Multiple Scattering Update msc93 – msc95

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MscModel - semiempirical model based on Lewis theory

Changes in the model from msc93 to msc95

1.sampling of the geometrical step length (no in msc93 by default, yes in msc95)
2.lateral displacement (mean value in msc93, sampling in msc95)
3.modification in angular distribution : tail modified in msc95
4.change in stepping for case $opt = 3$

$\longrightarrow$ better results and results are much more stable when cuts/step sizes are changed

All points 1.-4. contribute to the improvement, most of the improvement comes from 3.

Point 1. - 2. : sampling of z (geom.steplength) and r (lateral displacement)
shape of the distributions taken from single scattering simulation, mean values agree with the theory.
Point 4. - step size is restricted in msc : tlimit
if actual step size t > tlimit → t = tlimit
optimization : if $tlimit < 0.3 * safety \rightarrow tlimit = 0.3 * safety$
msc95: this optimization is removed for opt = 3 , i.e. smaller tlimit is allowed in order to get a more precise stepping.

Point 3. angular distribution

model function

$$g(u) = q[pg_1(u) + (1-p)g_2(u)] + (1-q)g_3(u) \qquad (1)$$

where $u = \cos(\theta)$

$0 \leq p, q \leq 1$

$g_i(u)$ are simple functions:

$$g_1(u) = C_1 \exp^{-a(1-u)} \qquad u_0 \leq u \leq 1 \qquad (2)$$

$$g_2(u) = C_2 \frac{1}{(b-u)^c} \qquad -1 \leq u \leq u_0 \qquad (3)$$

$$g_3(u) = C_3 \qquad -1 \leq u \leq 1 \qquad (4)$$

Here C_i are normalization constants, u_0, a, b, c are parameters of the model.

It can be seen easily that $g_1(u)$ is Gaussian in θ for small θ values, $g_2(u)$ describes a Rutherford-like tail for big θ and $g_3(u)$ is uniform in u.

The 6 model parameters are not independent, we require that

A. $g(u)$ should be continuous at $u = u_0 = 1 - \frac{\xi}{a}$

B. 1st derivative of $g(u)$ should be continuous at $u = u_0$

C. mean value of u is the same as the theoretical value,

so we have only 3 independent parameters in the model.

Choice of the free parameters:

up to version msc93

- a tuned from e- scattering data
- $\xi = 3$ fixed
- c from Hanson's e- scattering data (2 data sets only $\rightarrow$ c can not be too well determined)

version msc95

From conditions A. and B. it follows

$$b = 1 - \frac{\xi - c}{a} \tag{5}$$

Choice of the free parameters:

- a tuned from e- scattering data (same as in earlier versions)
- $b = 1$ fixed ($\rightarrow \xi = c$)
- c determined from the condition

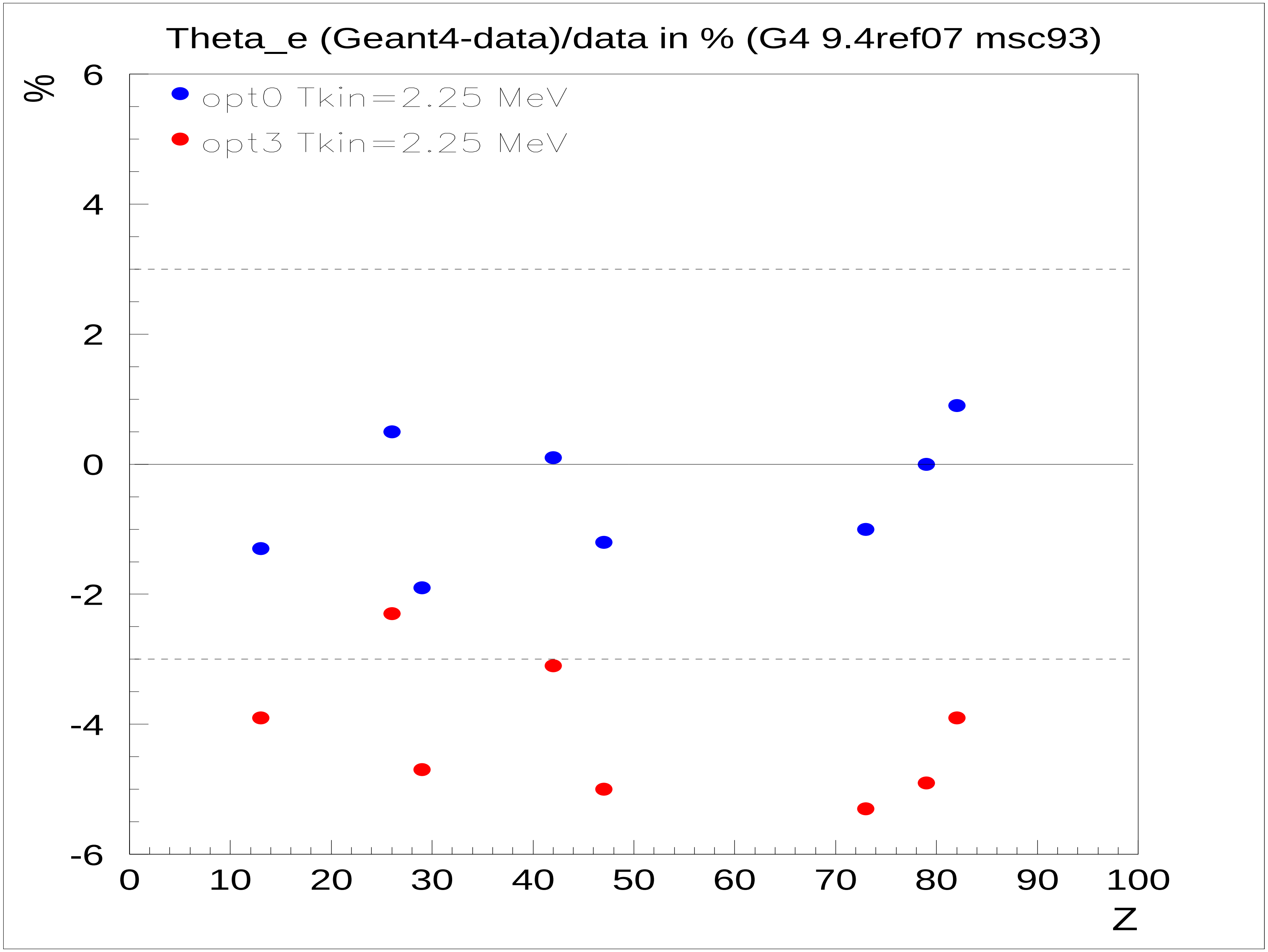
$$(q - 1)^2 = min \tag{6}$$

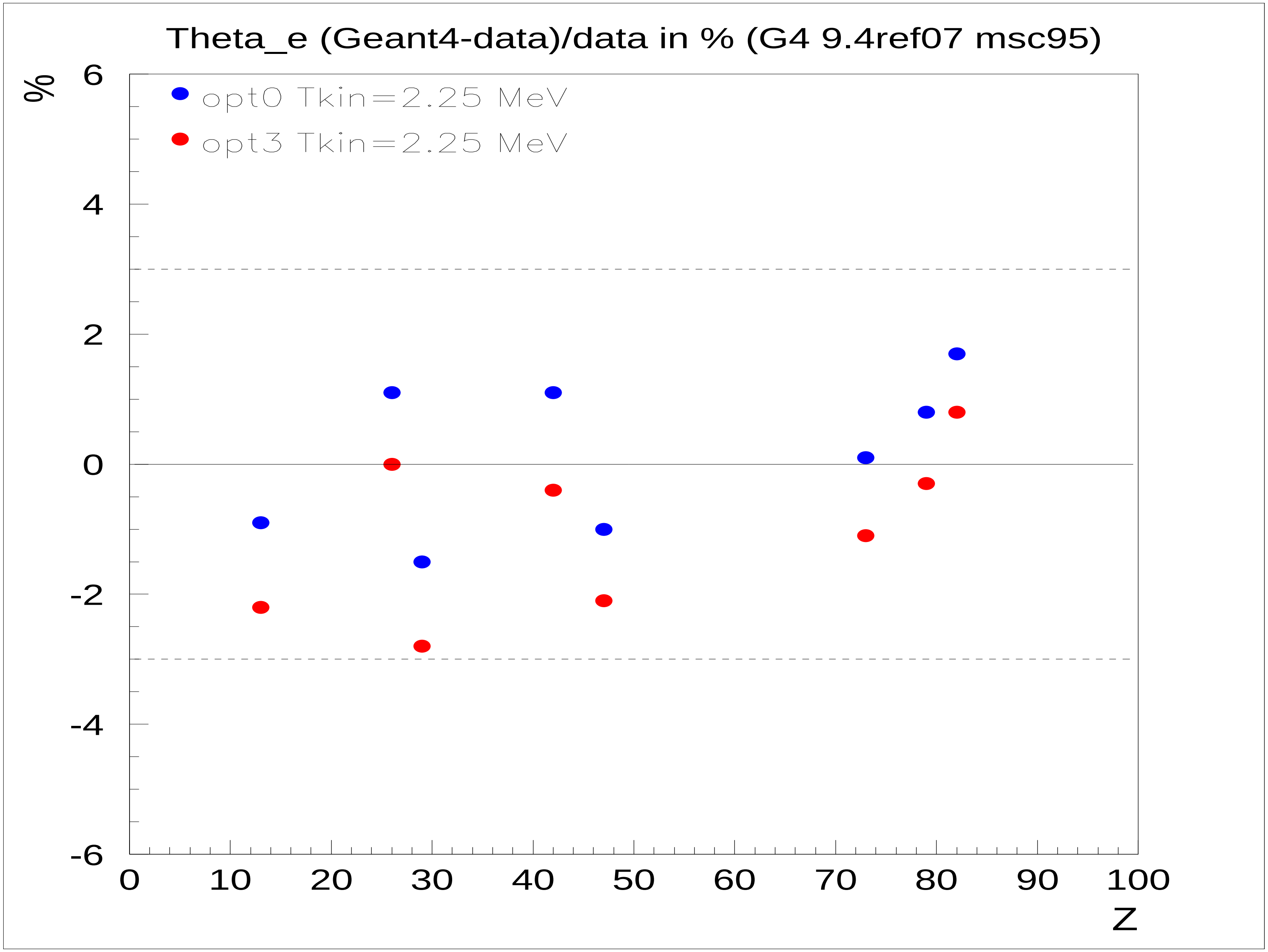
Note: if $q = 1$ we have only 2 terms in the model function $g(u)$, the 3rd term (uniform in u) is missing.

