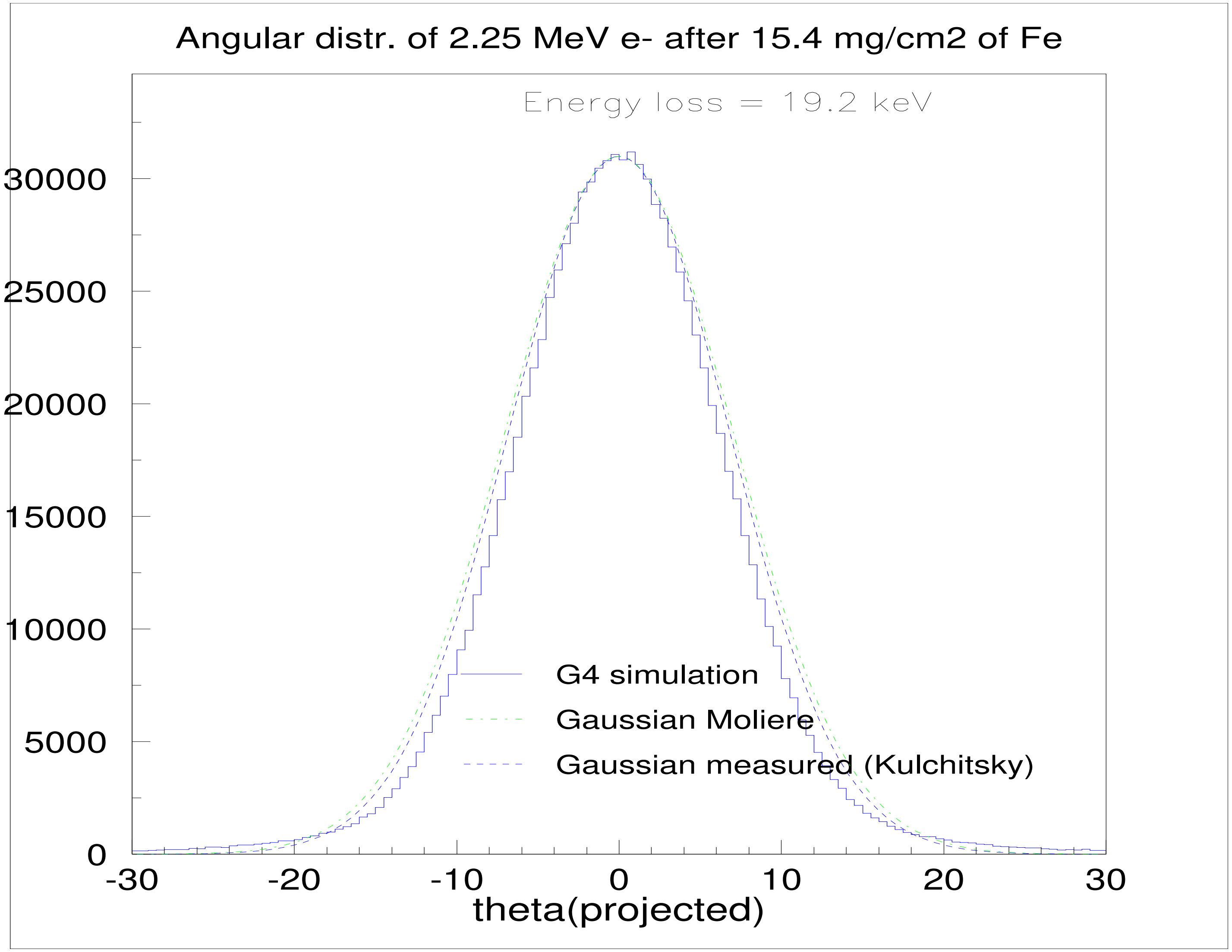


Angular distribution 5 MeV p, Al central part+some tail

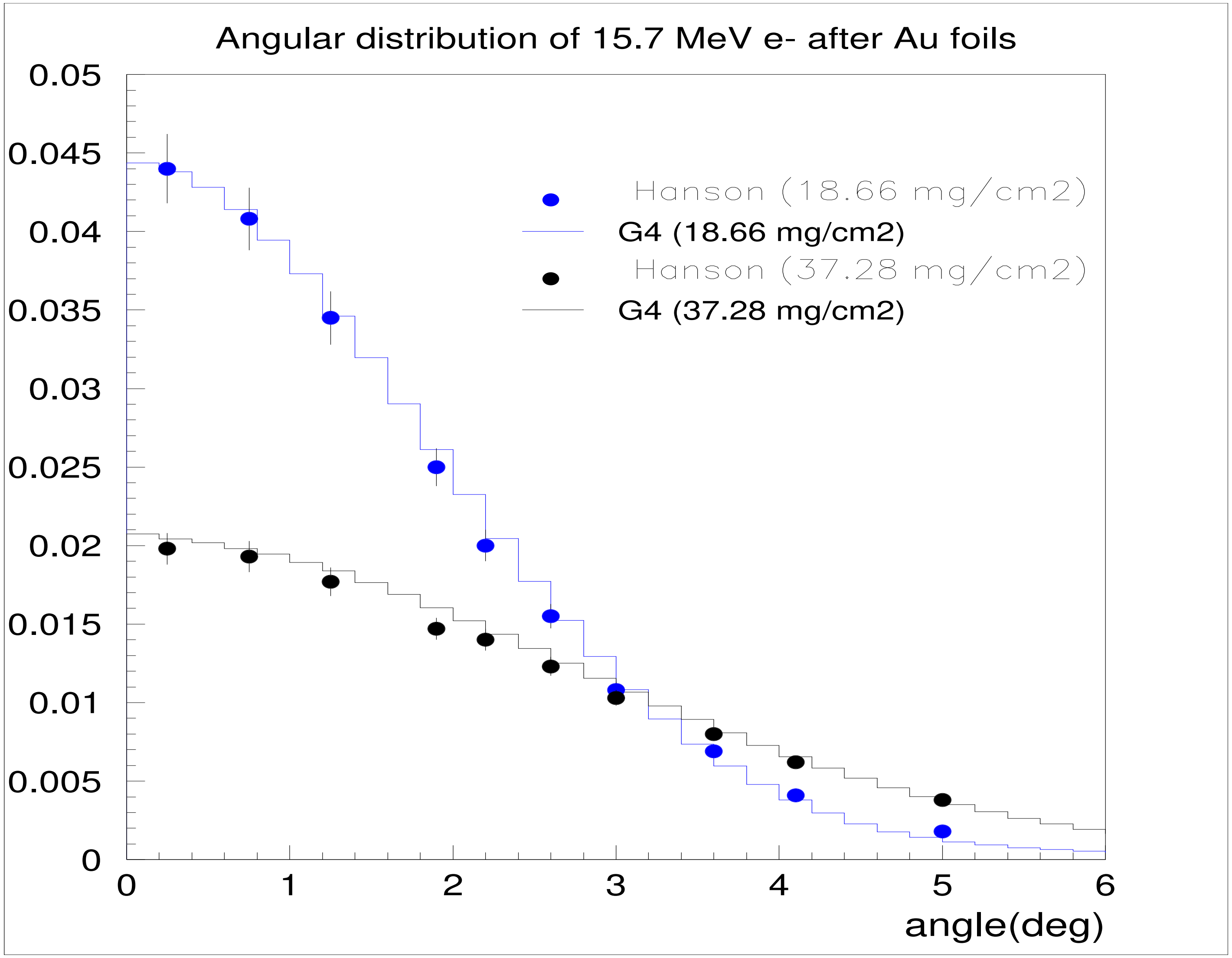


(error on data $\approx 5\%$).

