

Multiple Scattering in GEANT4

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Abstract

MSC model in G4 : its main features, development of the model and some G4/data and G4/G3 comparisons.

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 problem to be solved :

$$p(r, d, t) = ?$$

if the initial energy of the particle, the material parameters, all the cross sections are known ...

The transport is governed by the transport equation

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

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 as

- detailed (microscopic) simulations,
- condensed simulations
- and mixed simulation algorithms.

detailed simulation : exact, but time consuming if the energy is not small

condensed simulation: simulates the global effects of the collisions during a step, but uses approximations

mixed algorithms: "hard collisions" are simulated one by one + global effects of the "soft collisions".

⇒ Detailed simulation is used for low energy particles only

⇒ examples of the condensed simulations : EGS, GEANT3 - both use Moliere theory, **GEANT4**

⇒ mixed simulation algorithm is used e.g in PENELOPE.

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 'z' 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 'z' step.

path length correction(transformation): $t \iff z$

$t \implies z : F(z, t)$

$z \implies t : G(t, z)$

scattering angle distribution: $f(x, t)$, $x = \cos\theta$

lateral displacement : $R(r, t)$.

PHYSICS INPUT:**(first) transport mean free path**

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

where $\frac{d\sigma(\chi)}{d\Omega}$ is the differential cross section of the scattering,

$$N = N_{Avogadro} \frac{\rho}{A} ,$$

ρ is the density of the material,

A is the atomic weight,

$N_{Avogadro}$ is the Avogadro's number .

i-th transport mean free path is defined similarly with the substitution $(1 - \cos\chi) \implies (1 - P_i(\cos\chi))$,

$P_i(\cos\chi)$ - 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.

steps of MSC algorithm (are essentially the same for many condensed simulation):

1. selection of step length \Leftarrow physics processes + geometry
(MSC performs the $t \iff z$ 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)
 $t = \min(t_{proc1}, t_{proc2}, \dots, t_{procn})$
2. do the $t \rightarrow z$ transformation $z_{phys} \Leftarrow F(z, t)$
3. ask step limit z_{geom} from geometry
4. take the final (geom.) step size as $z_{step} = \min(z_{phys}, z_{geom})$
5. compute the corresponding true step length
 $t_{step} \Leftarrow G(t, z_{step})$

Model functions $F(z, t)$ and $G(t, z)$:

1. G4 standard (until now): not distributions, mean values only

$$z = F(z, t) = \lambda * (1 - \exp(-t/\lambda))$$

$$t = G(t, z) = -\lambda * \ln(1 - \frac{z}{\lambda})$$

(the formulae come from the theory).

2. G4 new : distributions with the theoretical mean values

$$F(z, t) : F(u) = \beta^2 * u * \exp(-\beta * u) , \text{ where } u = \frac{t}{z} - 1$$

$$(0 \leq u < \infty) , \beta \text{ is computed from } \langle u \rangle = \frac{t}{\langle z \rangle} - 1$$

$$G(t, z) : G(v) = \gamma^2 * v * \exp(-\gamma * v) , \text{ where } v = \frac{t}{z} - 1$$

$$(0 \leq v < \infty) , \gamma \text{ is computed from } \langle v \rangle = \frac{\langle t \rangle}{z} - 1$$

STEP 3

sample scattering angle θ from the model distribution $f(x, t)$
 ($x = \cos\theta$).

$f(x, t)$:

1. G4 standard (until now):

$$f(x, t) = p * \frac{(a + 1)^2 * (a - 1)^2}{2 * a} * \frac{1}{(a - x)^3} + (1 - p) * \frac{1}{2} \quad (3)$$

where $a = 1 + \alpha * \frac{t}{\lambda}$, $\alpha = 0.9$, $0 \leq p \leq 1$.

2. G4 new :

$$f(x, t) = q * f_0(x, t) + (1 - q) * \{p * f_1(x, t) + (1 - p) * f_2(x, t)\} \quad (4)$$

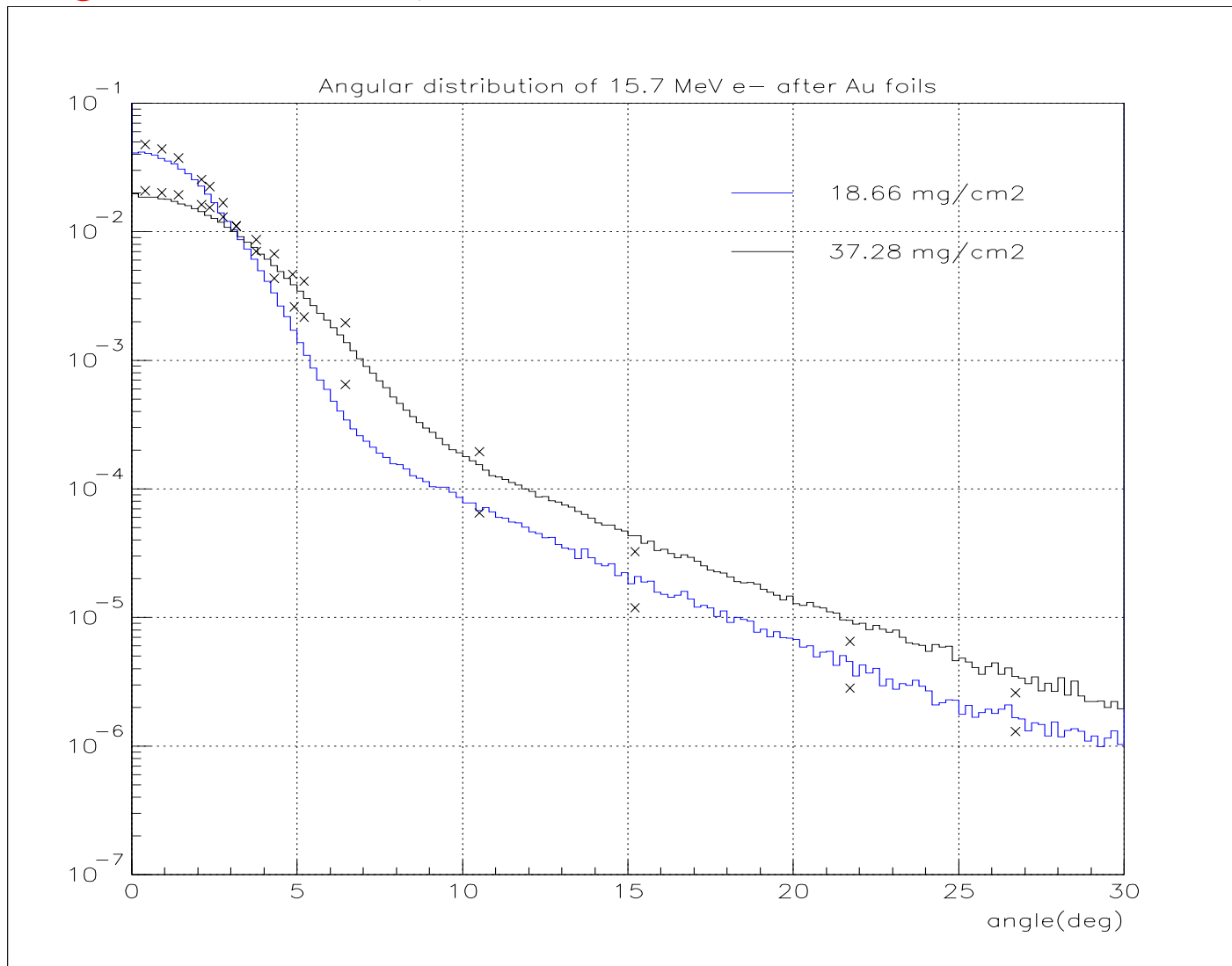
where $0 \leq p, q \leq 1$, $f_i(x, t)$ -s are relatively simple functions
 of x and the variable $\tau = \frac{t}{\lambda}$.