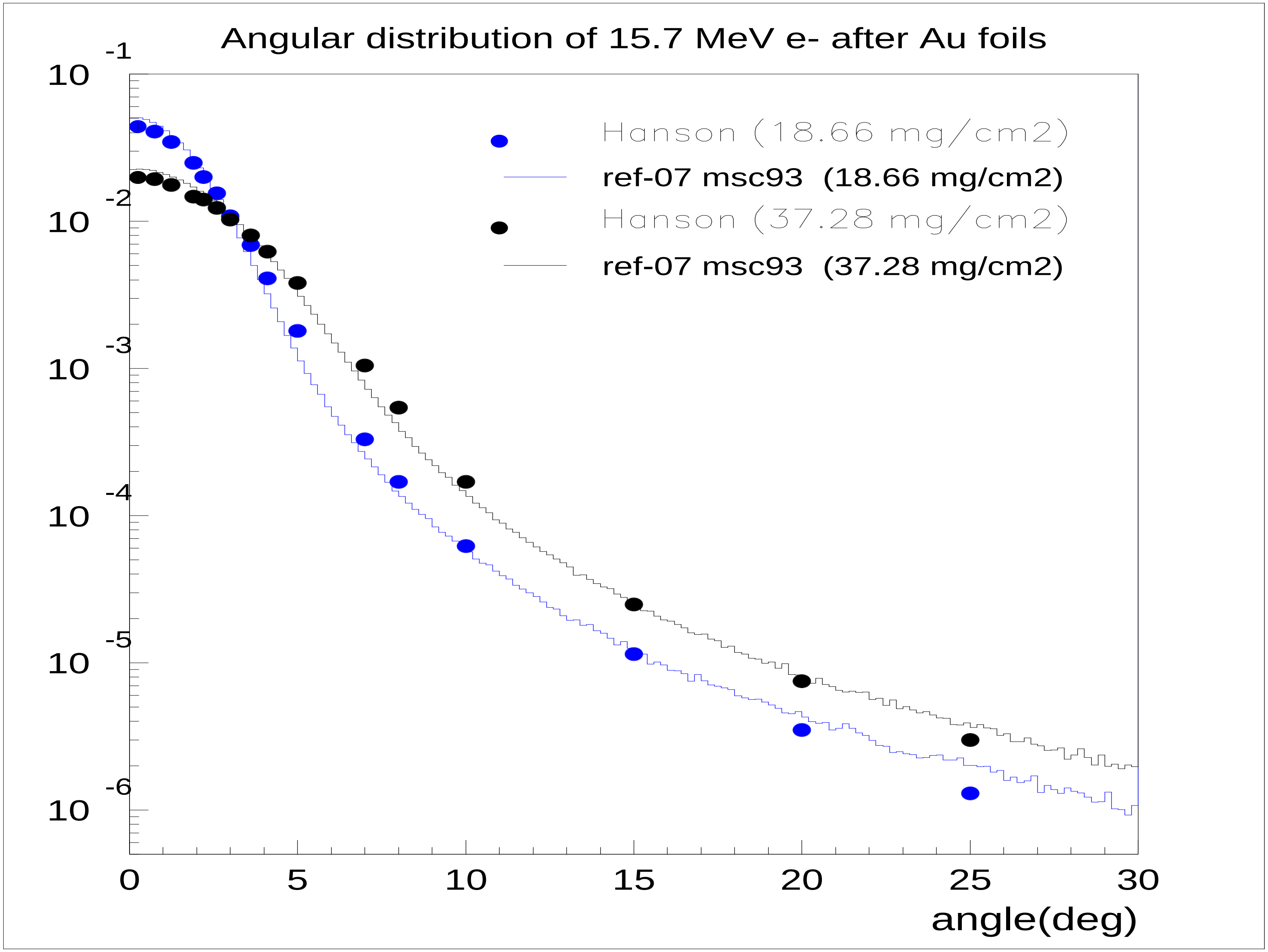
This last condition ensures the very weak step and cut dependence of the results.

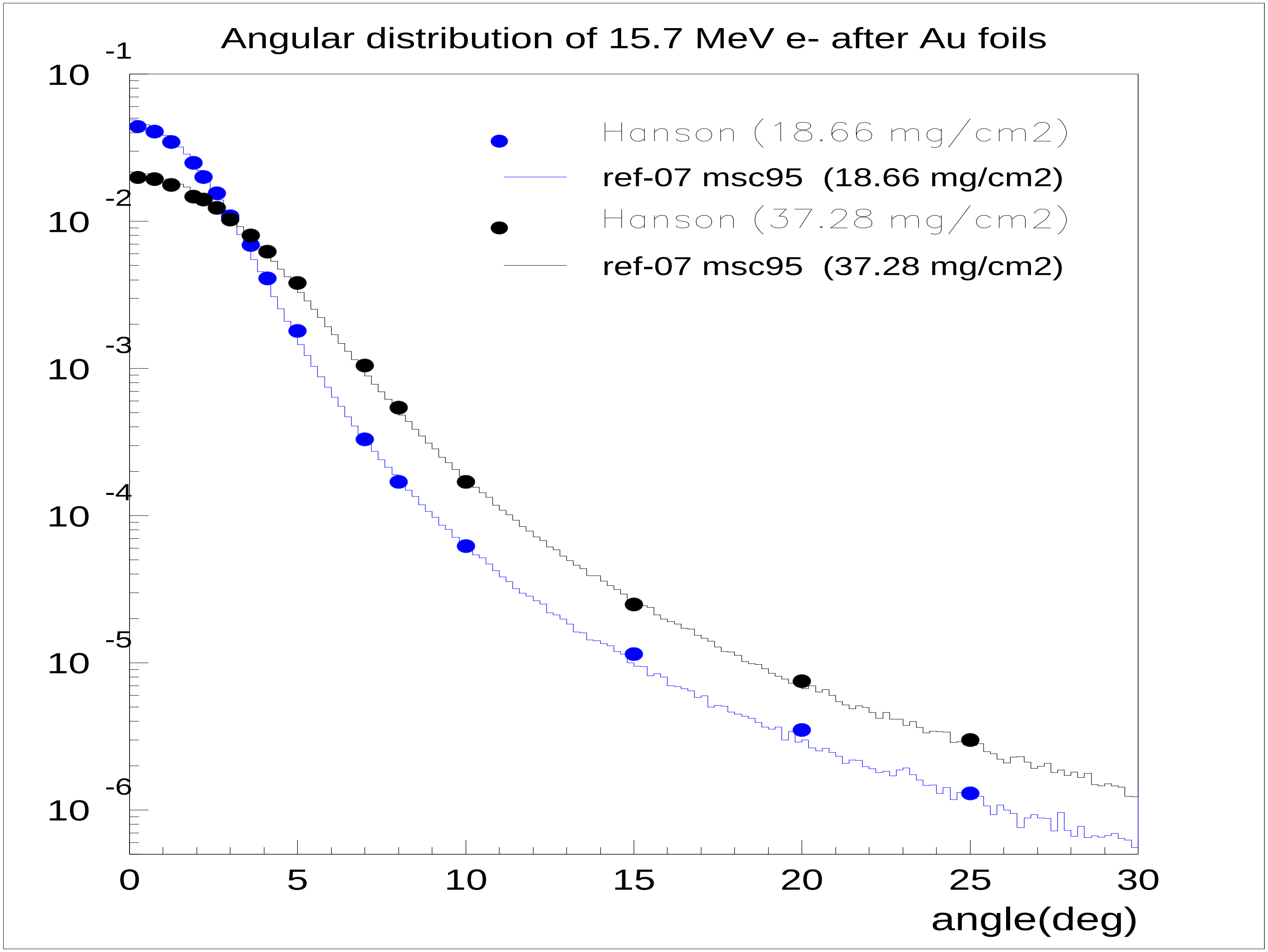
Test/validation results group 1 : angular distributions, backscattering