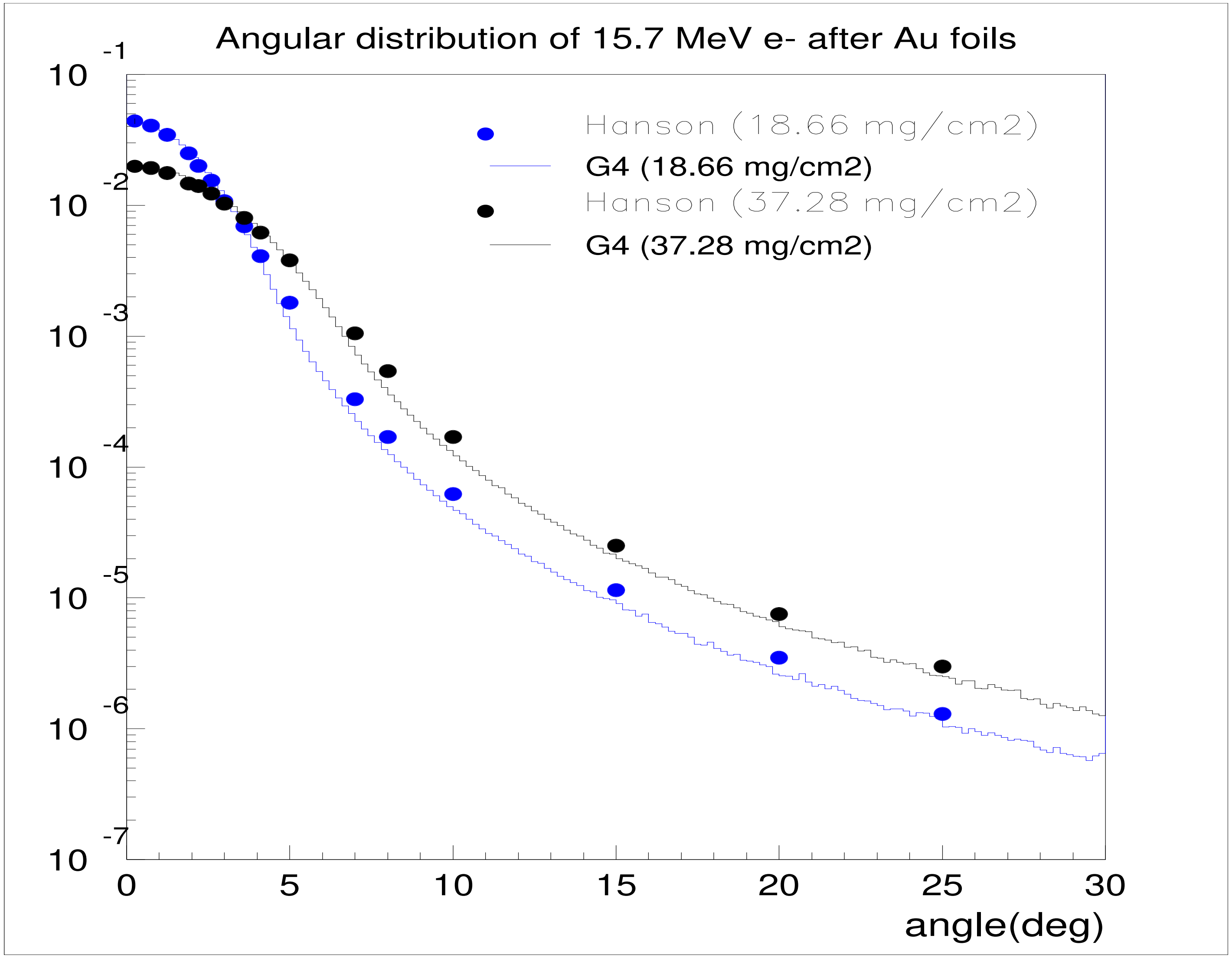
Angle distributions, 2.25 MeV e-, Fe



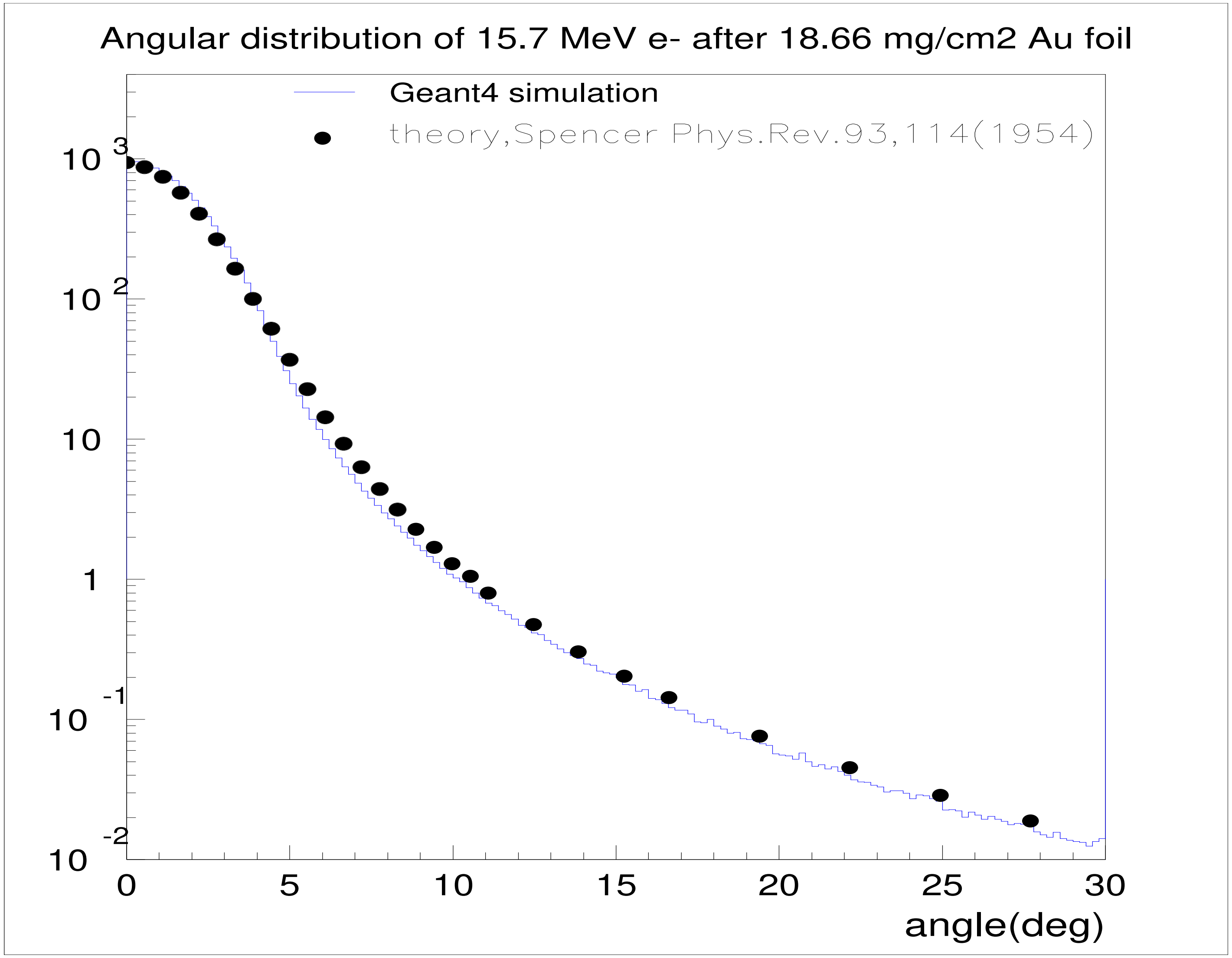
Angle distributions central part



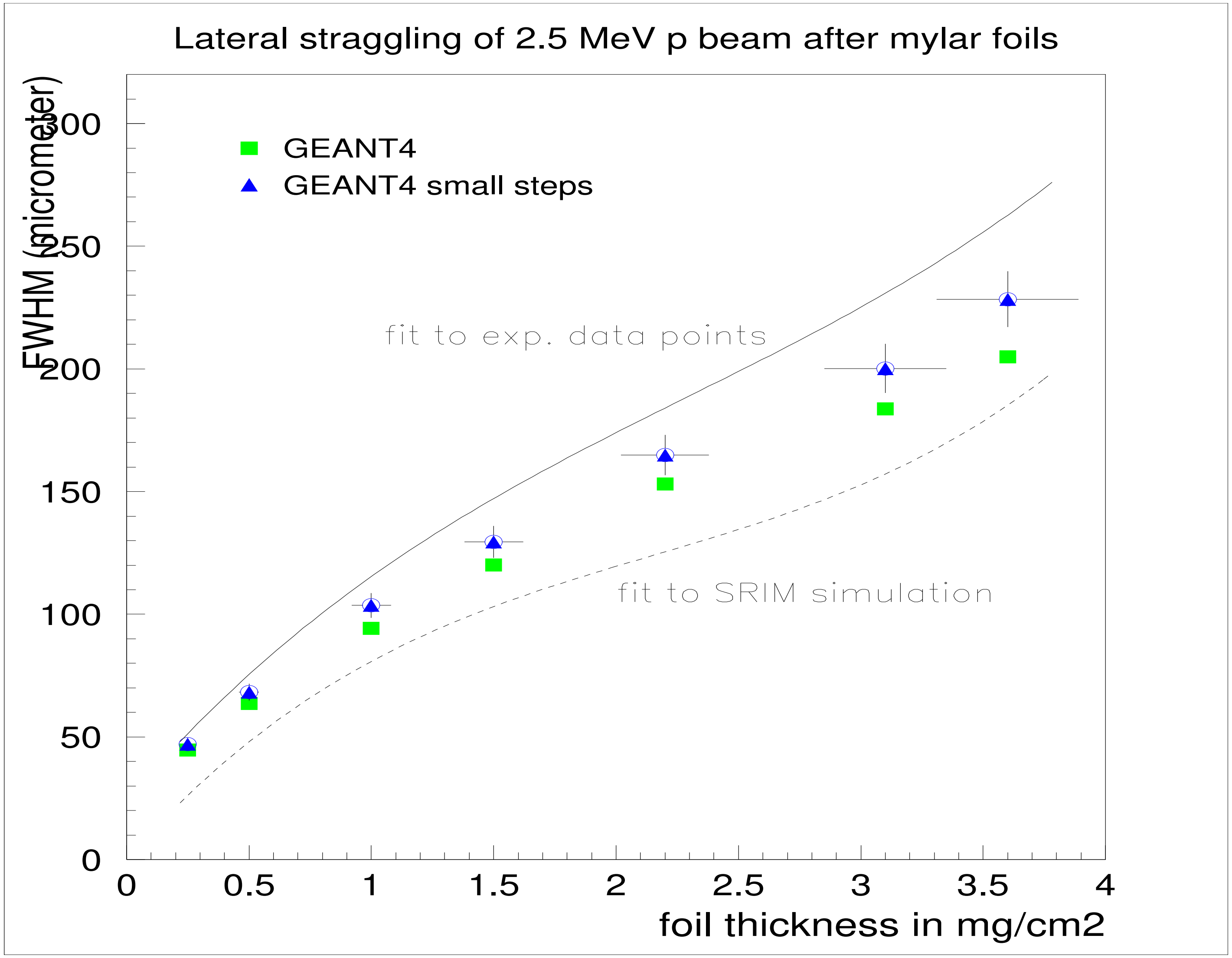