STEP 4

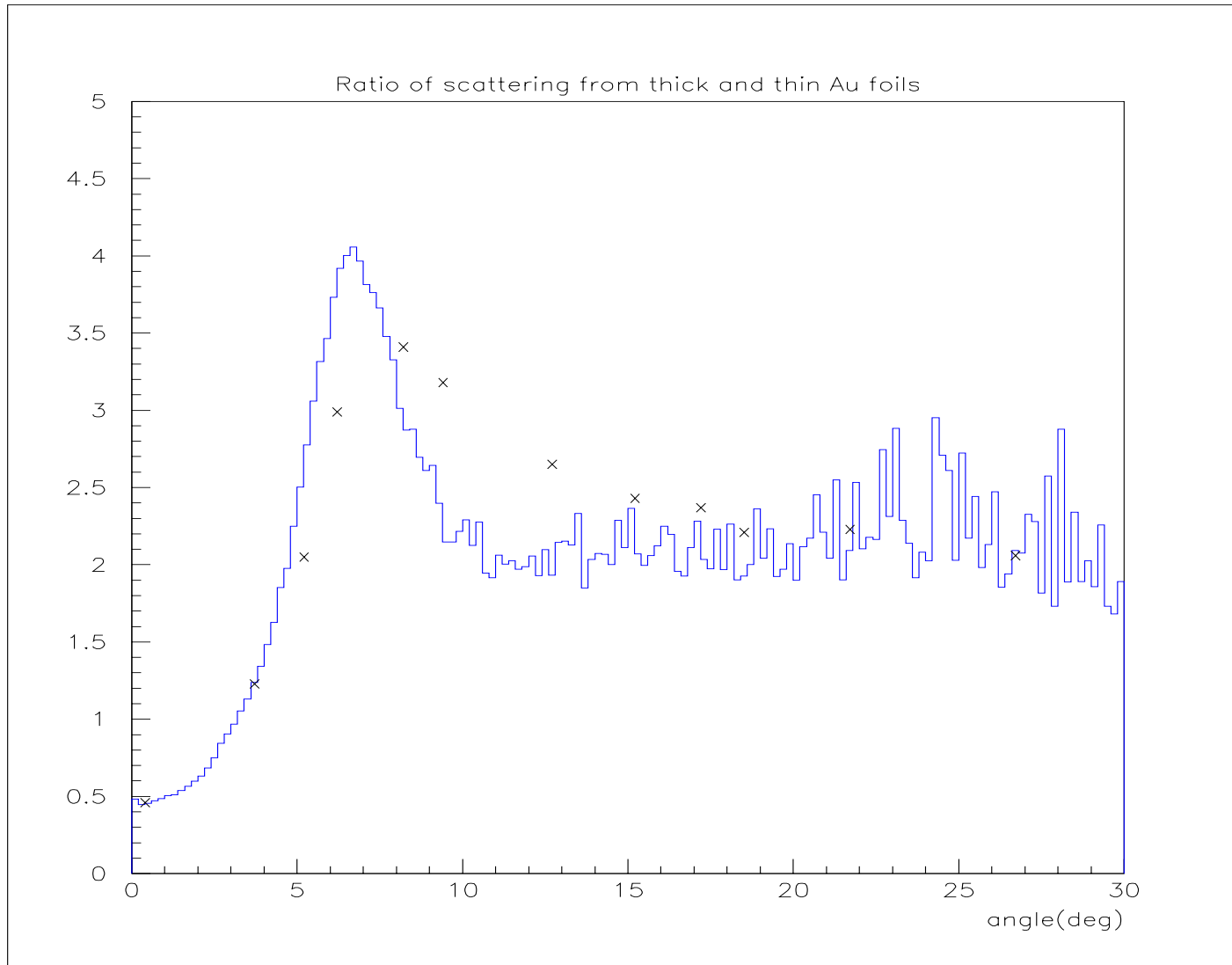
compute the mean lateral displacement according to the theoretical formula and change the position of the particle correspondingly.