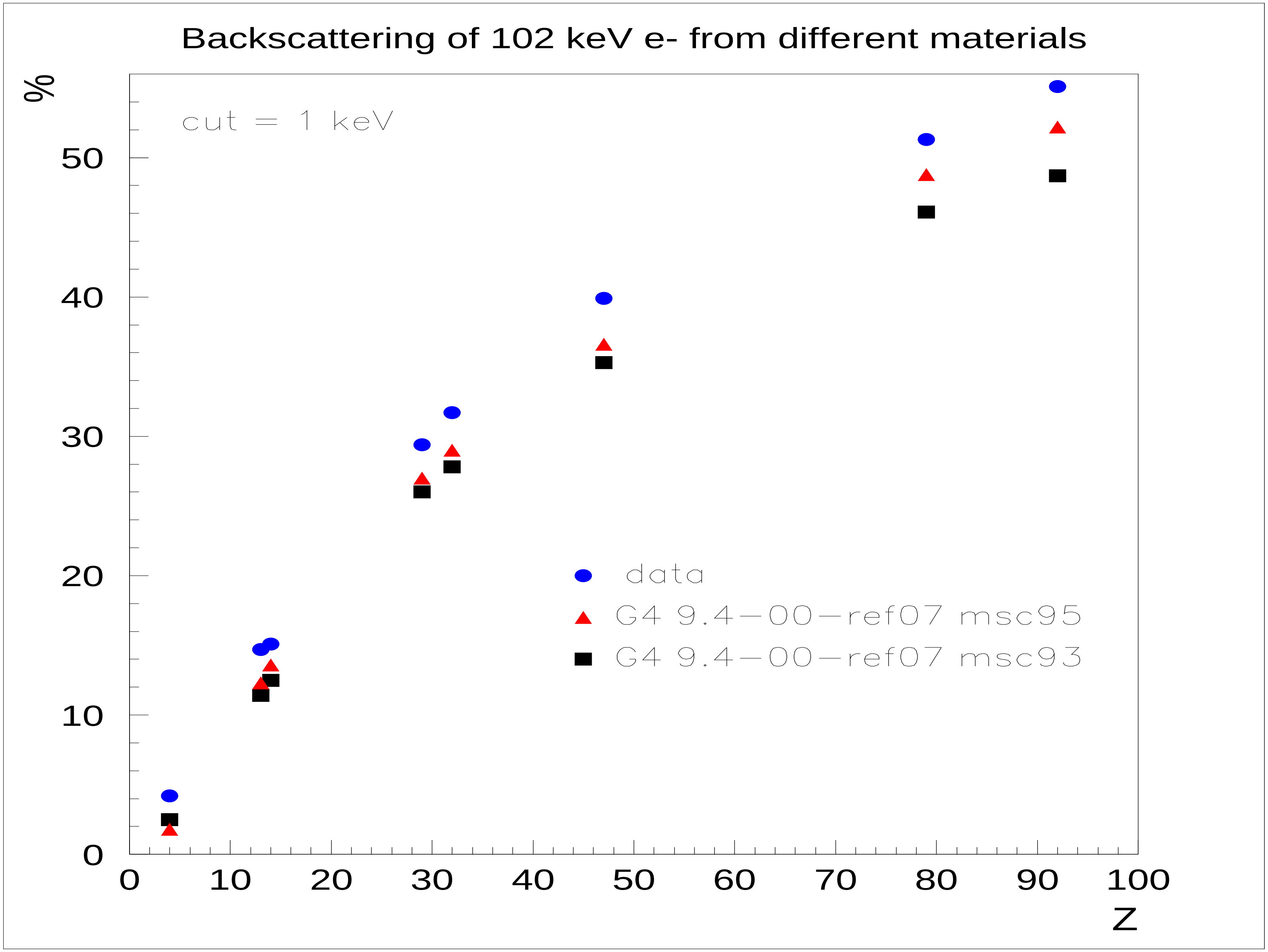
msc93 - msc95 - data comparisons


Theta_e (Geant4-data)/data in % (G4 9.4ref07 msc93)
%
opt0 Tkin=2.25 MeV
opt3 Tkin=2.25 MeV
6
4
2
0
-2
-4
-6
0
10
20
30
40
50
60
70
80
90
100
Z

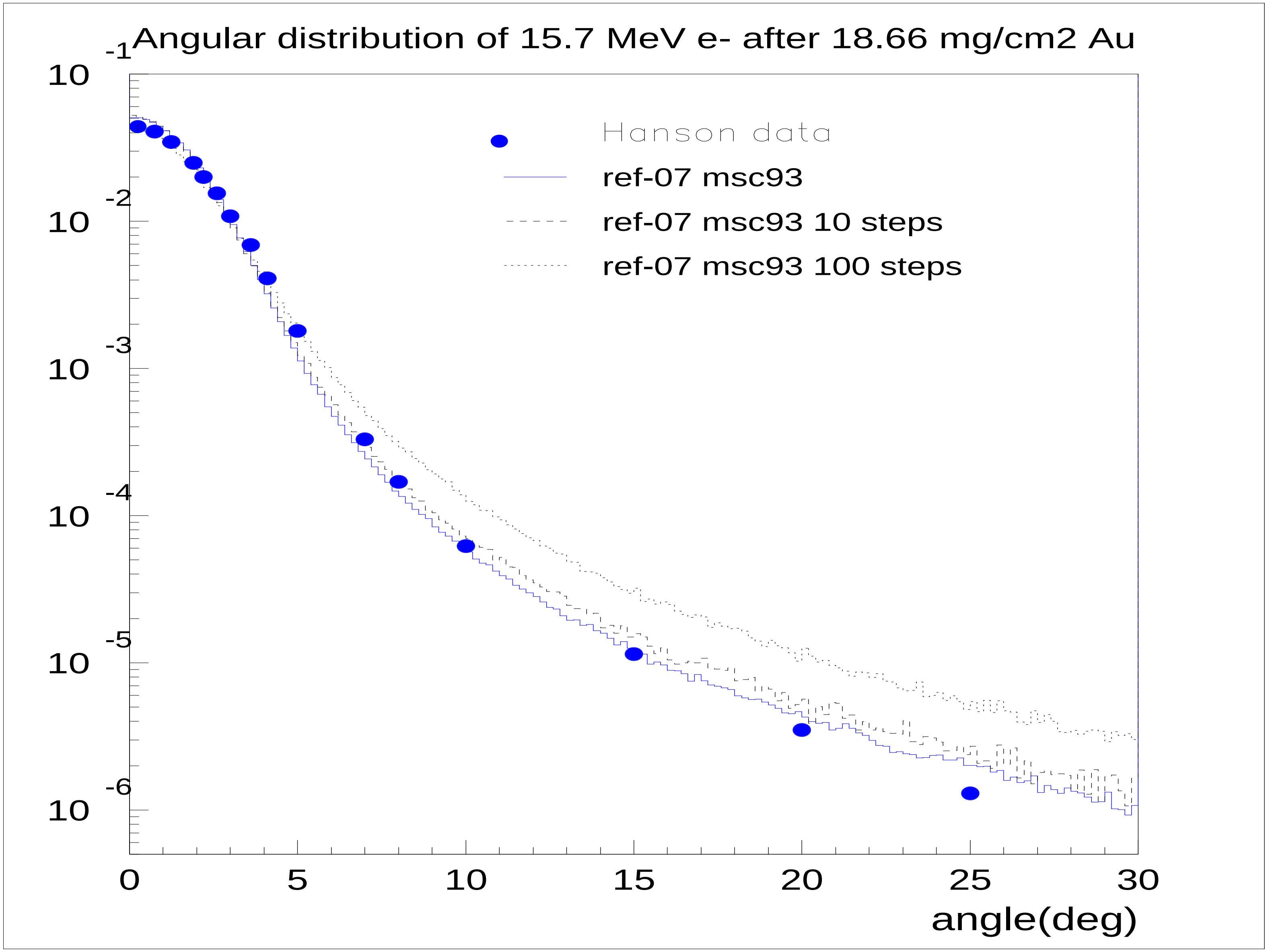

Theta_e (Geant4-data)/data in % (G4 9.4ref07 msc95)
%
6
4
2
0
-2
-4
-6
opt0 Tkin=2.25 MeV
opt3 Tkin=2.25 MeV
0
10
20
30
40
50
60
70
80
90
100
Z