Angle distributions central part + tail



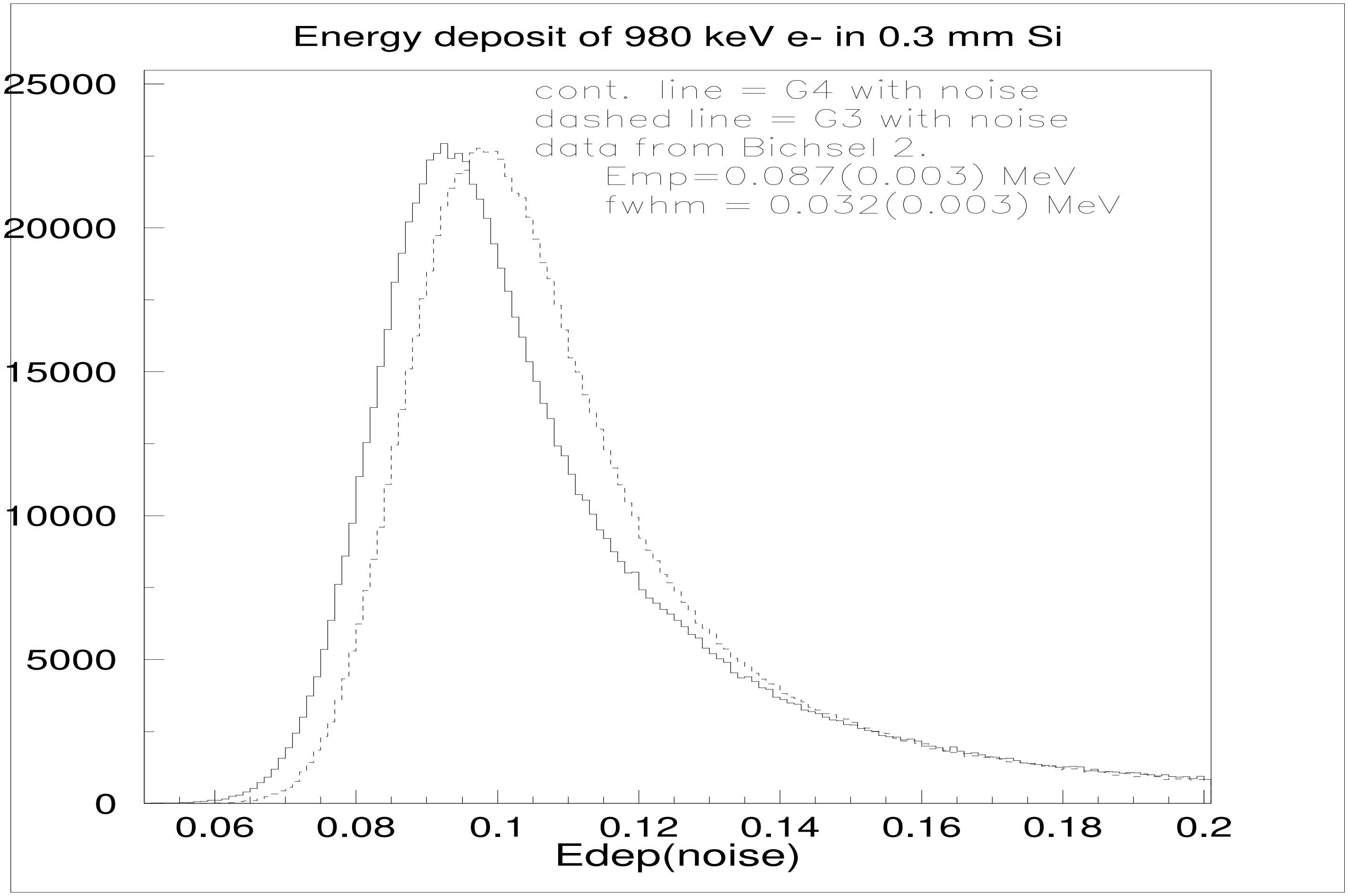
Angle distributions G4 + theory



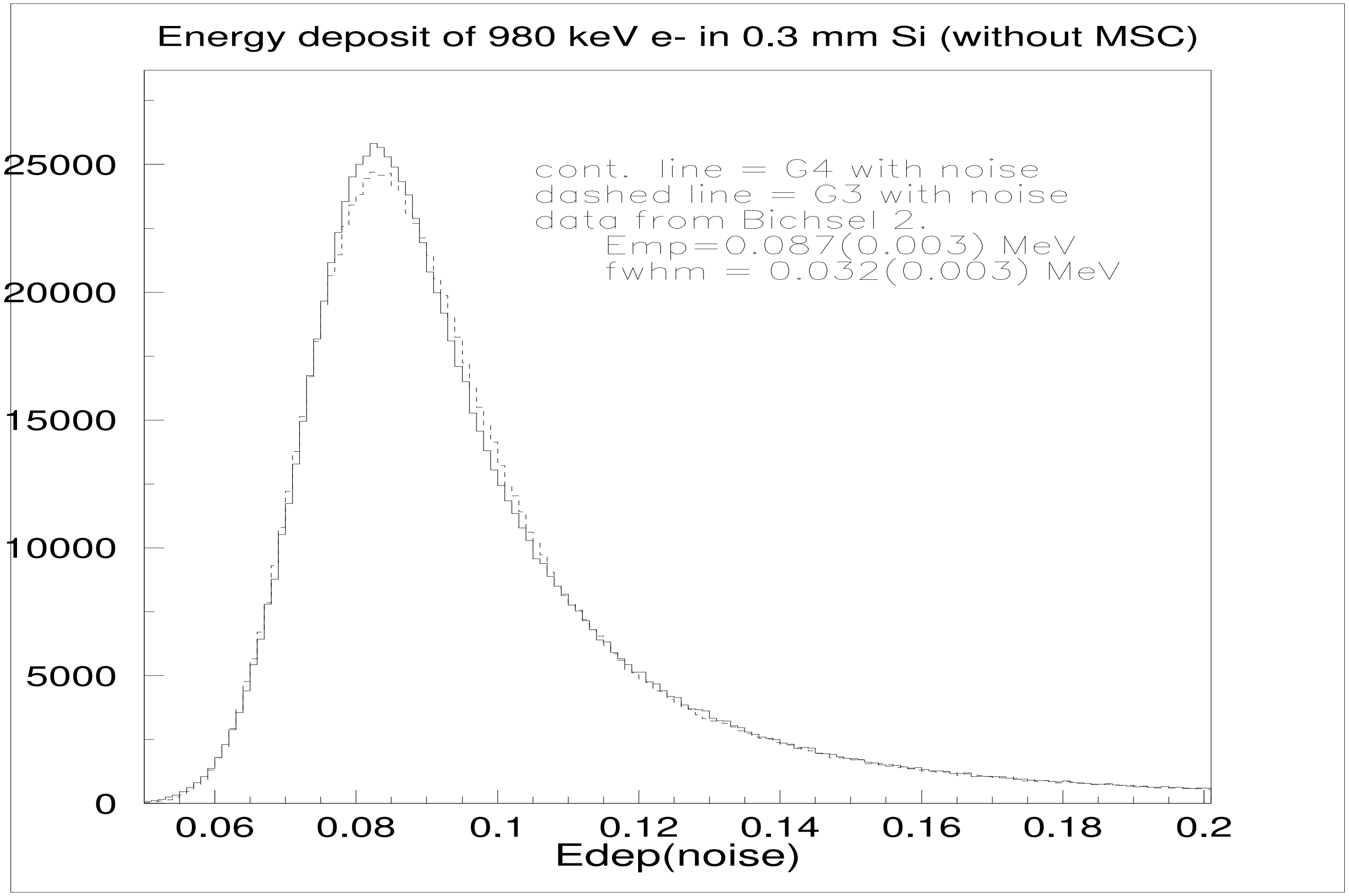
Lateral straggling of 2.5 MeV p after Mylar foils