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

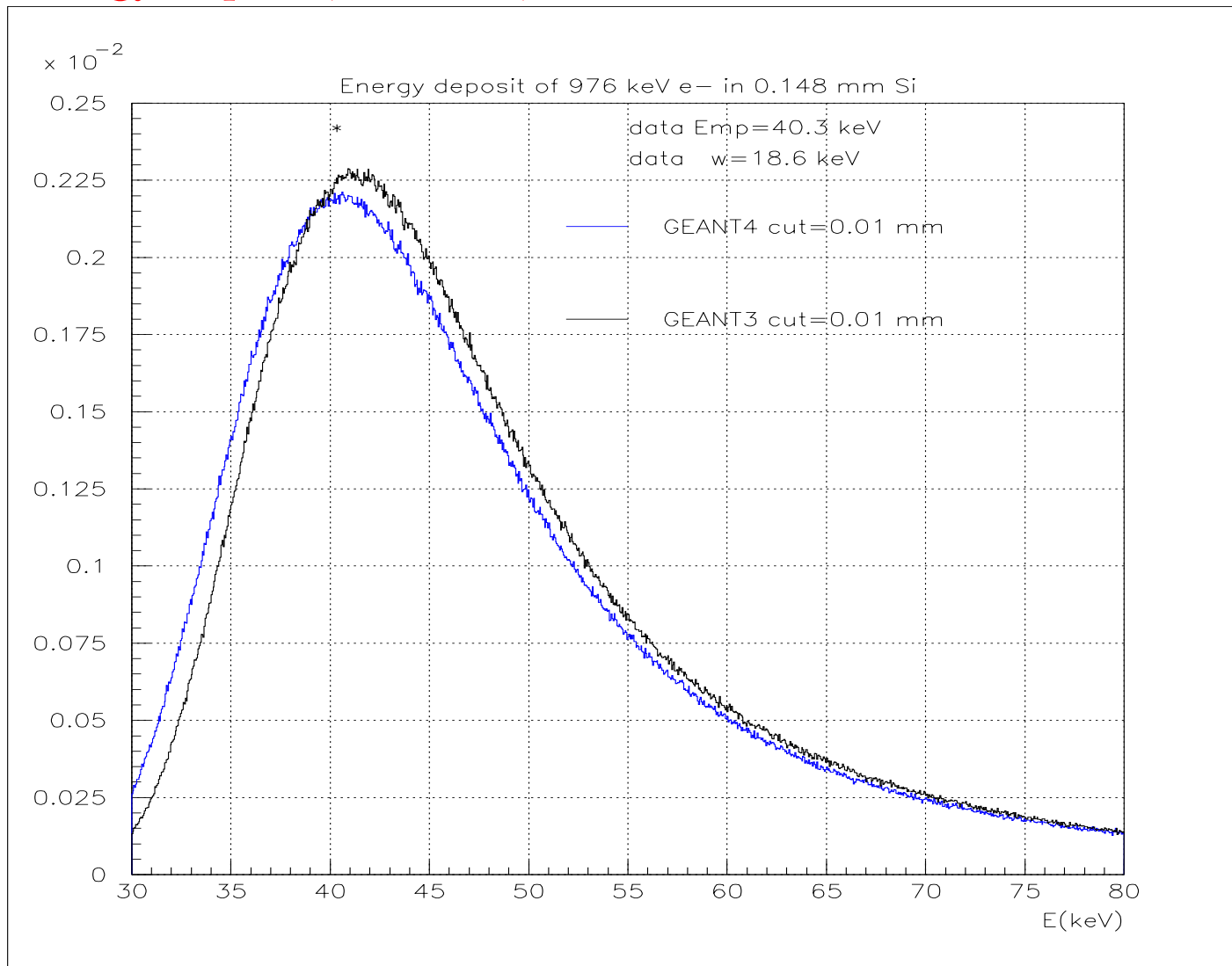
Angle distributions, G4 new



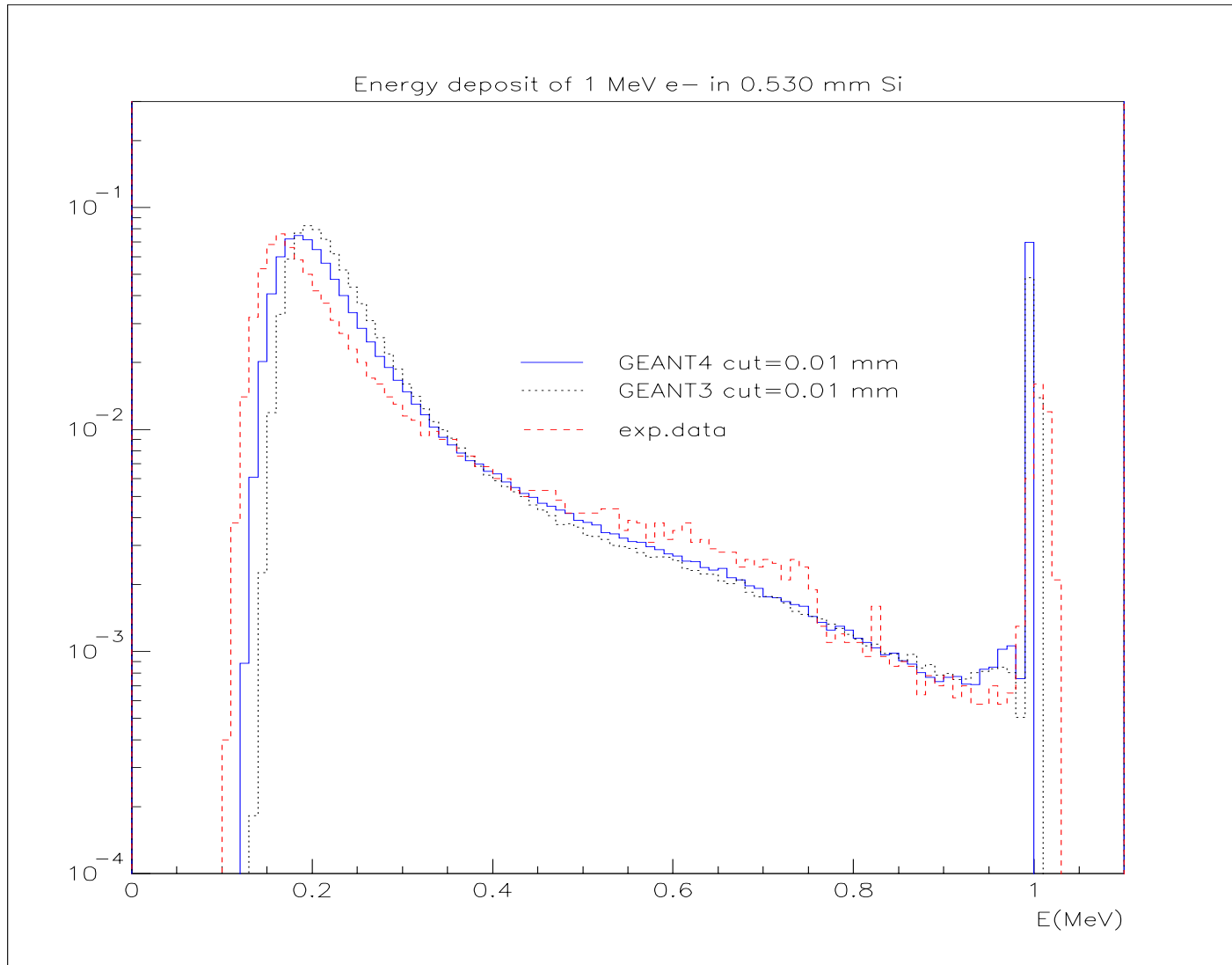
Angle distributions, G4 new



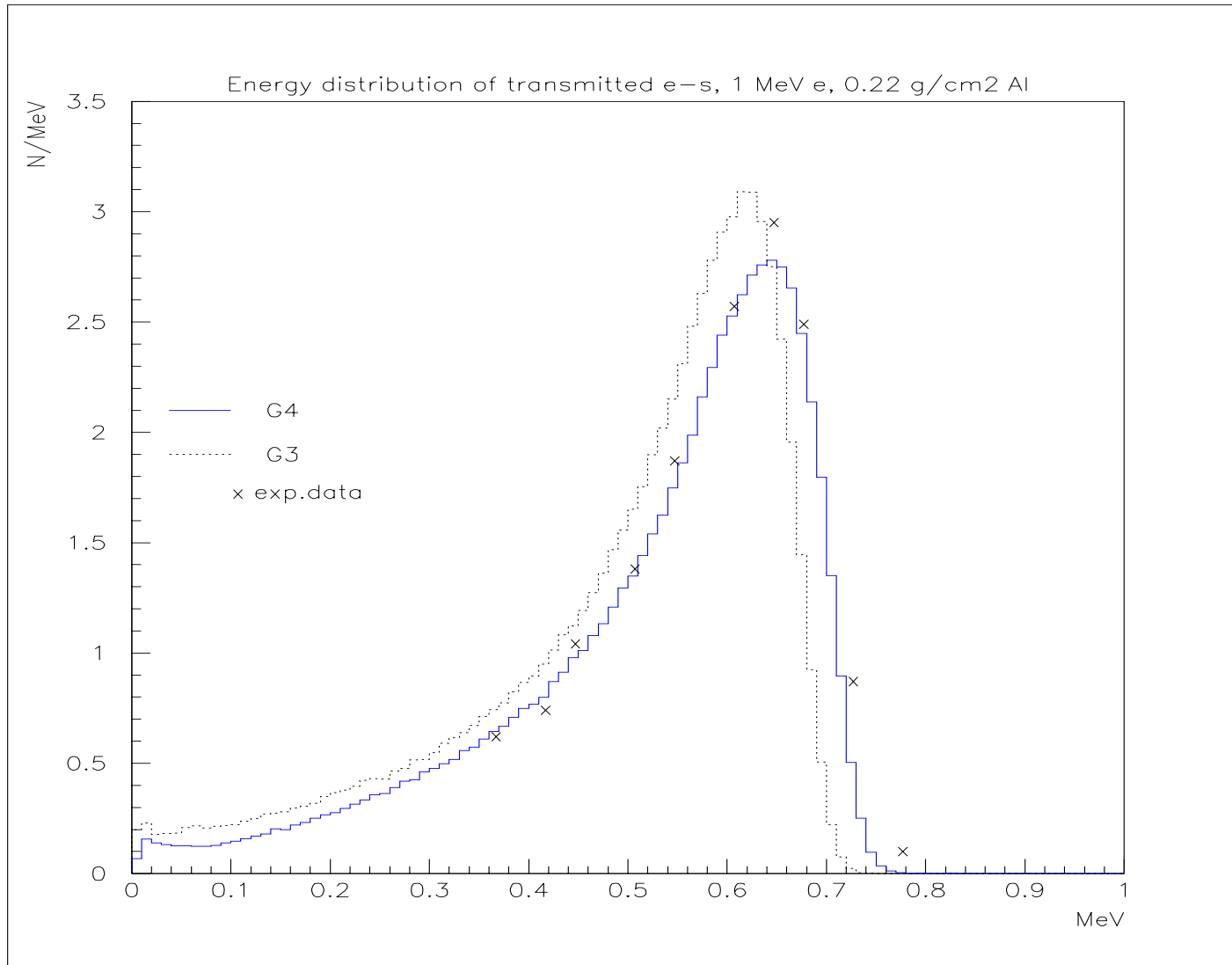
Energy deposit, G4 new, G3 and data



Energy deposit, G4 new, G3 and data



Transmission, G4 new, G3 and data



Backscattering is a difficult problem for condensed simulations.