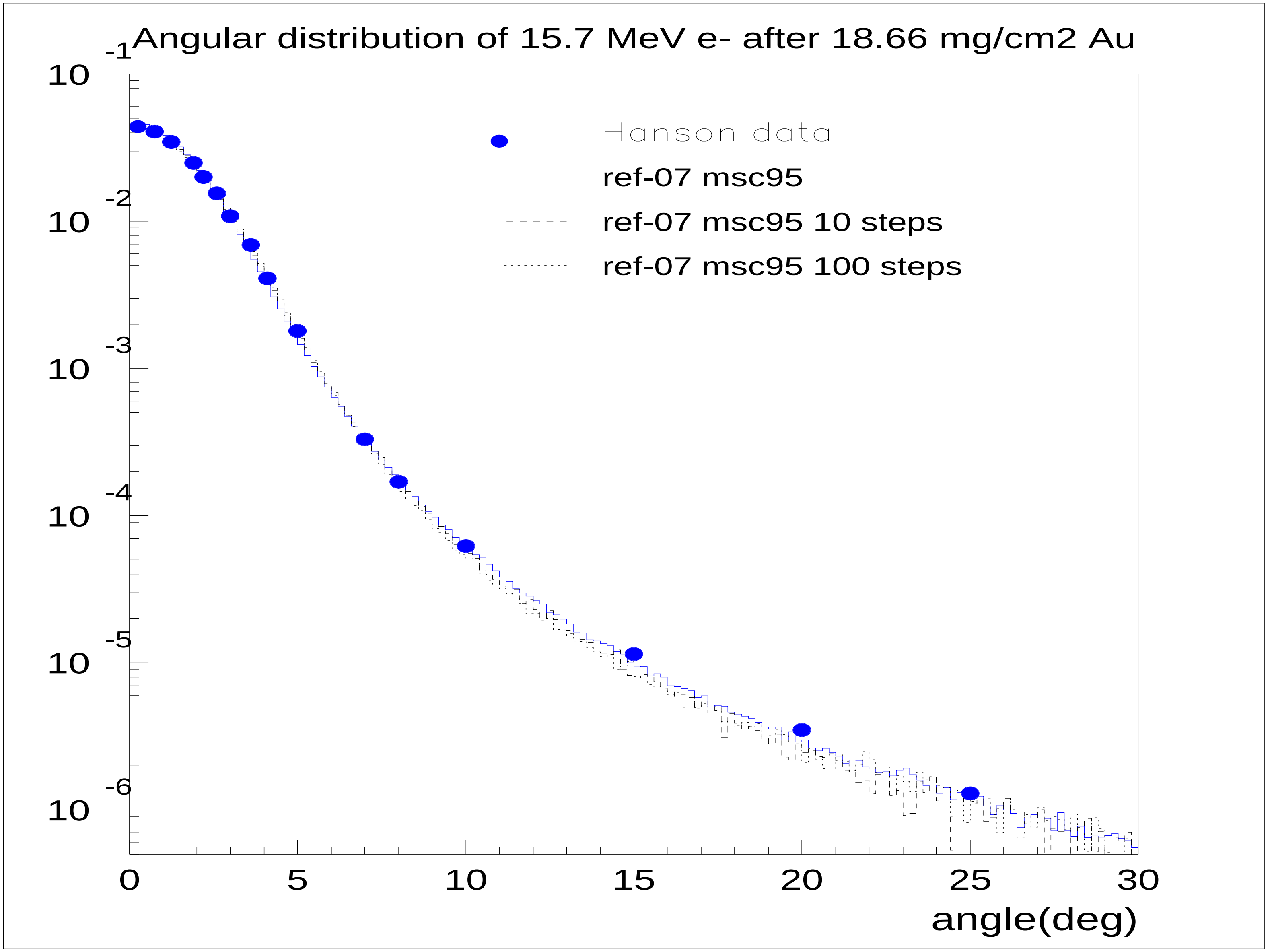

Angular distribution of 15.7 MeV e- after Au foils
Hanson (18.66 mg/cm2)
ref-07 msc93 (18.66 mg/cm2)
Hanson (37.28 mg/cm2)
ref-07 msc93 (37.28 mg/cm2)
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
0
5
10
15
20
25
30
angle(deg)

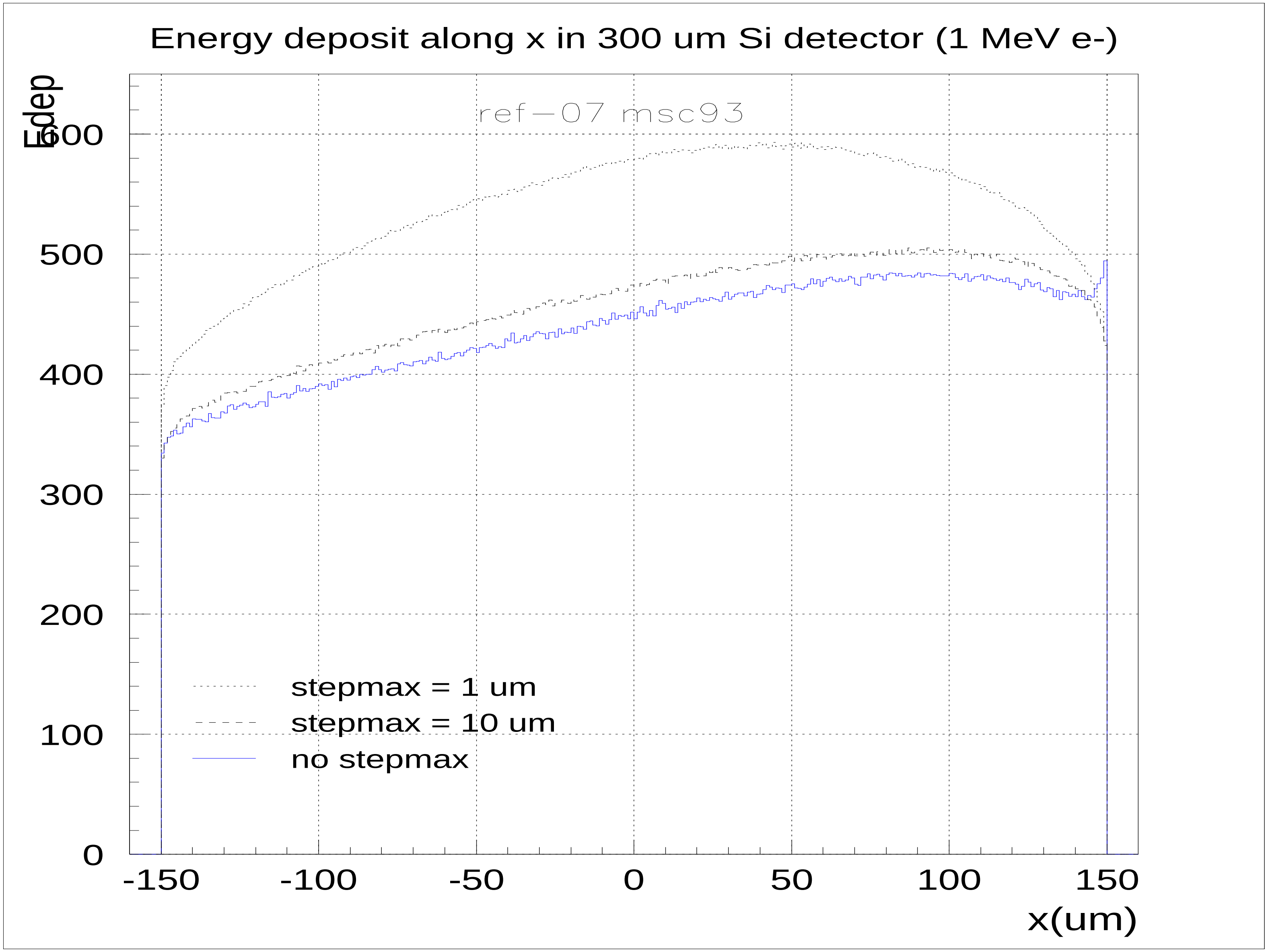

Angular distribution of 15.7 MeV e- after Au foils
Hanson (18.66 mg/cm2)
ref-07 msc95 (18.66 mg/cm2)
Hanson (37.28 mg/cm2)
ref-07 msc95 (37.28 mg/cm2)
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
0
5
10
15
20
25
30
angle(deg)