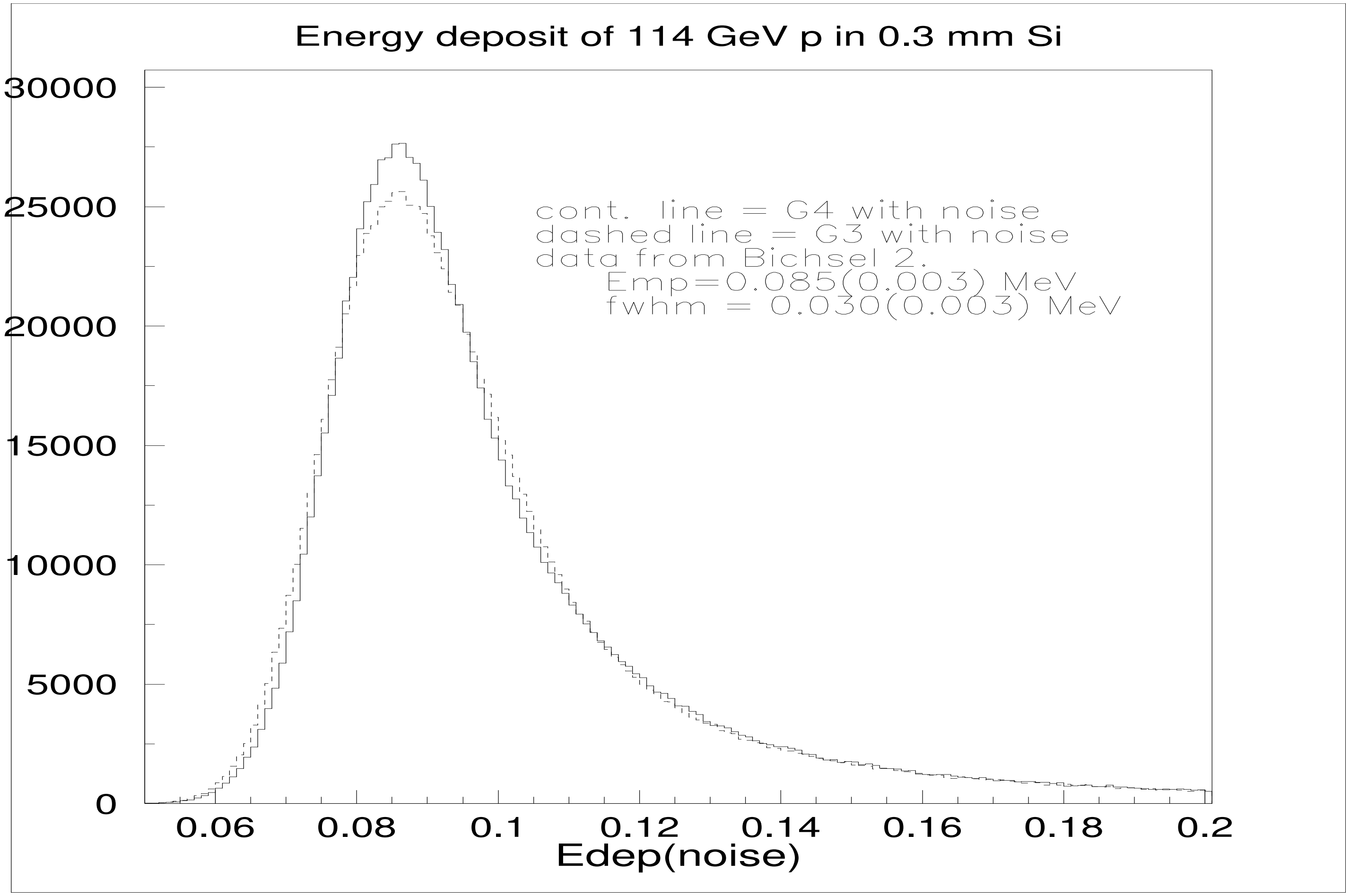
Energy deposit G4,G3,data



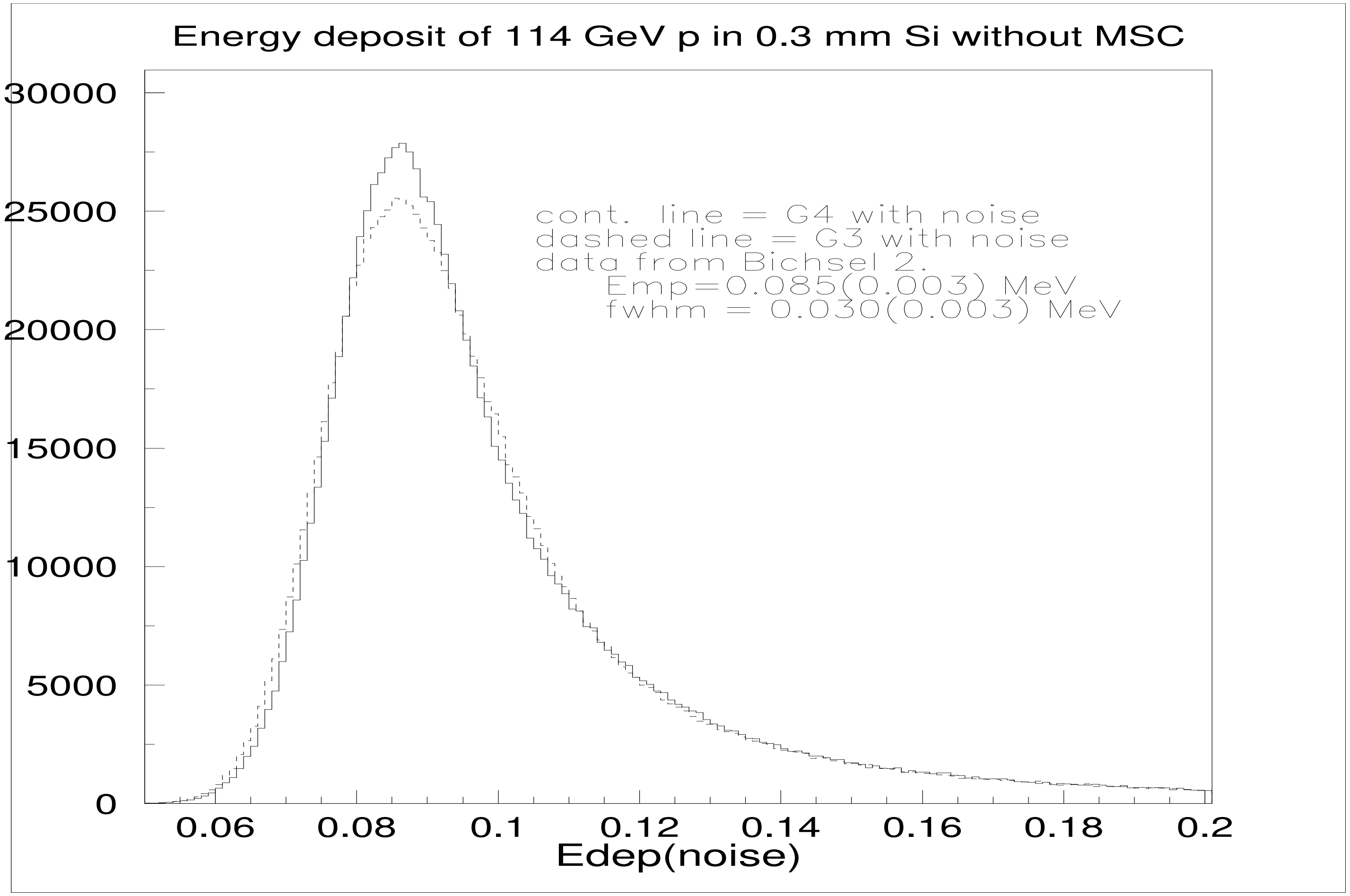
Energy deposit G4,G3,data without MSC



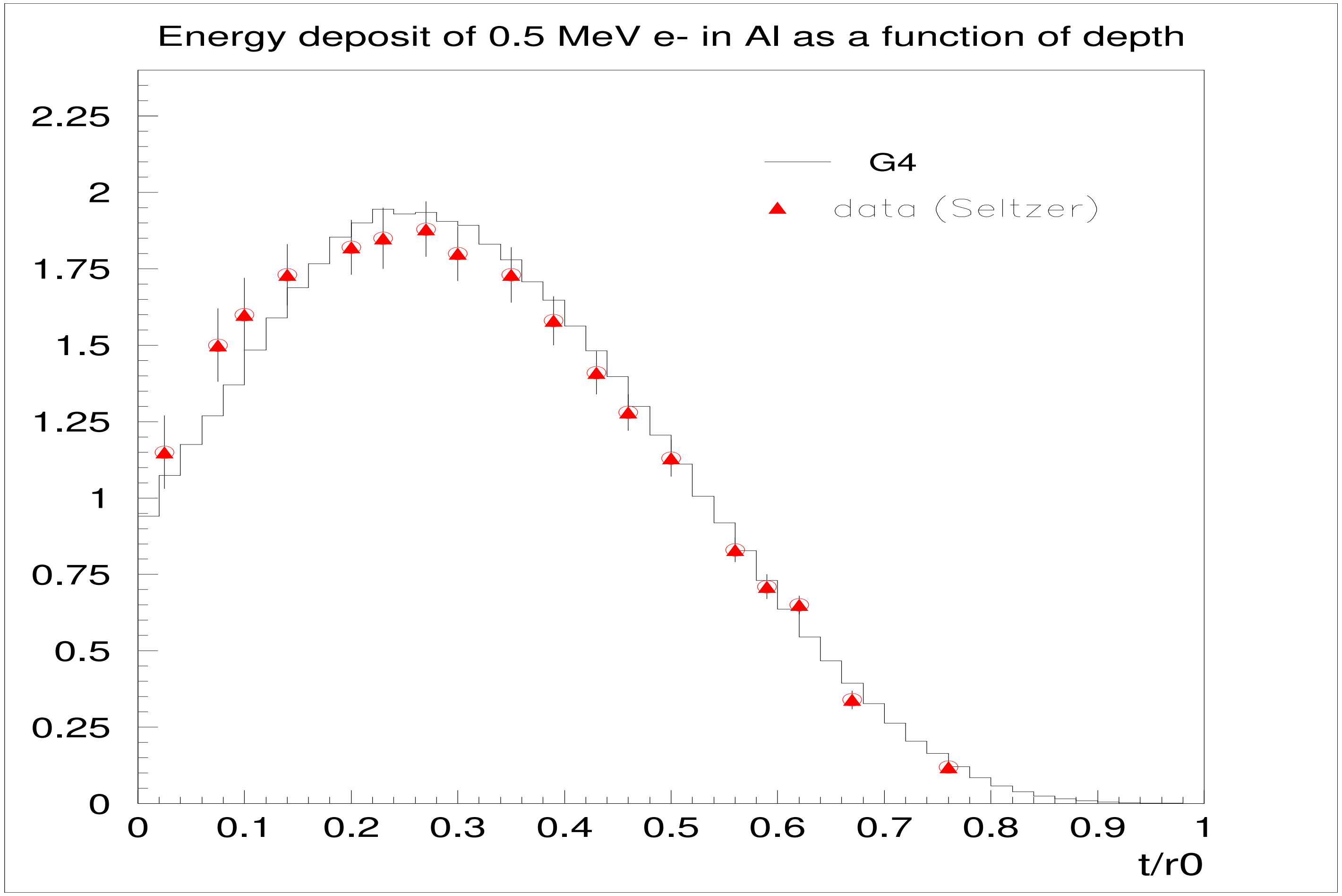