One step to the good direction in the new G4 MSC algorithm: limit the step in MSC when entering a volume . (This is NOT the user limit, the step is limited by MSC near to boundaries only!) Algorithm:

$t_{lim} = \max(\lambda, t_{min})$ where $t_{min} = 0.001$ micrometer.

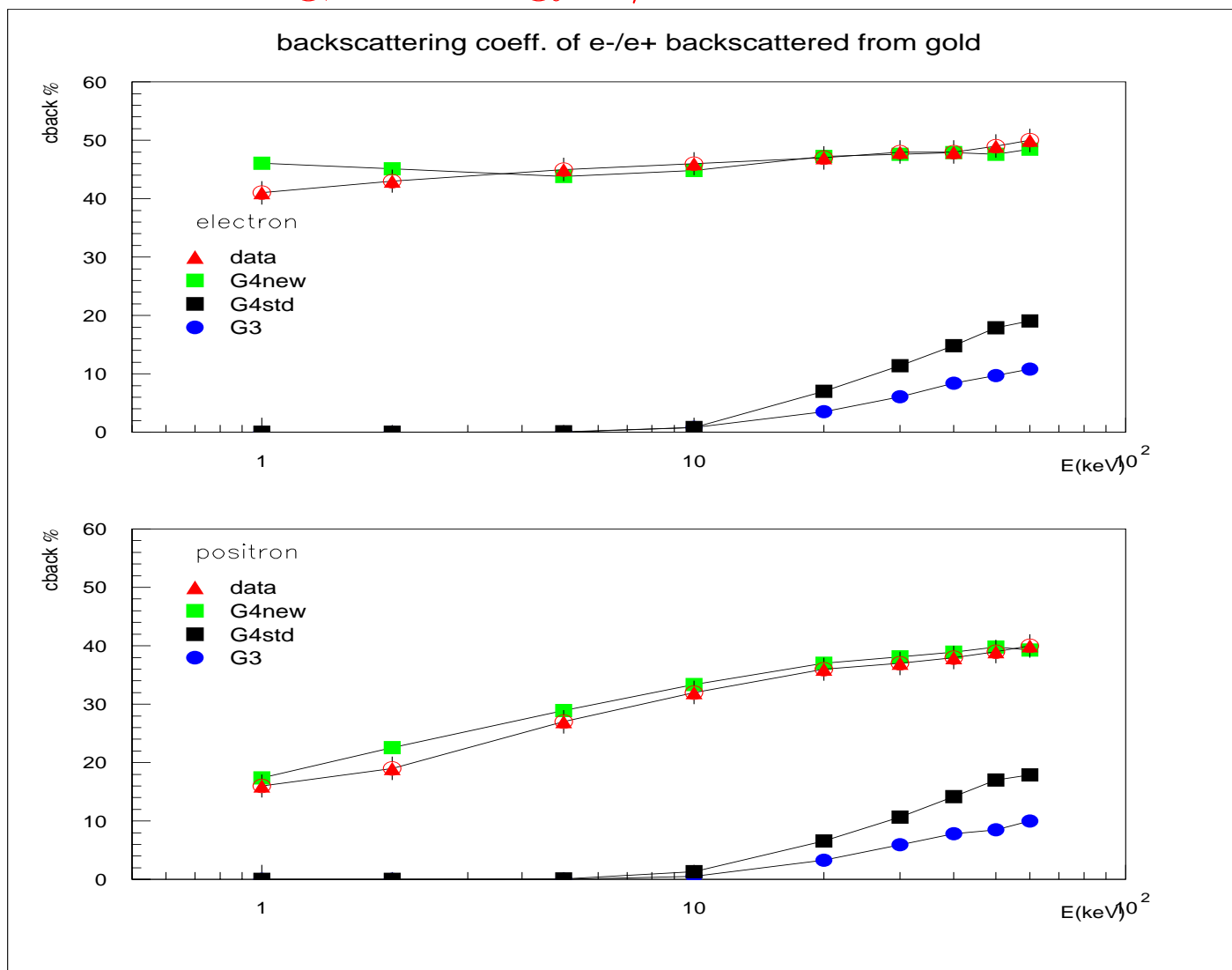
if(*safety* < t_{lim}) and ($tstep > t_{lim}$)

$tstep = fact * \lambda$ and MSC limits the step.