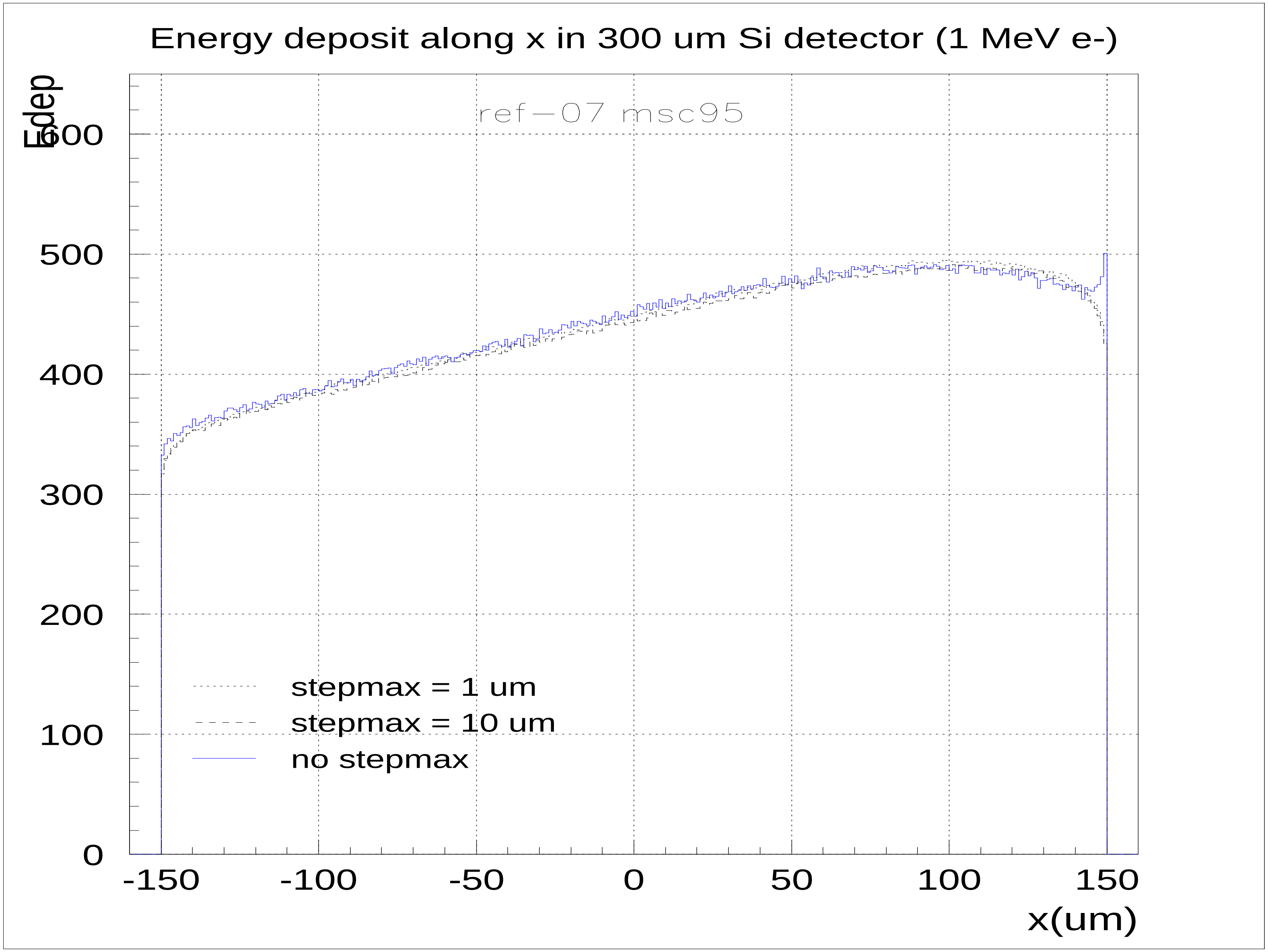

Backscattering of 102 keV e- from different materials
%
cut = 1 keV
data
G4 9.4−00−ref07 msc95
G4 9.4−00−ref07 msc93
0
10
20
30
40
50
0
10
20
30
40
50
60
70
80
90
100
Z

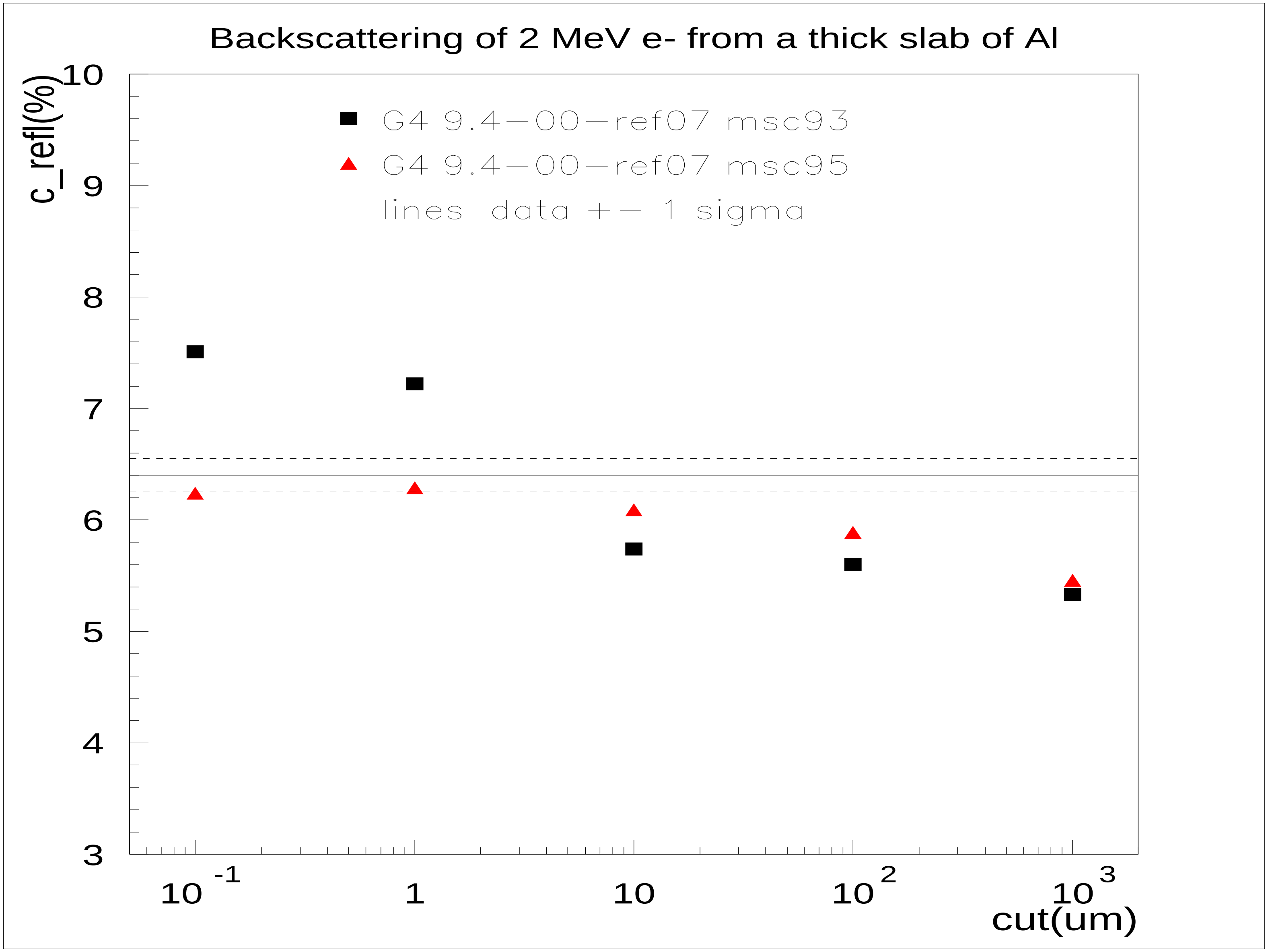
Test/validation results group 2 : stability against step size/cut changes – angular distributions, energy deposit distributions, backscattering


Angular distribution of 15.7 MeV e- after 18.66 mg/cm2 Au
Hanson data
ref-07 msc93
ref-07 msc93 10 steps
ref-07 msc93 100 steps
angle(deg)

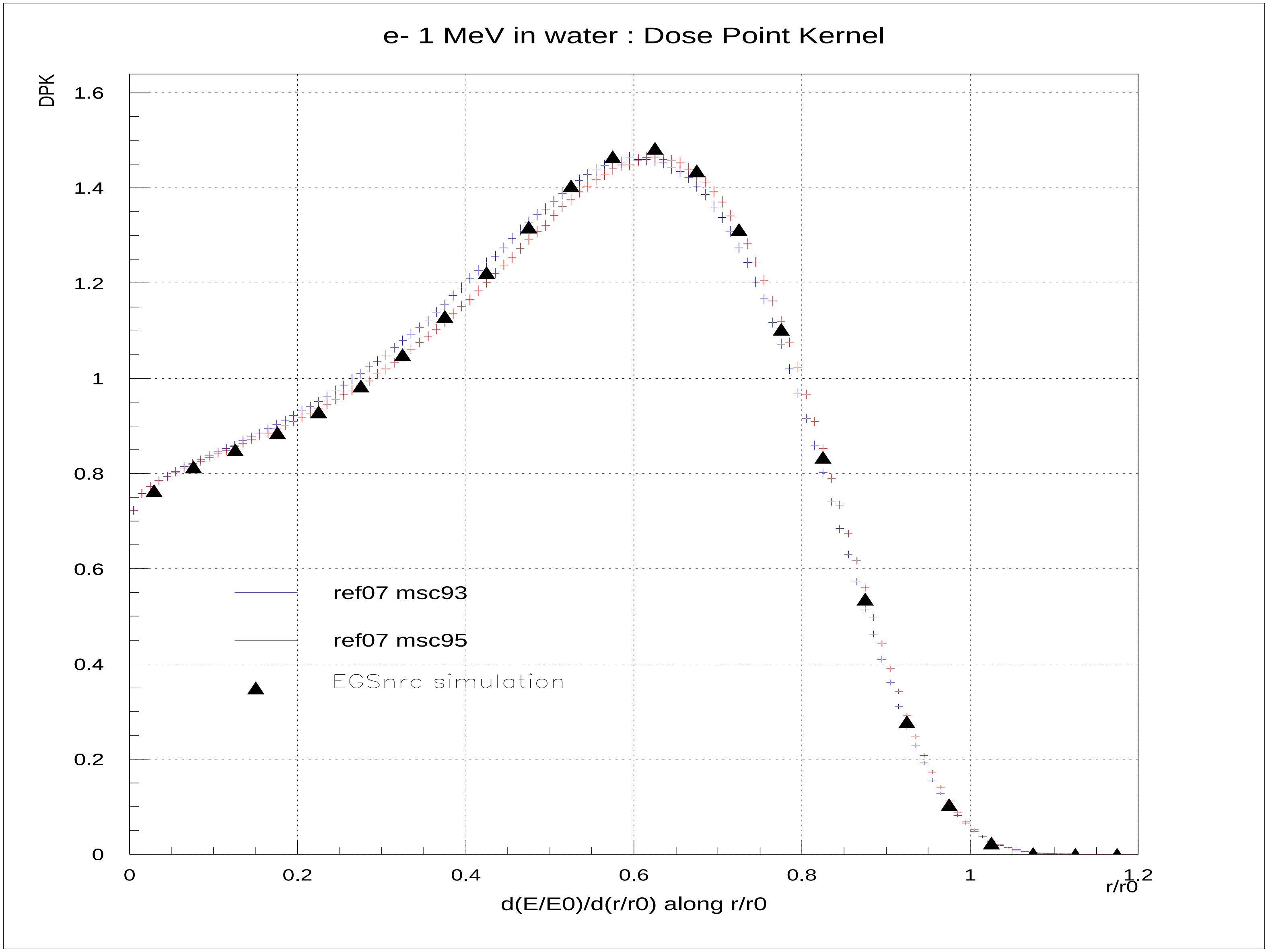

Angular distribution of 15.7 MeV e- after 18.66 mg/cm2 Au
Hanson data
ref-07 msc95
ref-07 msc95 10 steps
ref-07 msc95 100 steps
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
0
5
10
15
20
25
30
angle(deg)