Energy deposit/2 G4,G3,data



Energy deposit/2 G4,G3,data without MSC

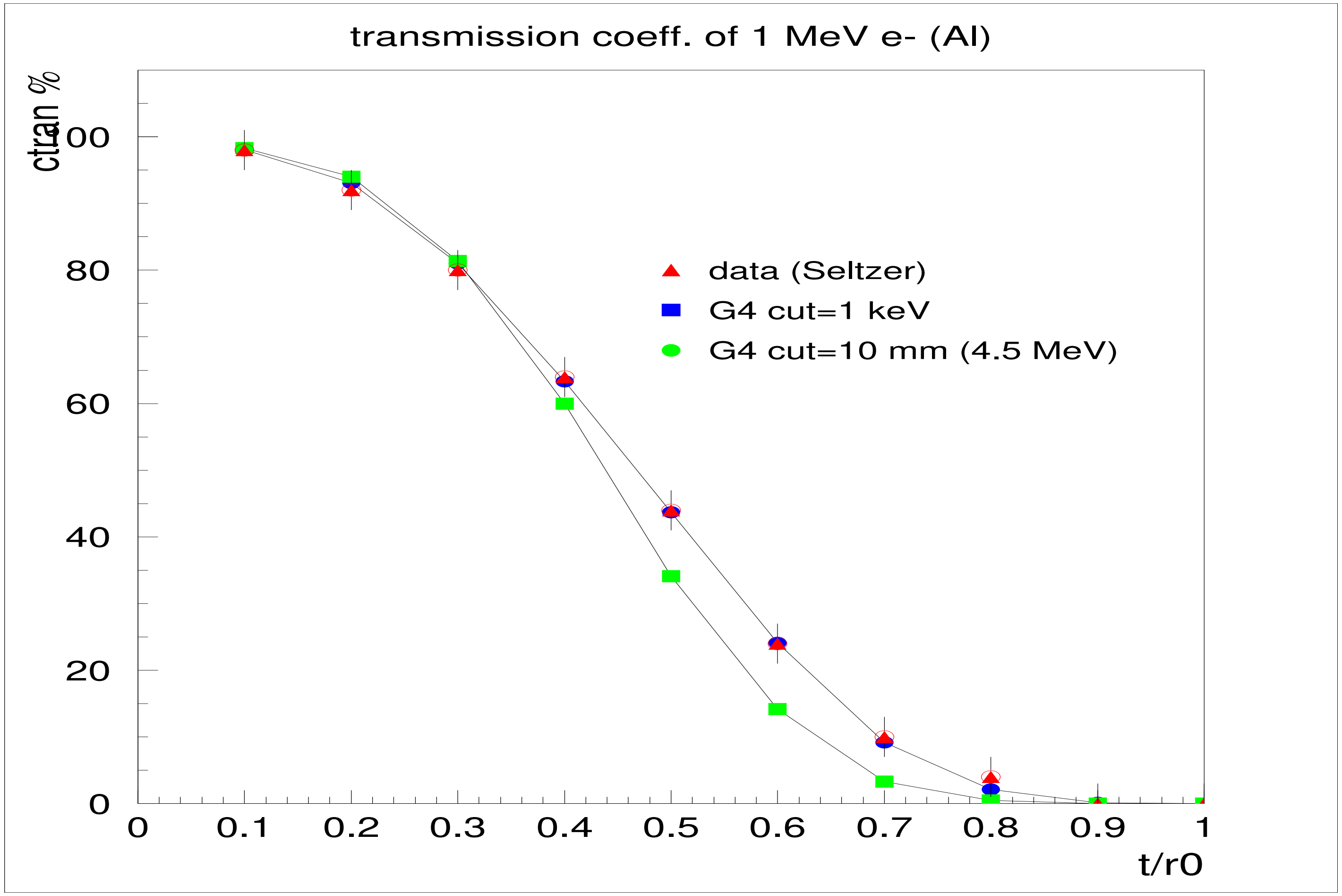


Depth-dose distribution



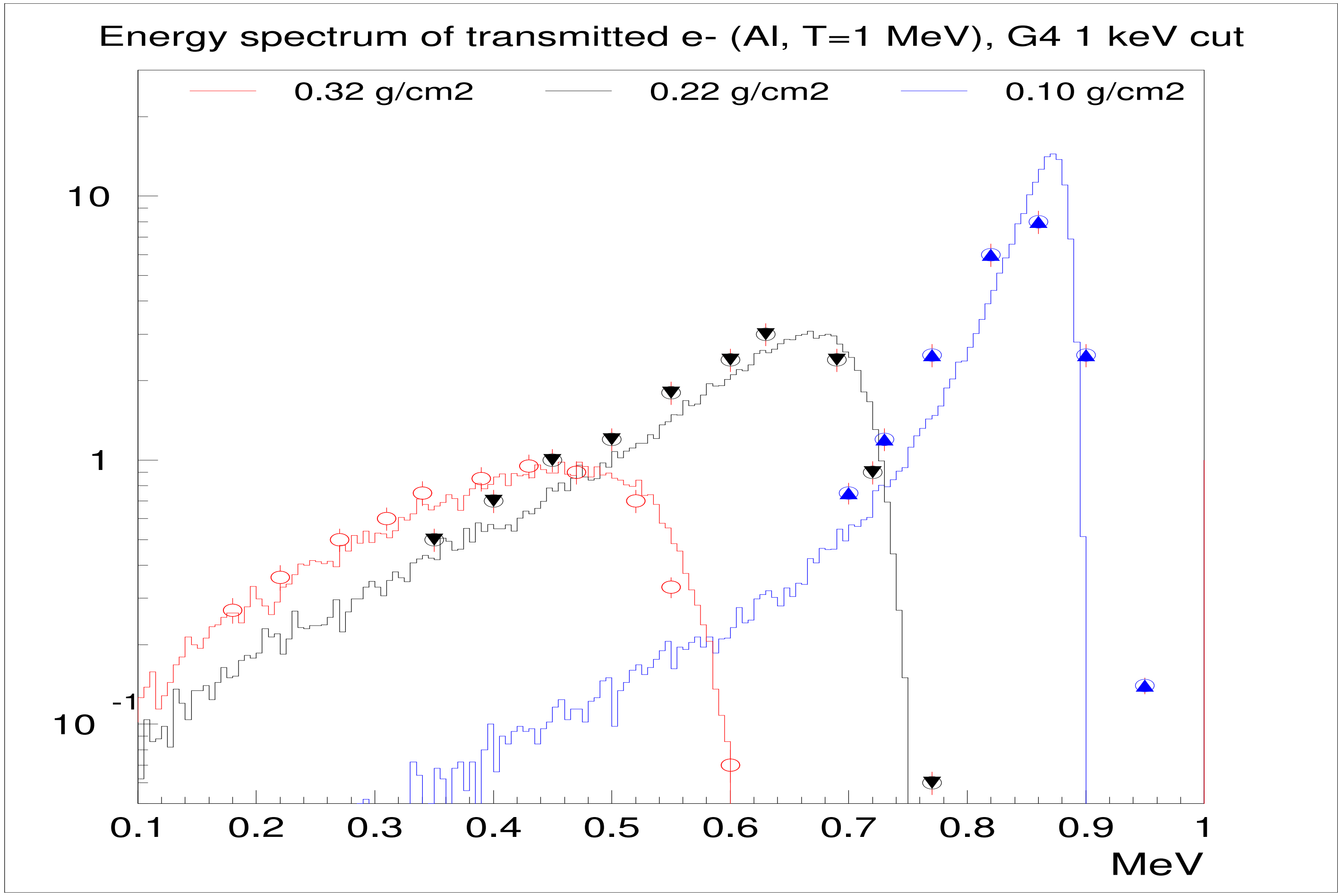