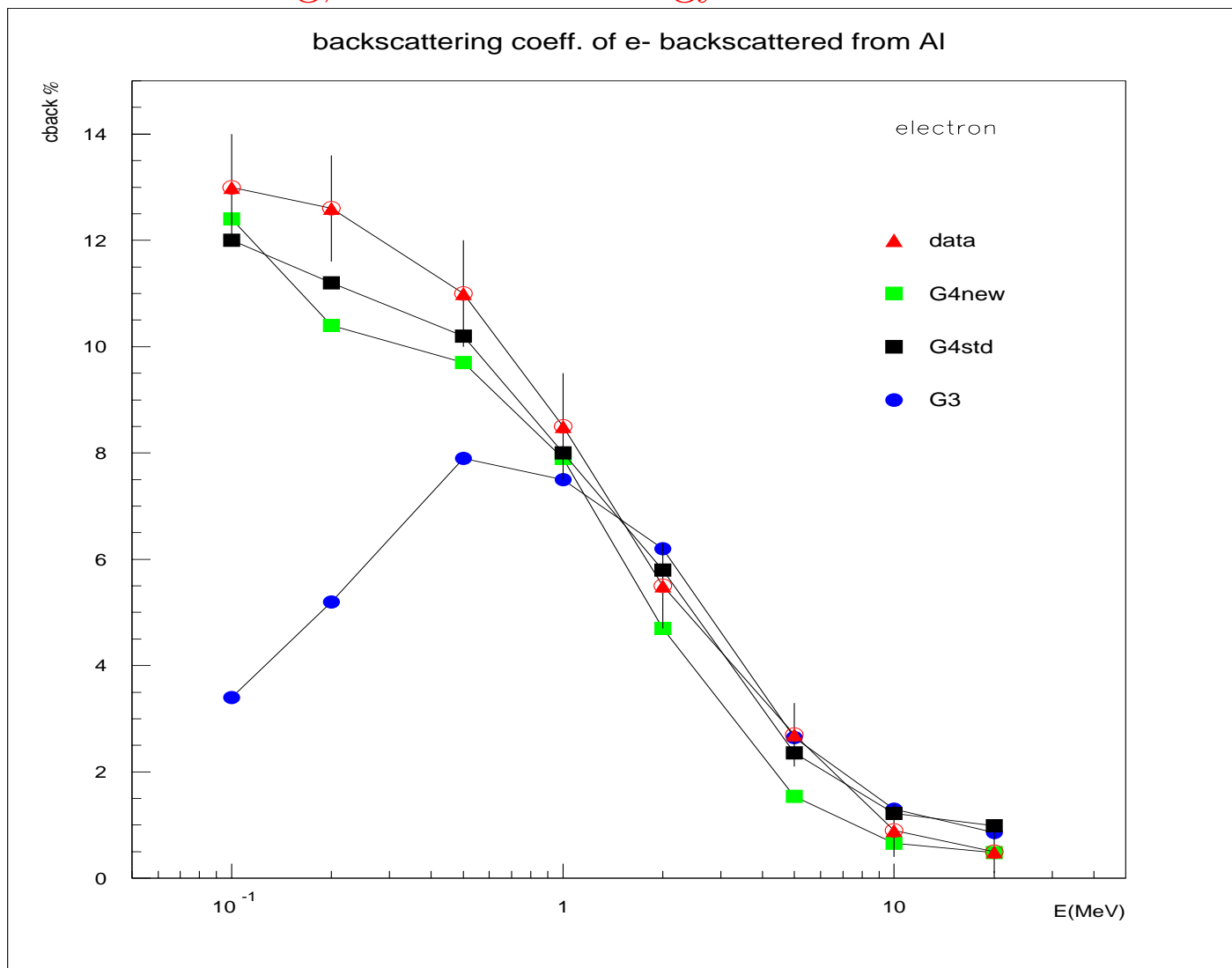
This means a restriction of the step length for low energy particles only.

Some results of this very simple algorithm follow ...