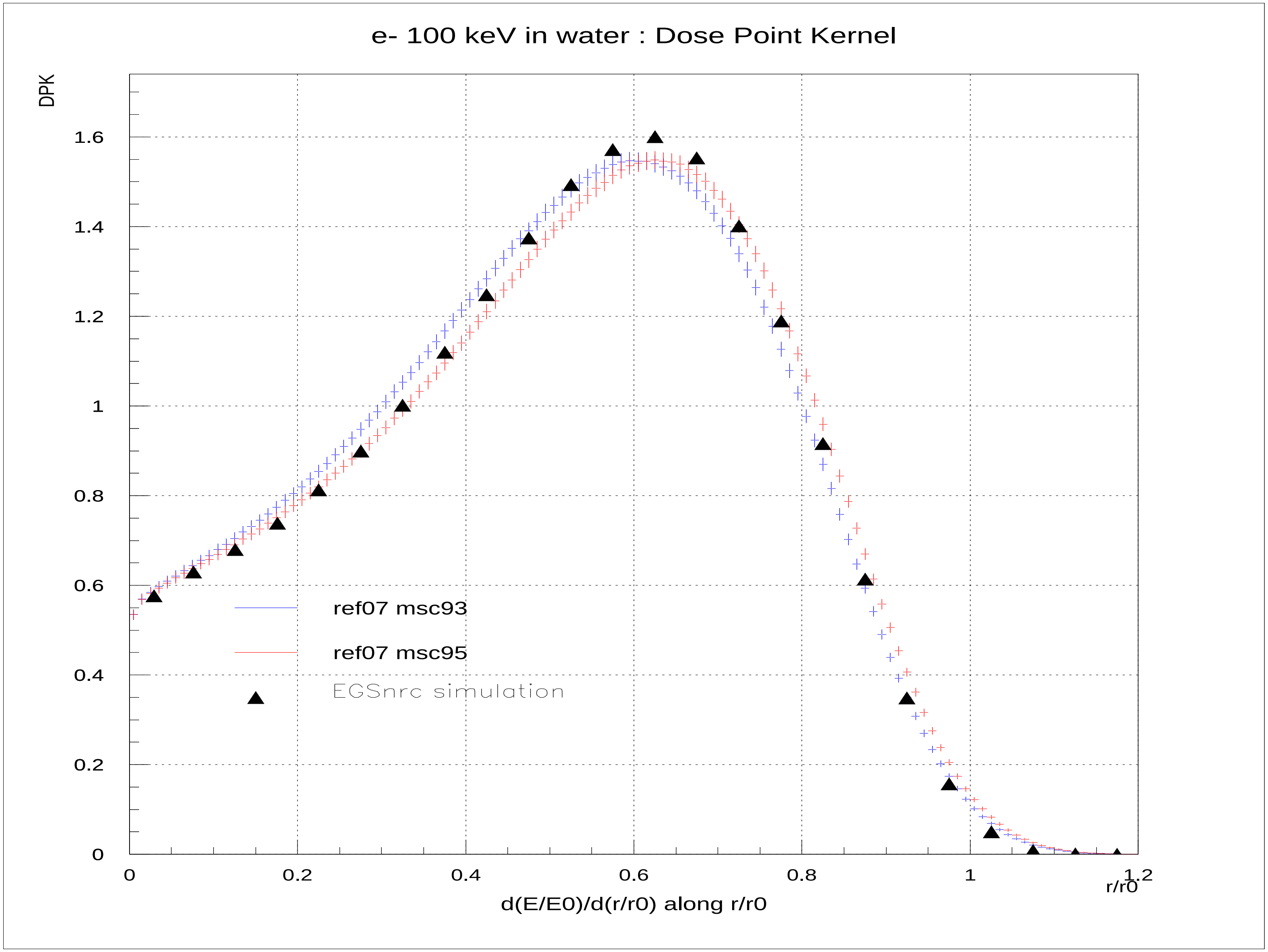

Energy deposit along x in 300 um Si detector (1 MeV e-)
ref−07 msc93
Edep
600
500
400
300
200
100
0
-150
-100
-50
0
50
100
150
x(um)
stepmax = 1 um
stepmax = 10 um
no stepmax

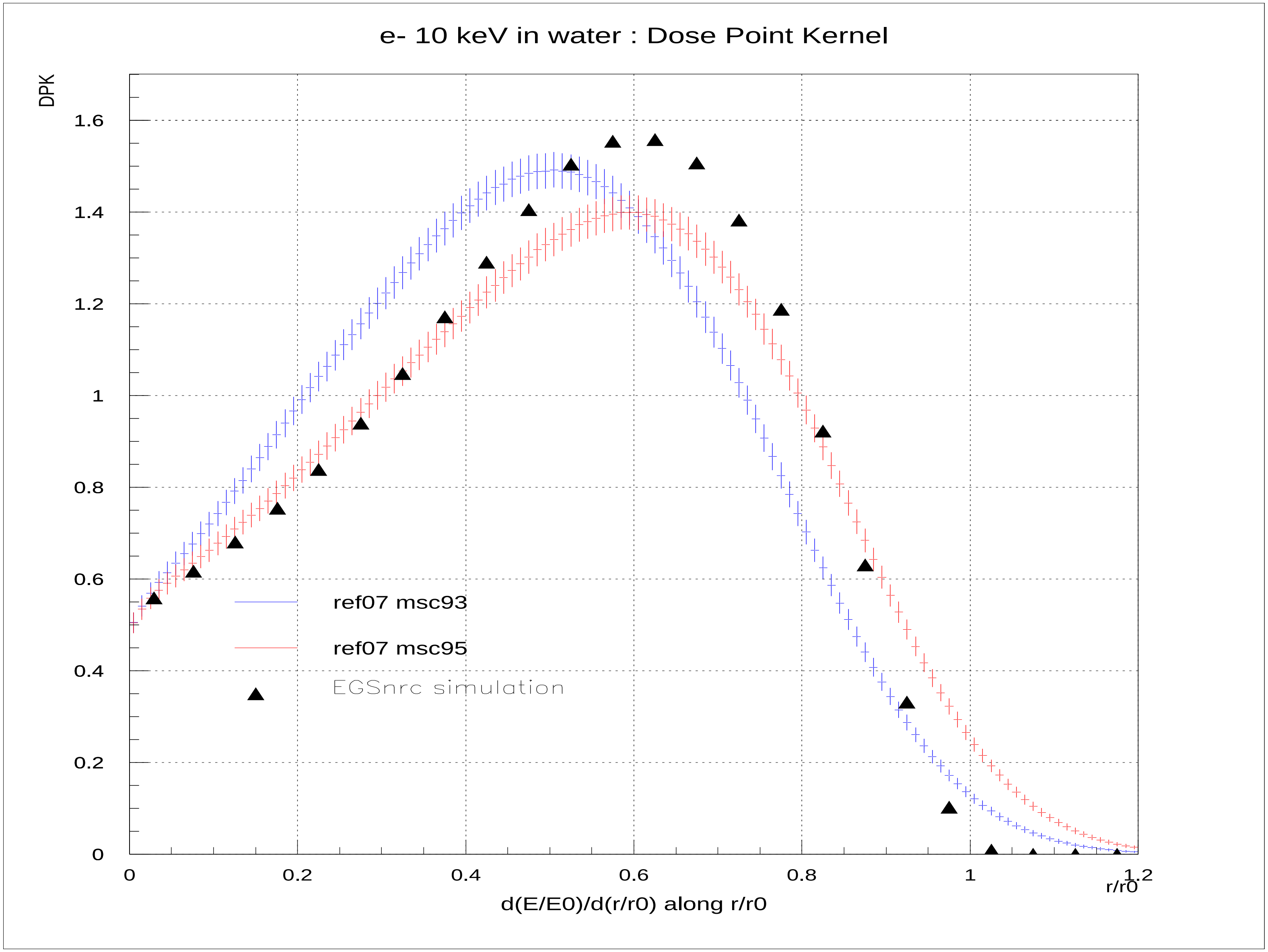

Energy deposit along x in 300 um Si detector (1 MeV e-)
ref−07 msc95
Edep
600
500
400
300
200
100
0
-150
-100
-50
0
50
100
150
x(um)
stepmax = 1 um
stepmax = 10 um
no stepmax


Backscattering of 2 MeV e- from a thick slab of Al
c_refl(%)
10
9
8
7
6
5
4
3
G4 9.4−00−ref07 msc93
G4 9.4−00−ref07 msc95
lines data +− 1 sigma
10 -1
1
10
10 2
10 3
cut(um)

Test/validation results group 3 : dose point kernel for e- in water – msc93 msc95 EGSnrc comparisons


e- 1 MeV in water : Dose Point Kernel
DPK
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1
1.2
r/r0
ref07 msc93
ref07 msc95
EGSnrc simulation
d(E/E0)/d(r/r0) along r/r0


e- 100 keV in water : Dose Point Kernel
DPK
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1
1.2
r/r0
d(E/E0)/d(r/r0) along r/r0
ref07 msc93
ref07 msc95
EGSnrc simulation


e- 10 keV in water : Dose Point Kernel
DPK
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1
1.2
r/r0
d(E/E0)/d(r/r0) along r/r0
ref07 msc93
ref07 msc95
EGSnrc simulation

For low energy neither msc93 nor msc95 are close to EGSnrc, but it seems msc95 is closer than msc93.