(error on data $\approx 5 - 10\%$).

Transmission of 1 MeV e- through Al layers



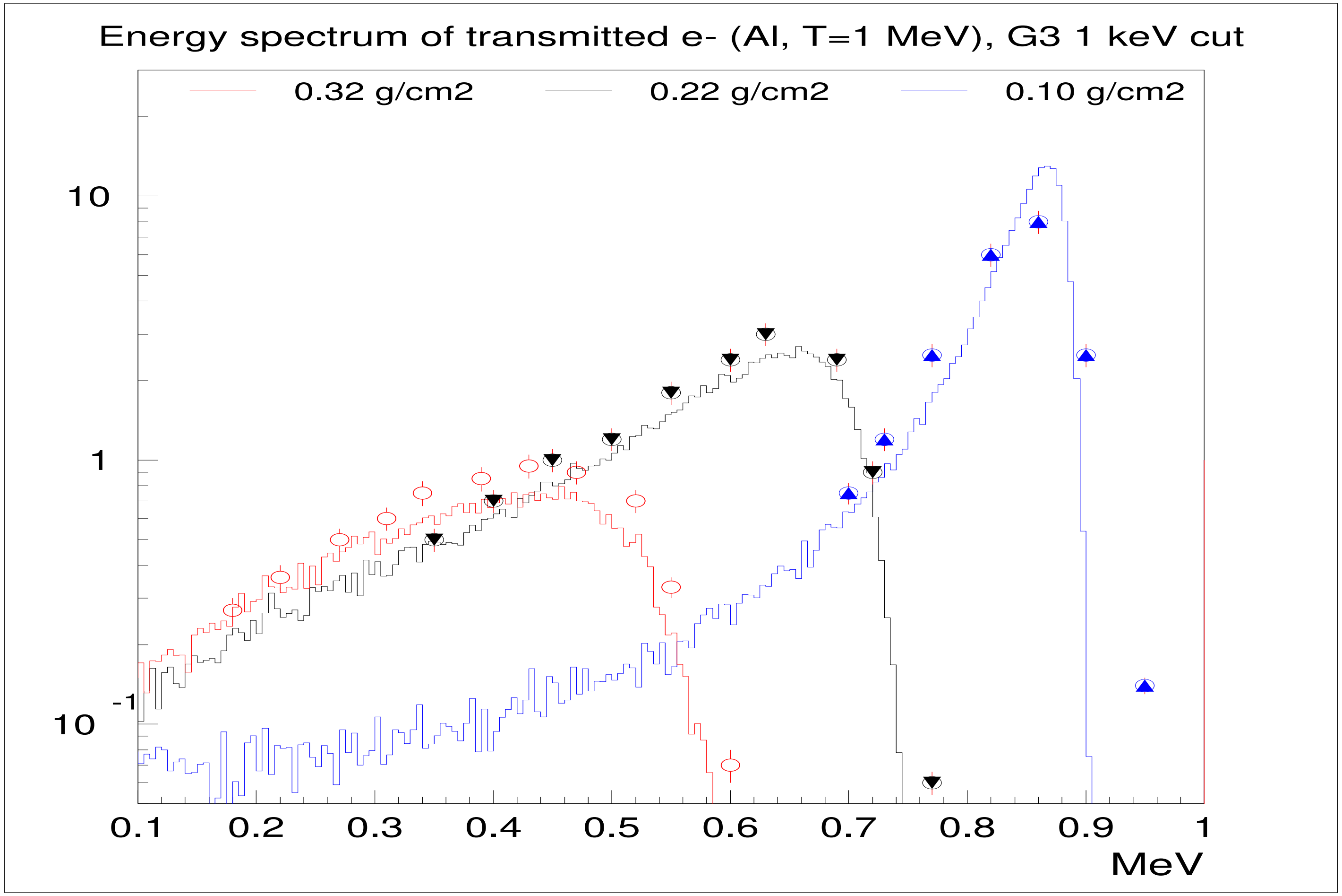
(error on data $\approx 5 - 10\%$).