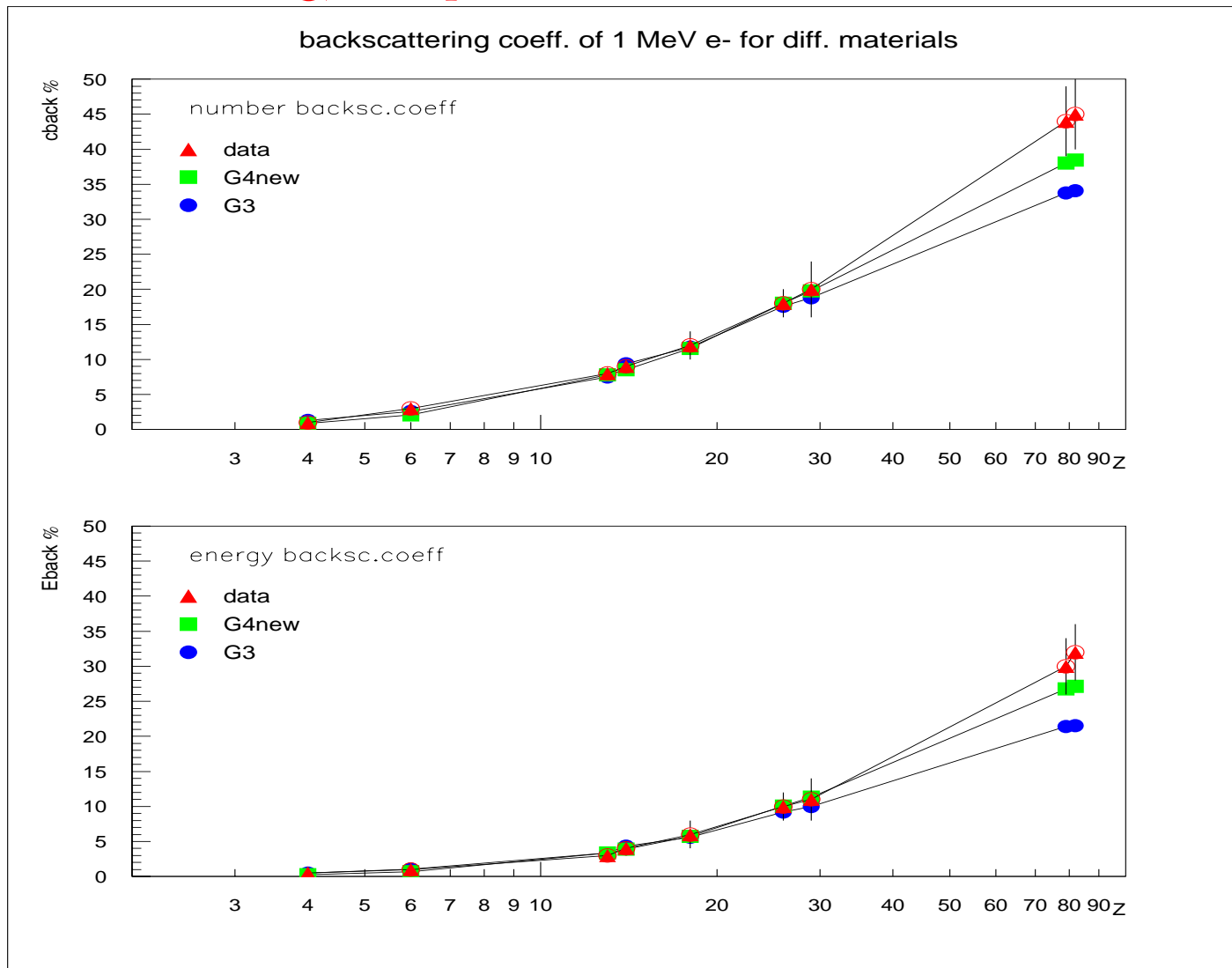
Backscattering, low energy e-/e+



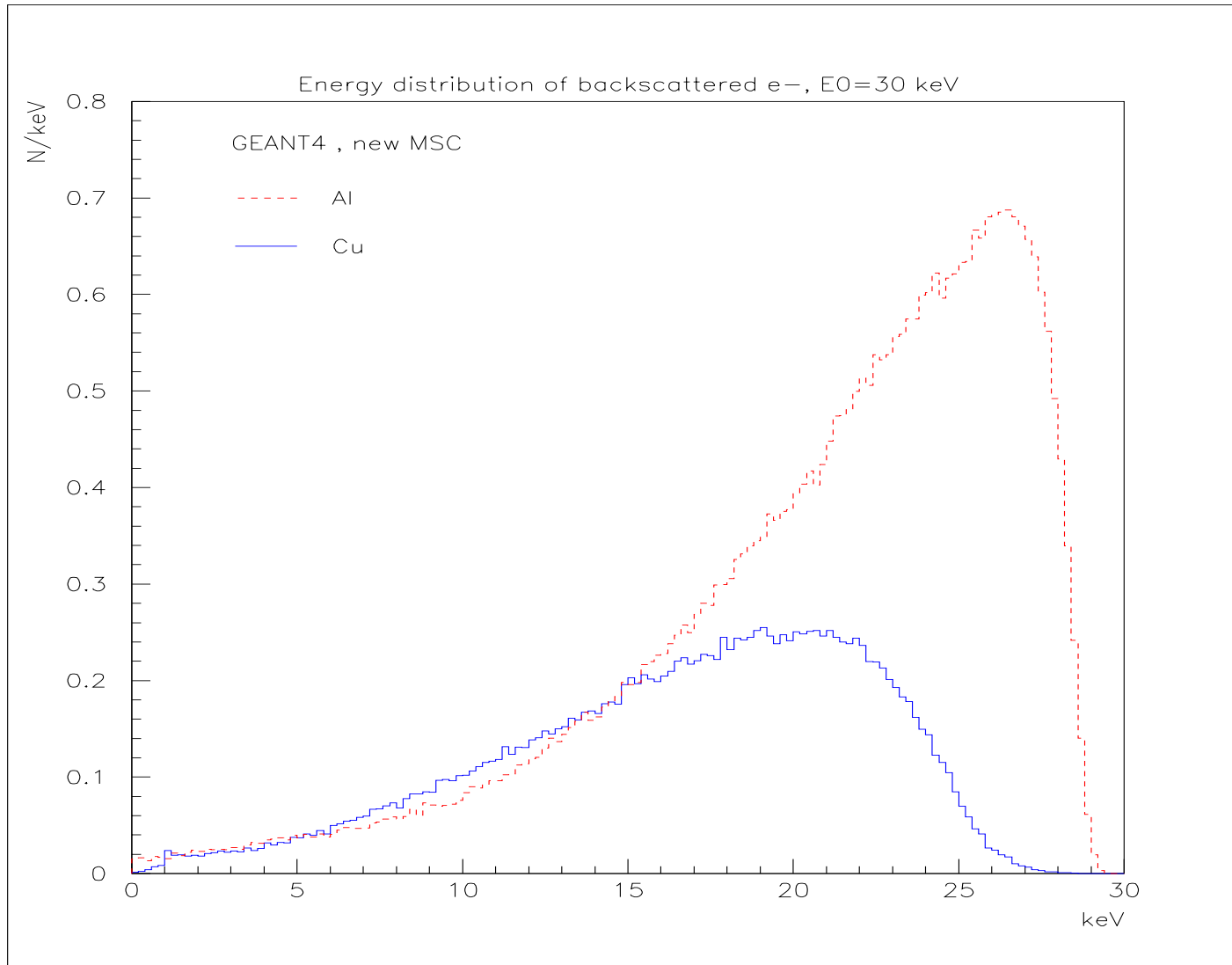
Backscattering, not so low energy



Backscattering, Z dependence



Backscattering, energy spectra



The new MSC version brought -sometime big- changes in the physics results for low energy particles.

Is there any effect/change for a high energy setup ?

The answer is **yes**.

Example : 30(23 mm Fe + 0.4 mm Si) SICAPO calorimeter, 6 GeV e- initiated showers.