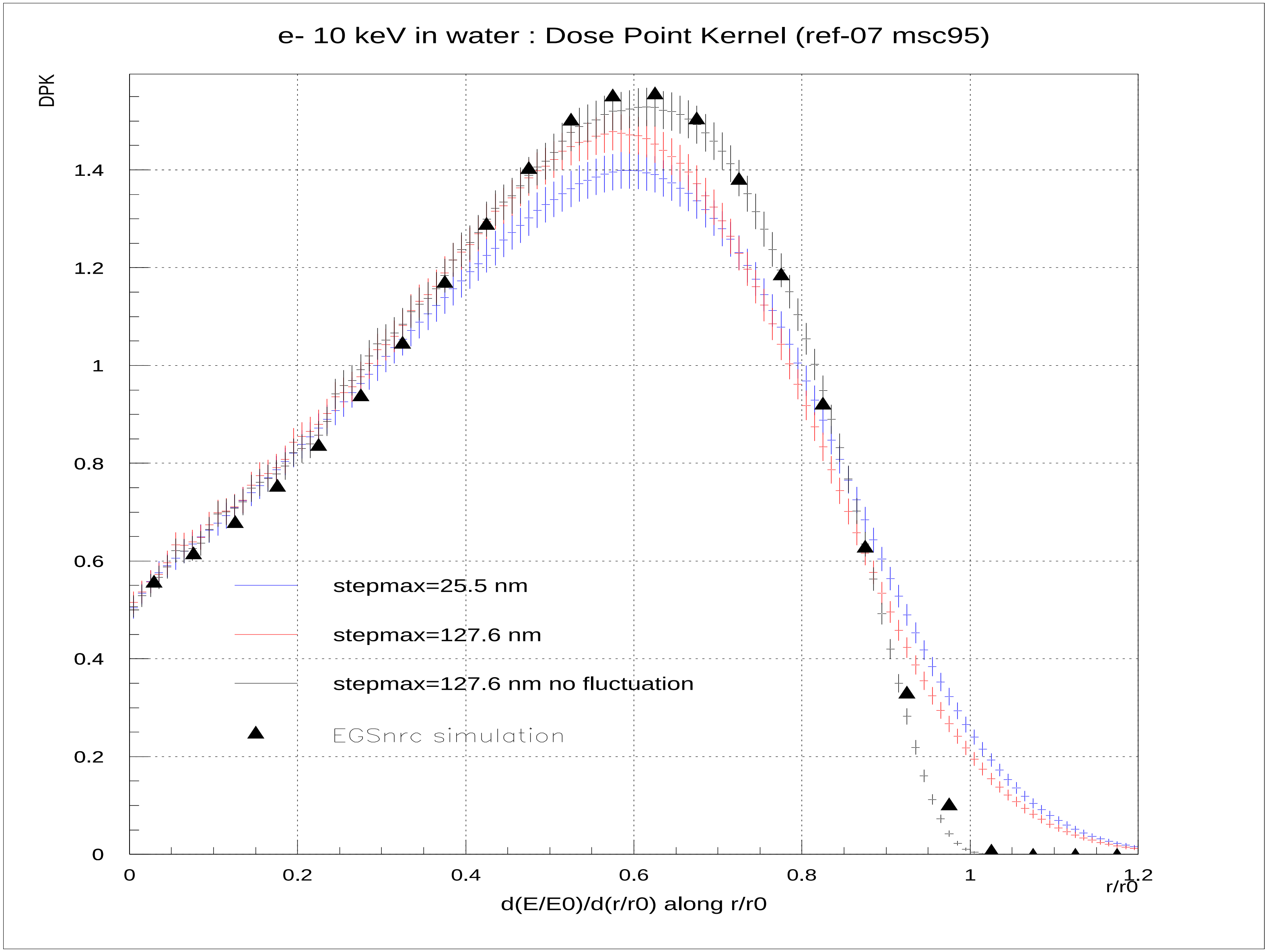
Questions/problems:

The distribution depends on the used stepmax value and stepmax is extremely small for 10 keV stepmax = 25.5 nm. Stepmax is determined from the bin size of the dose point kernel plot.

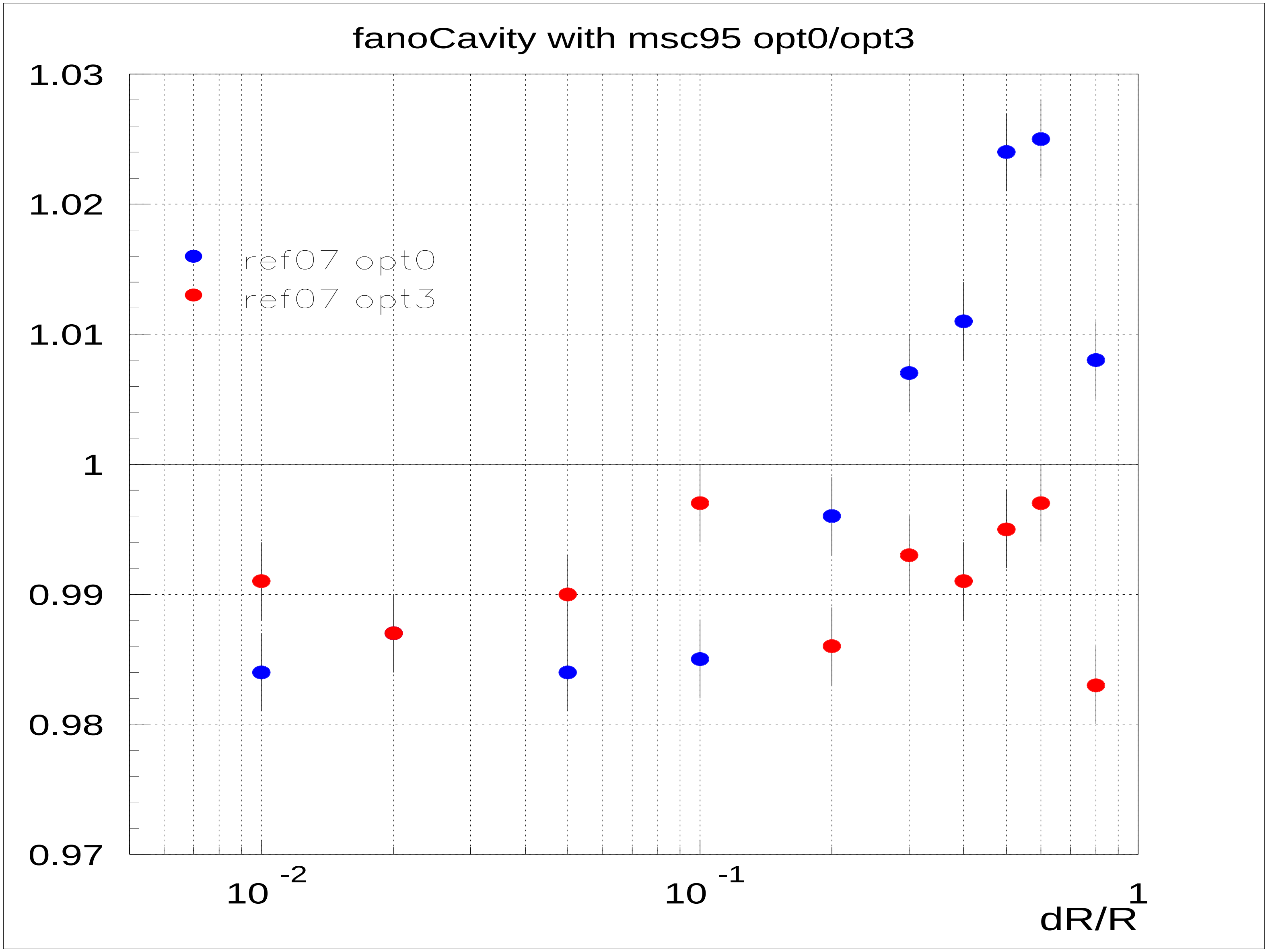
Msc and energy loss fluctuations: how good are they for very small steps?

How good is EGSnrc at 10 keV?