Energy spectra of transmitted e-,Al



(data from Rester, error on data ≈ 10%).

Energy spectra of transmitted e-,Al,GEANT3



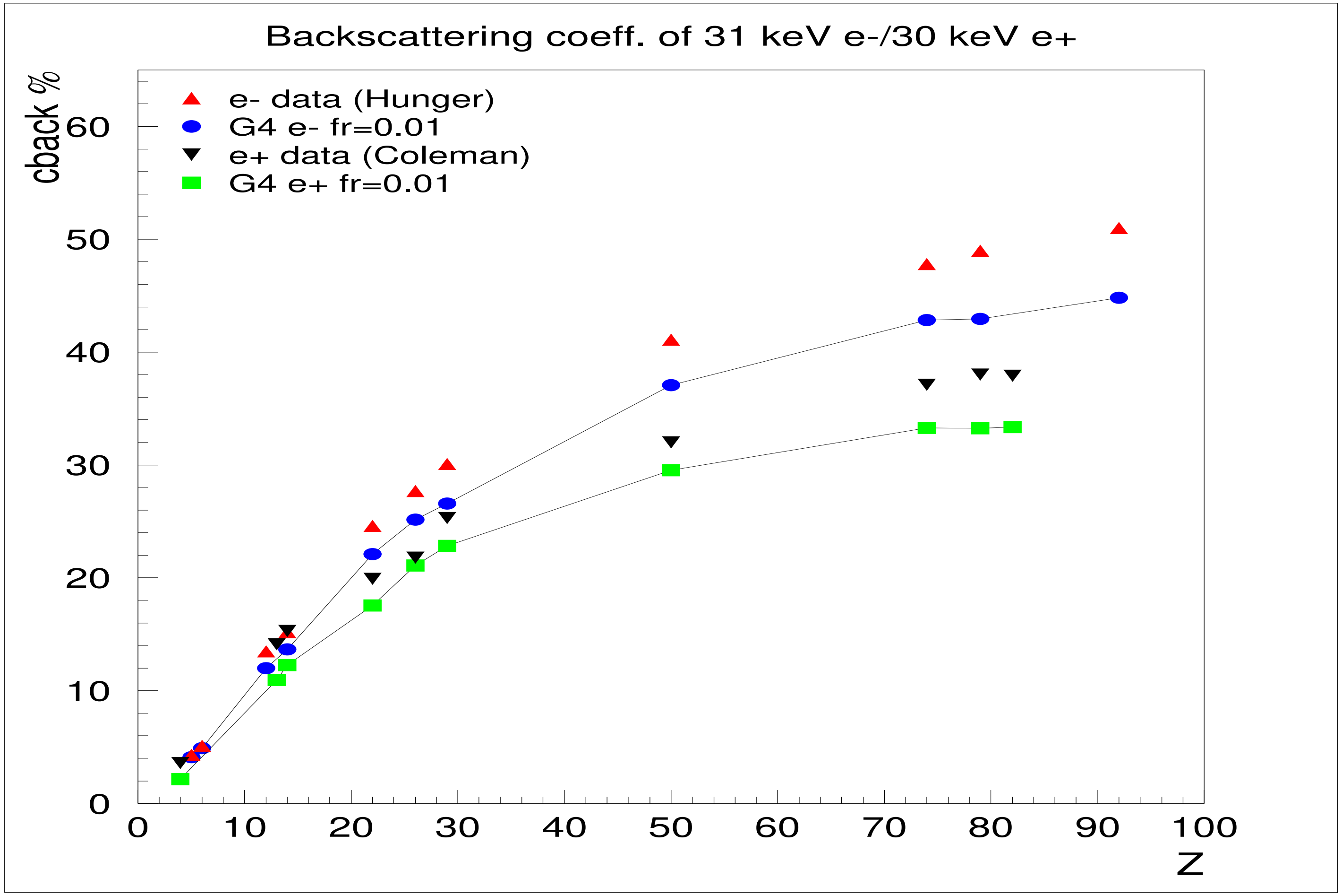
(data from Rester, error on data ≈ 10%).

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 !

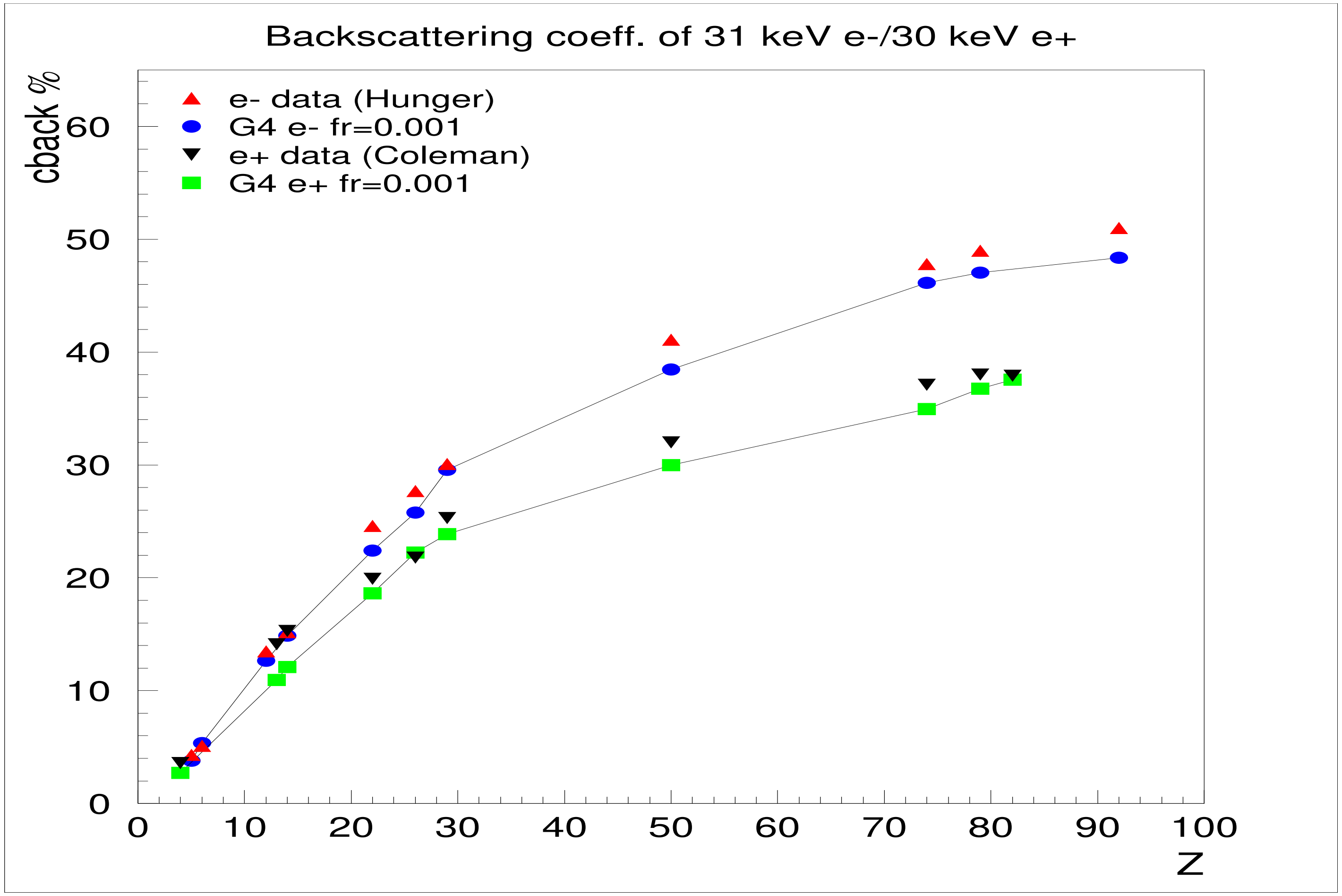
(Limiting the step length at boundaries is not enough, to get good backscattering we need good angle distribution as well!)