Showers in sampling calorimeters

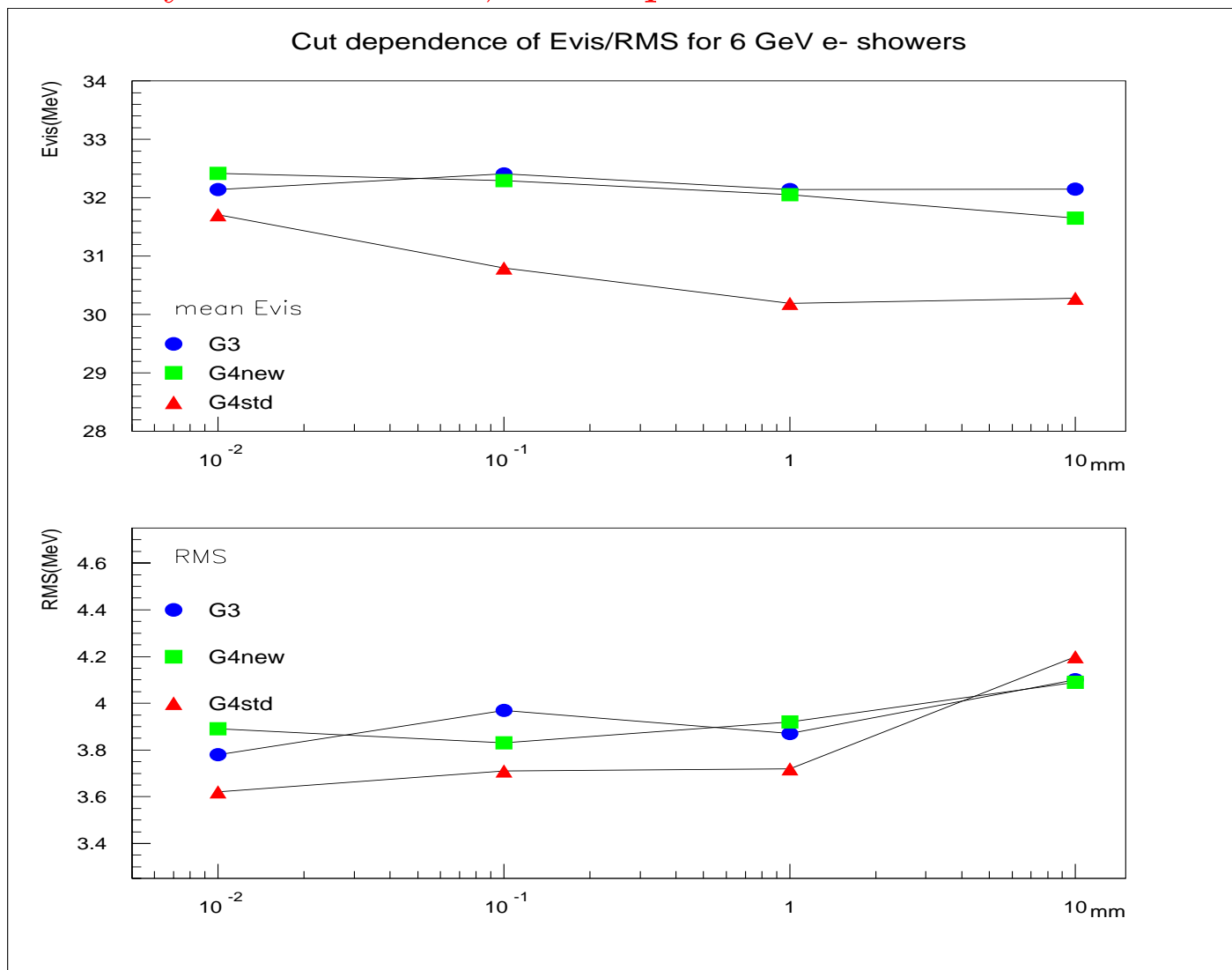
1000 showers/run with 0.01 mm cut.(diff en.cut in Fe/Si in G3!)

program version	E_{vis} in MeV	RMS (MeV)	ex.time(sec)
GEANT3	32.14	3.78	970.
G4 std	31.71	3.62	1520.
G4 new	32.42	3.89	1600.
G4 new(no bound)	32.00	3.79	1600.



- more E_{vis} and bigger RMS in G4 new than in G4 std
- G4 new is slower than G4 std by 5 % and this change in speed is not due to the boundary algorithm

Stability of the results, cut dependence



→ cut dependence of E_{vis} seen in ATLAS HEC and EM barrel for electrons is probably cured with the new MSC !!!!

another exercise: 20 GeV muons in the same calorimeter, 10000 showers/run (motivation: $E_{vis_{G3}} > E_{vis_{G4}}$ by 3 % in the ATLAS TileCal Fe + Scint calorimeter)

results (for cut = 1 mm)

program	$E_{vis}(\text{MeV})$	RMS(MeV)	$\Delta = 100 * \frac{E_{vis} - E_{vis_{G3}}}{E_{vis_{G3}}}$
G3	6.17	3.21	-
G4 std	6.03	2.93	-2.3
G4 new	6.18	3.36	+0.2

→ G4 std gives smaller E_{vis} than G3 while

$E_{vis_{G4new}} = E_{vis_{G3}}$ (stat.error of $E_{vis} \sim 0.5\%$ here.) The results are similar for cut = 0.1 mm).

Conclusions:

- the new MSC version exists and works rather well
- G4 with the new MSC gives better physics results than G4 std (and at least for the simple setups simulated here G4 new results are better than G3 results)
- G4 new is slightly slower than G4 with standard MSC
- backscattering can be simulated

Things to do:

- write-up (preprint,paper) - top priority
- results \implies EM Web gallery
- some more tuning on angle distribution (tail is overestimated, but G3 tends to underestimate the tail ...)
- correlations (e.g. $z - \cos\theta$)
- ...