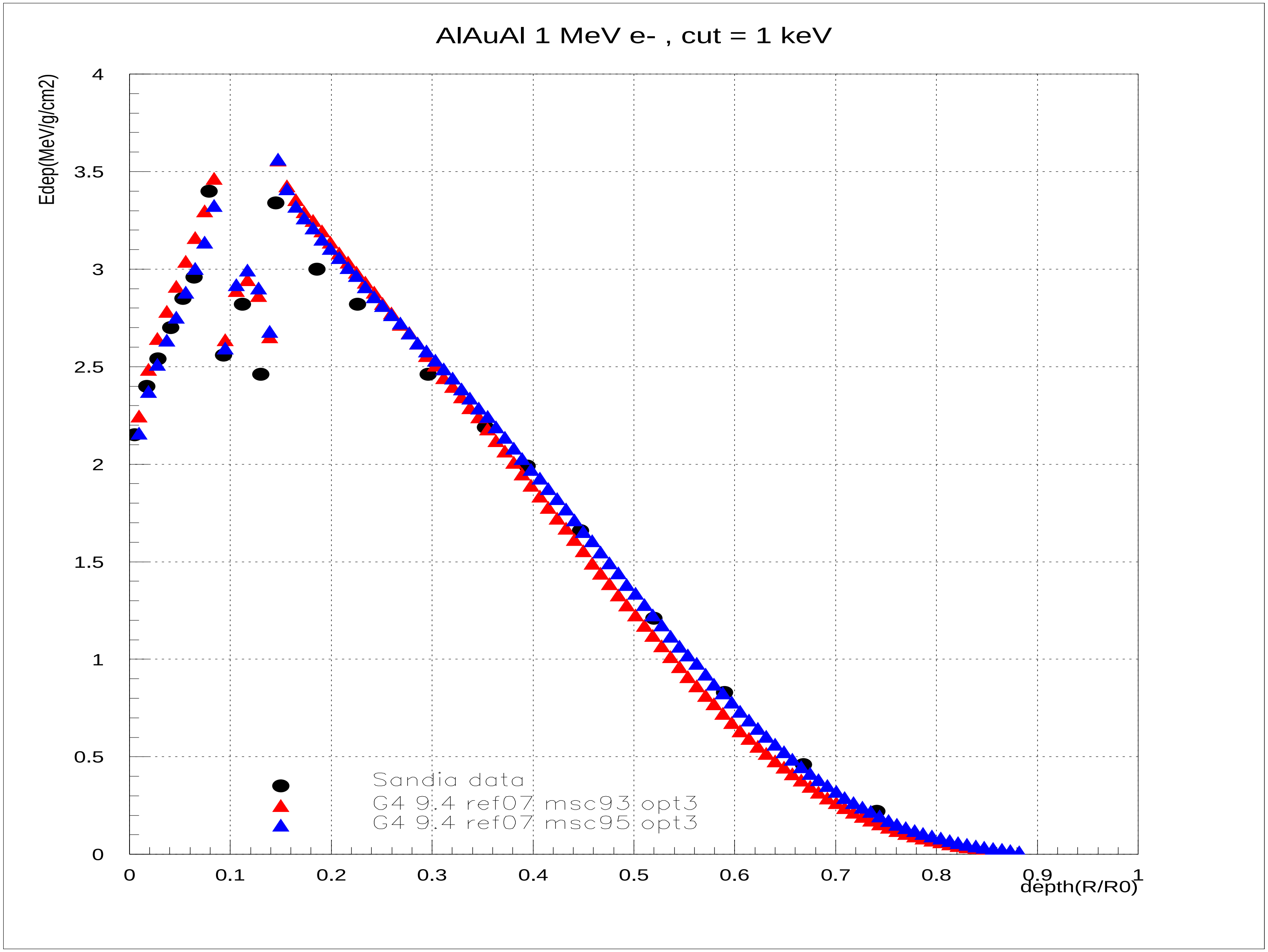
for illustration see next slide


e- 10 keV in water : Dose Point Kernel (ref-07 msc95)
DPK
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1
1.2
r/r0
d(E/E0)/d(r/r0) along r/r0
stepmax=25.5 nm
stepmax=127.6 nm
stepmax=127.6 nm no fluctuation
EGSnrc simulation

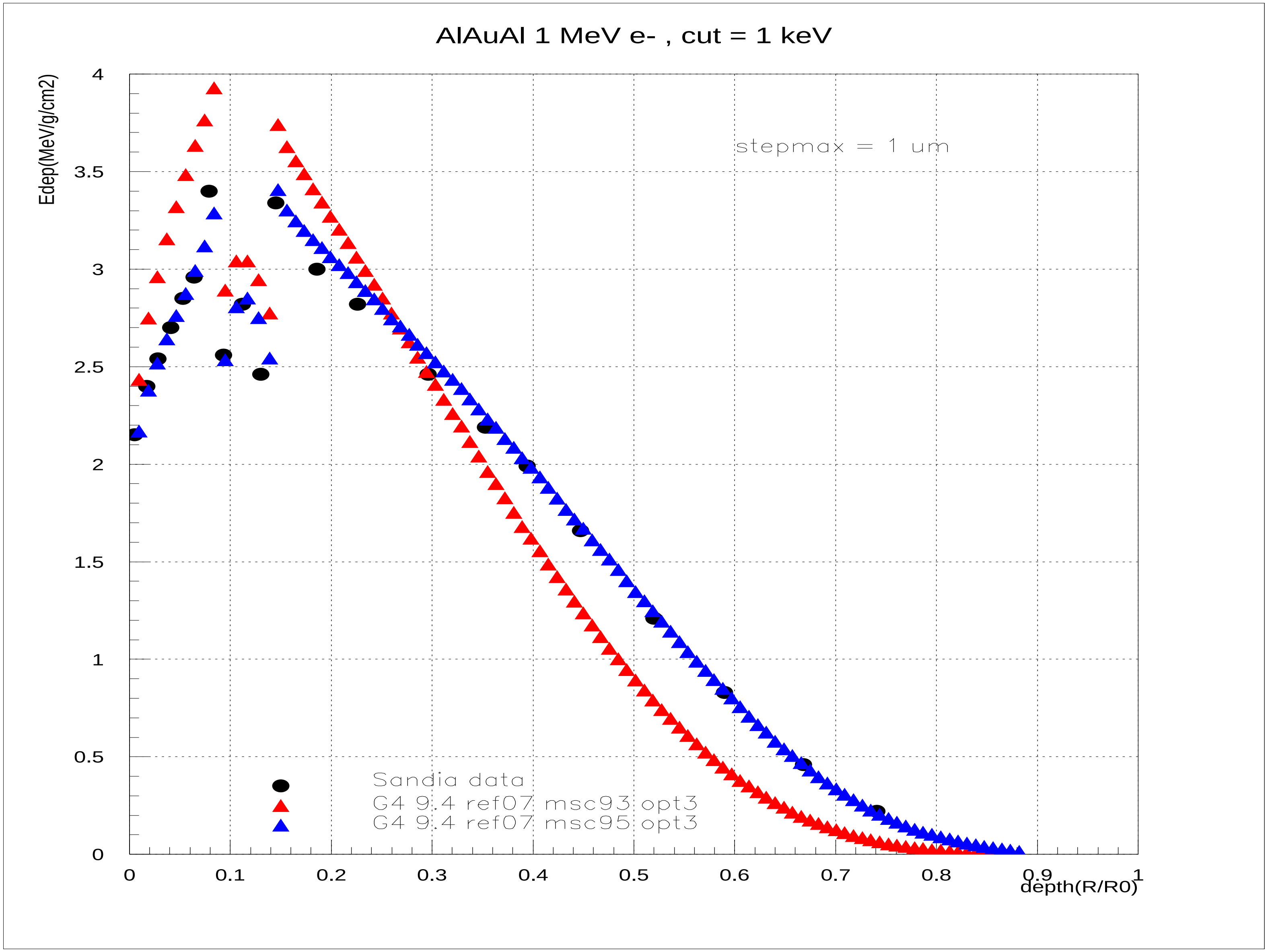
Fano cavity test: msc95 gives small improvement for opt=0 and definitive improvement for opt=3. I have here msc95 plot only, msc93 result can be seen on cern.ch
https://vnivanch/verification/verification/electromagnetic/fanoCavity


fanoCavity with msc95 opt0/opt3
1.03
1.02
1.01
1
0.99
0.98
0.97
ref07 opt0
ref07 opt3
10 -2
10 -1
1
dR/R

Last example : energy deposit distribution in a multilayer slab
171 um Al + 22 um Au + 1517 um Al, 1 MeV e-
msc93 - msc95 - Sandia data comparison, opt 3 simulation.
Both msc93 and msc95 are relatively close to data, alhough msc93 distribution looks a little short, see next slide.


AlAuAl 1 MeV e- , cut = 1 keV
Edep(MeV/g/cm2)
depth(R/R0)
0
0.5
1
1.5
2
2.5
3
3.5
4
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
Sandia data
G4 9.4 ref07 msc93 opt3
G4 9.4 ref07 msc95 opt3

We are interested at the spatial distribution of the energy deposit, so the next slide shows the results with a small stepmax = 1 um. It can be seen that in this case msc93 gives a too short and distorted distribution while msc95 is nearly perfect. This example shows again that msc95 has a better stability when we change the size of the step.


AlAuAl 1 MeV e- , cut = 1 keV
Edep(MeV/g/cm2)
stepmax = 1 um
Sandia data
G4 9.4 ref07 msc93 opt3
G4 9.4 ref07 msc95 opt3
depth(R/R0)
0
0.5
1
1.5
2
2.5
3
3.5
4
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9

Conclusion :

- msc95 gives better angular distributions than msc93
- the stability of the results is far better in msc95.

Timing: msc95 with opt=3 is ≈ same for thin layers, slower by 5 - 10 % for fanoCavity, slower by 10-15 % for the multilayer case msc95 with opt=0 has about the same timing than msc93 with opt=0 (at least on my Mac)