Backscattering of 31 keV e-/30 keV e+, diff. targets, fr = 0.01



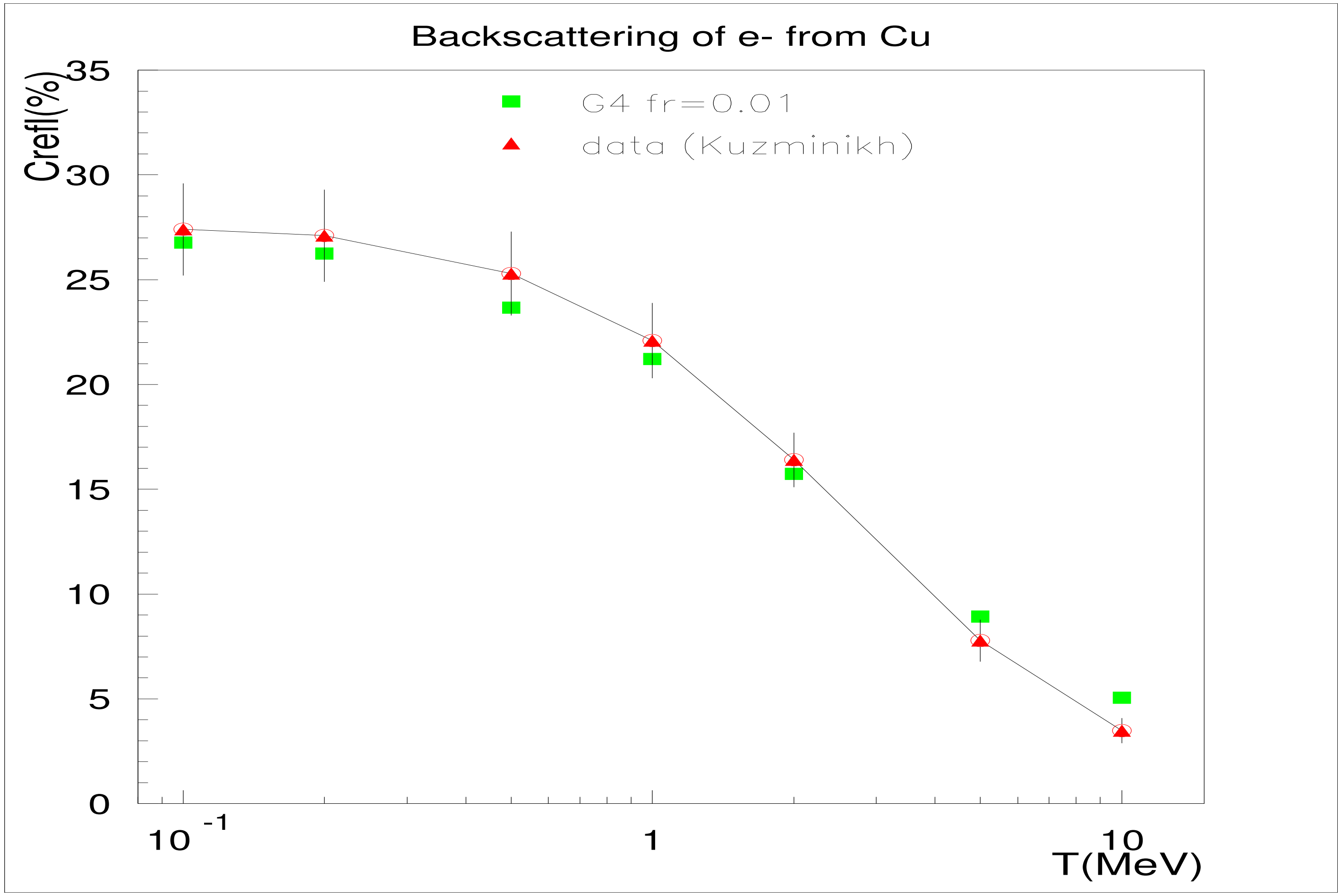
(error on data $\approx 2 - 5\%$).

Backscattering of 31 keV e-/30 keV e+, diff. targets, fr = 0.001



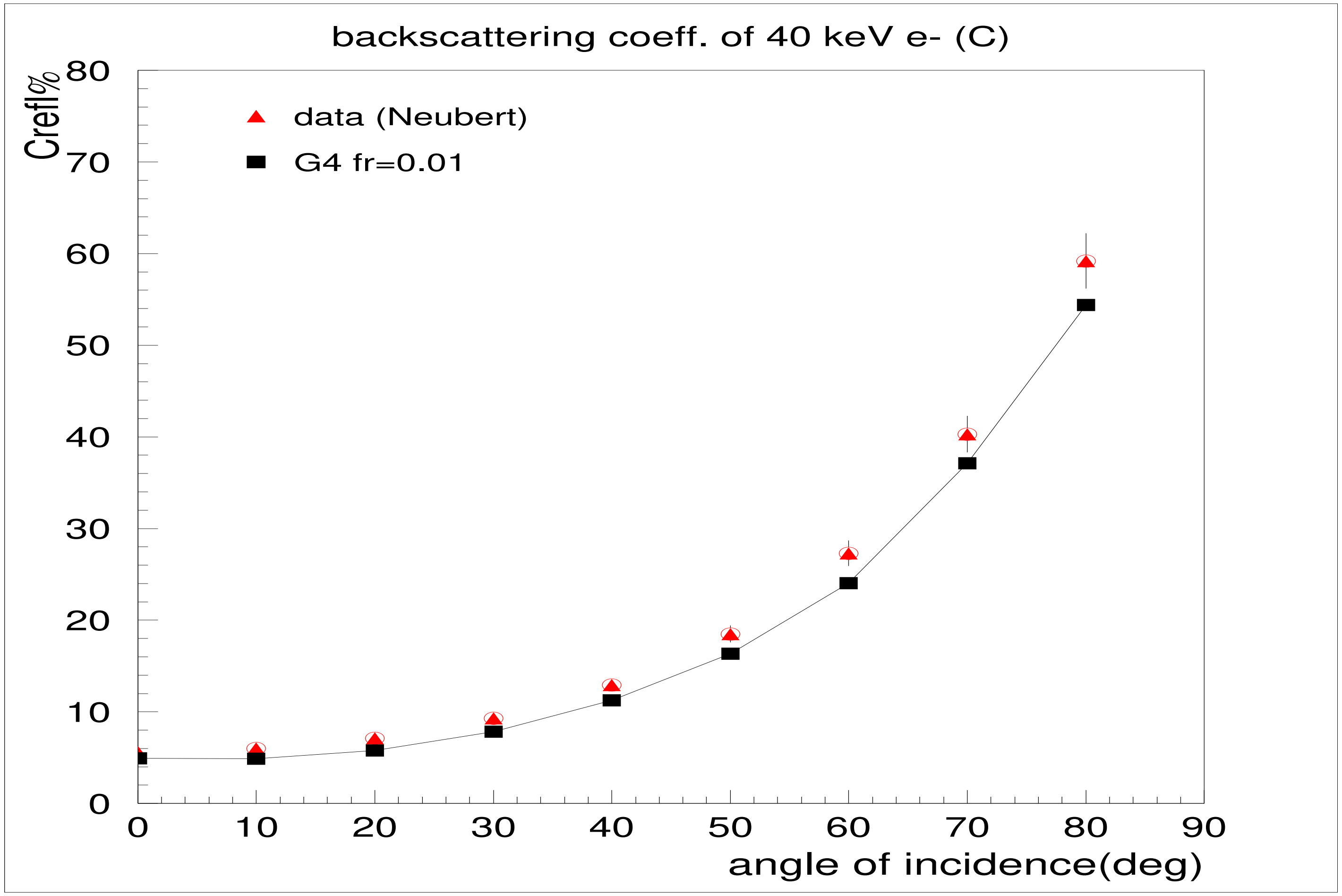
(error on data $\approx 2 - 5\%$).

Backscattering of e- from Cu, fr=0.01 energy dependence



(error on data ≈ 8%).

Backscattering of 40 keV e- from Al, fr = 0.01



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