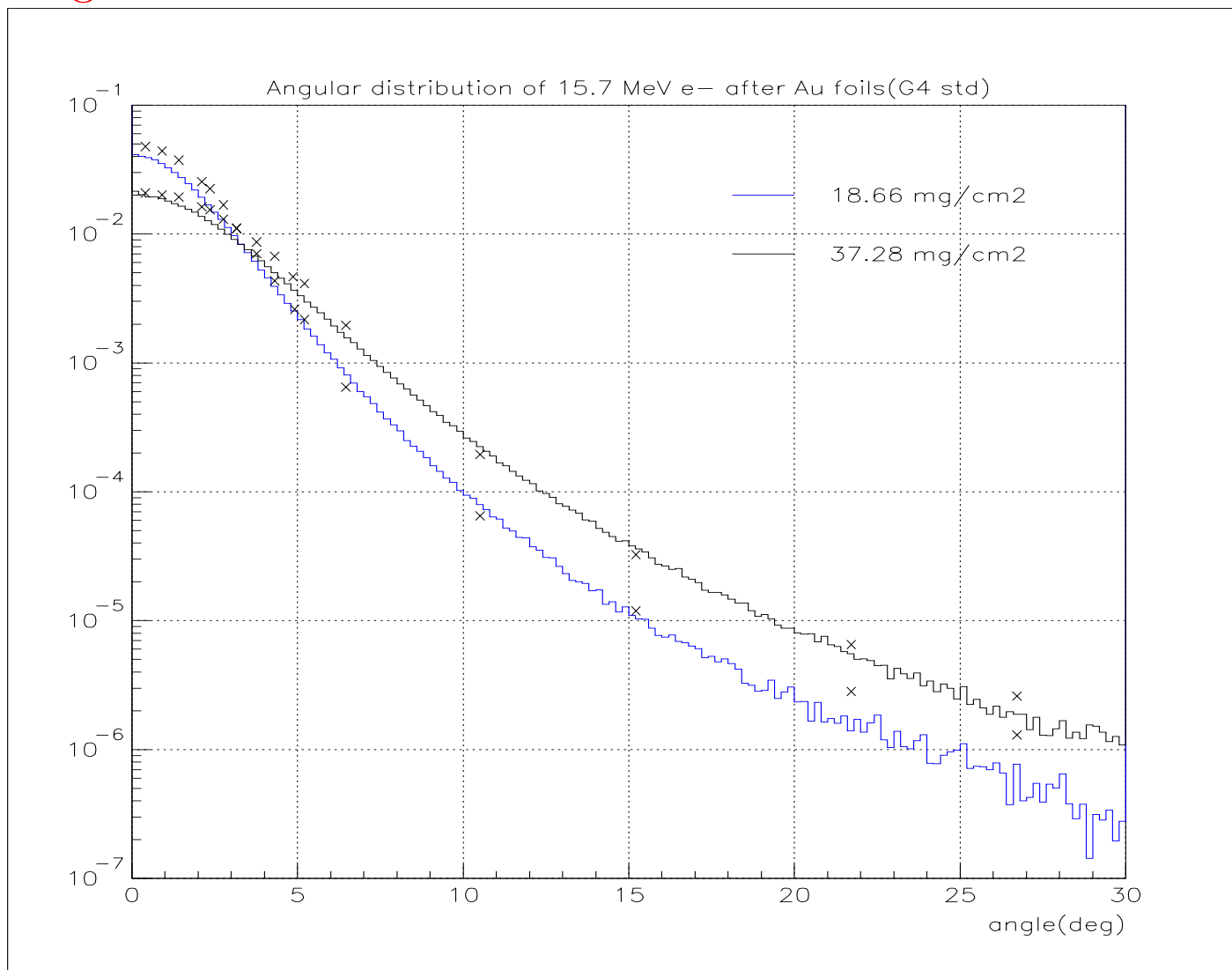
How to use the new MSC version:

it is in the CVS HEAD under the name `G4MultipleScatteringx`

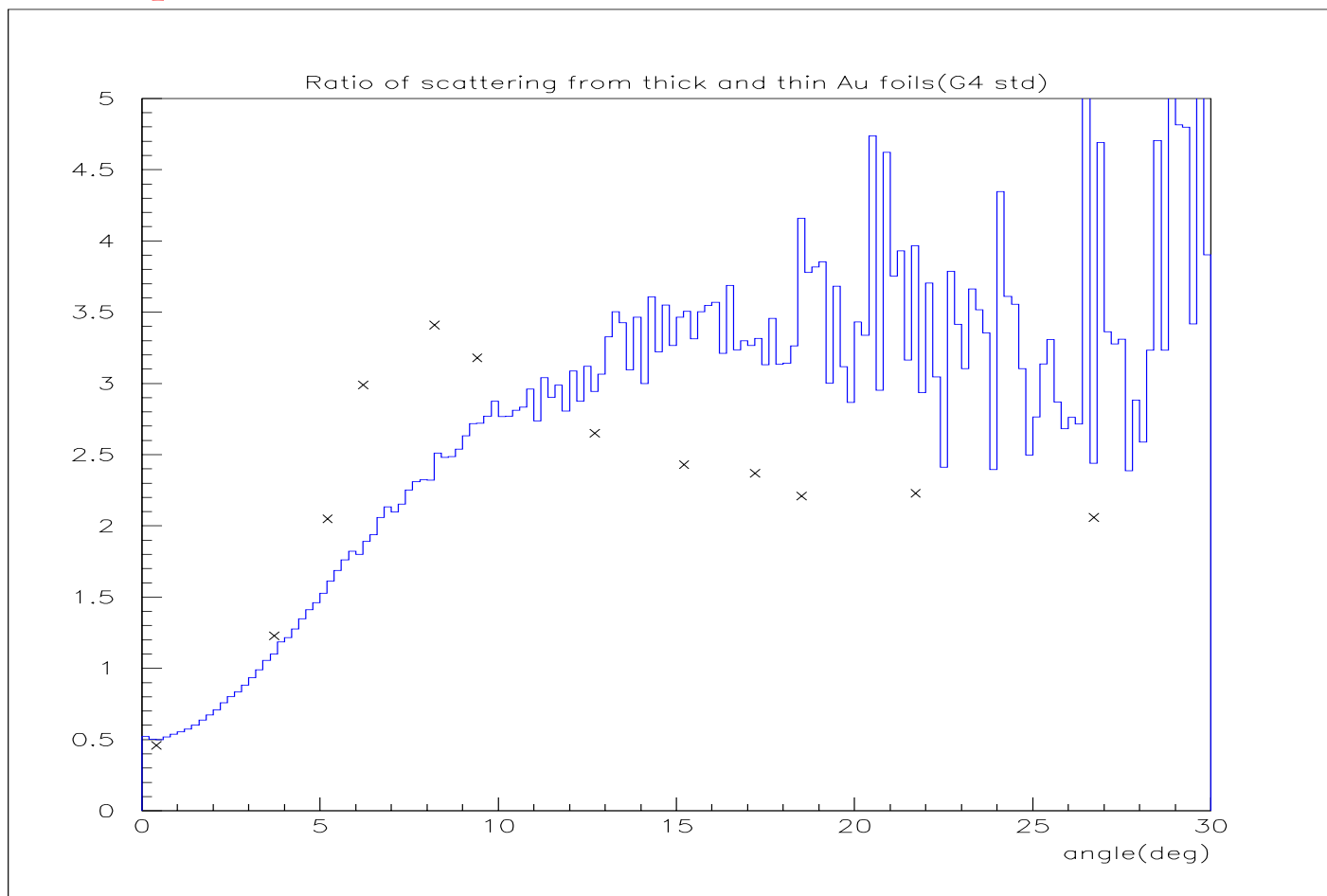
- update your working directory
- perform a change `G4MultipleScattering` \implies `G4MultipleScatteringx` in your `PhysicsList`

Try to use this new MSC, I need your feedback and sooner or later this will be the default !

Angle distributions with G4 std MSC



Angle distributions with G4 std MSC, motivation for MSC development!



Angle distributions with G3

