Geant4 and Fano cavity : where are we ?

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Outline

The Fano cavity setup allows to test the quality of low energy electrons transport algorithms

Fano cavity principle

Electron transport algorithm in Geant4

step limitation - end of step

Evolution of the electron transport algorithm

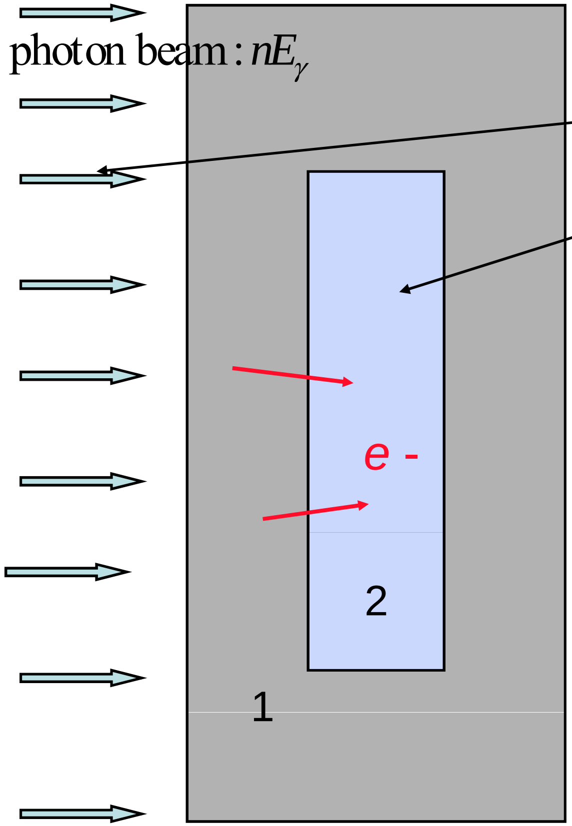
mean energy loss and energy fluctuation computation

multiple scattering

Global effect

Fano cavity principle

Materials 1 and 2 : same A, but different density ρ1 and ρ2 $\Rightarrow \left(\frac{1}{\rho}\frac{dE}{dx}\right)_1 = \left(\frac{1}{\rho}\frac{dE}{dx}\right)_2$



beam energy fluence : $\Phi = \frac{nE_\gamma}{S_1}$

dose in material 2 : D

energy transfert coefficient : $\mu_{tr}(E_\gamma) = \sigma_{tot}(E_\gamma)\frac{\langle T \rangle}{E_\gamma}$

$\langle T \rangle$ is the mean kinetic energy of emited e^-

Under *charged particle equilibrium* condition :

$$\frac{D}{\Phi(E_\gamma)} = \left(\frac{\mu_{tr}(E_\gamma)}{\rho}\right)_1 = \text{const}$$

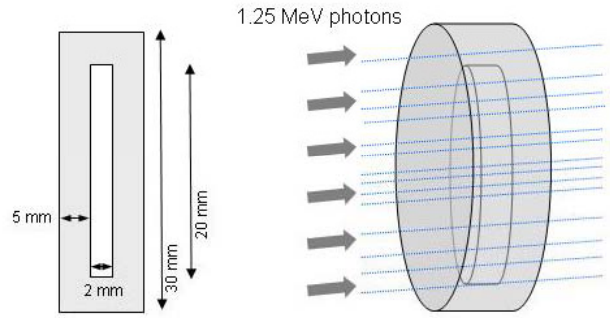
i.e. independent of the tracking parameters of the simulation

Geant4 v 6.2 results

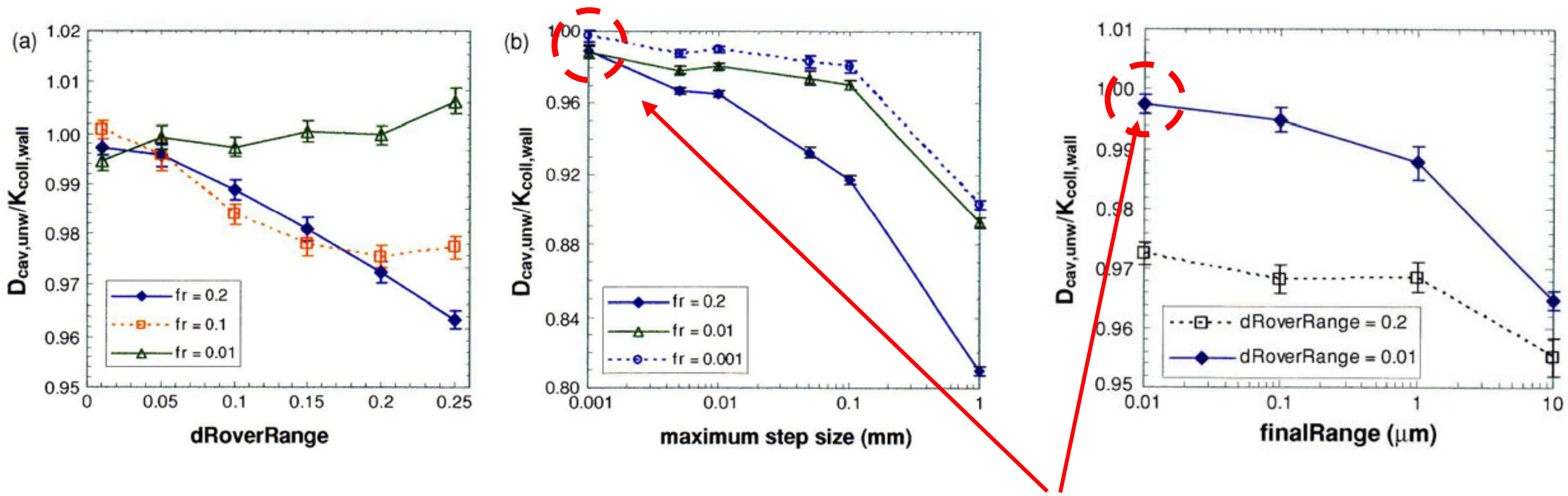
E. Poon and al. (Phys. Med. Biol, Feb 2005)

Evaluation of the consistency of the cavity response for different parameters of Geant4

Defining $K = \left(\frac{\mu_{tr}}{\rho}\right)\Phi$ basic equation becomes $\frac{D}{K} = 1$



Ionization chamber



Most accurate results for Fano test

G4 6.2 default parameters : dRoverRange=1, RangeFactor=0.2

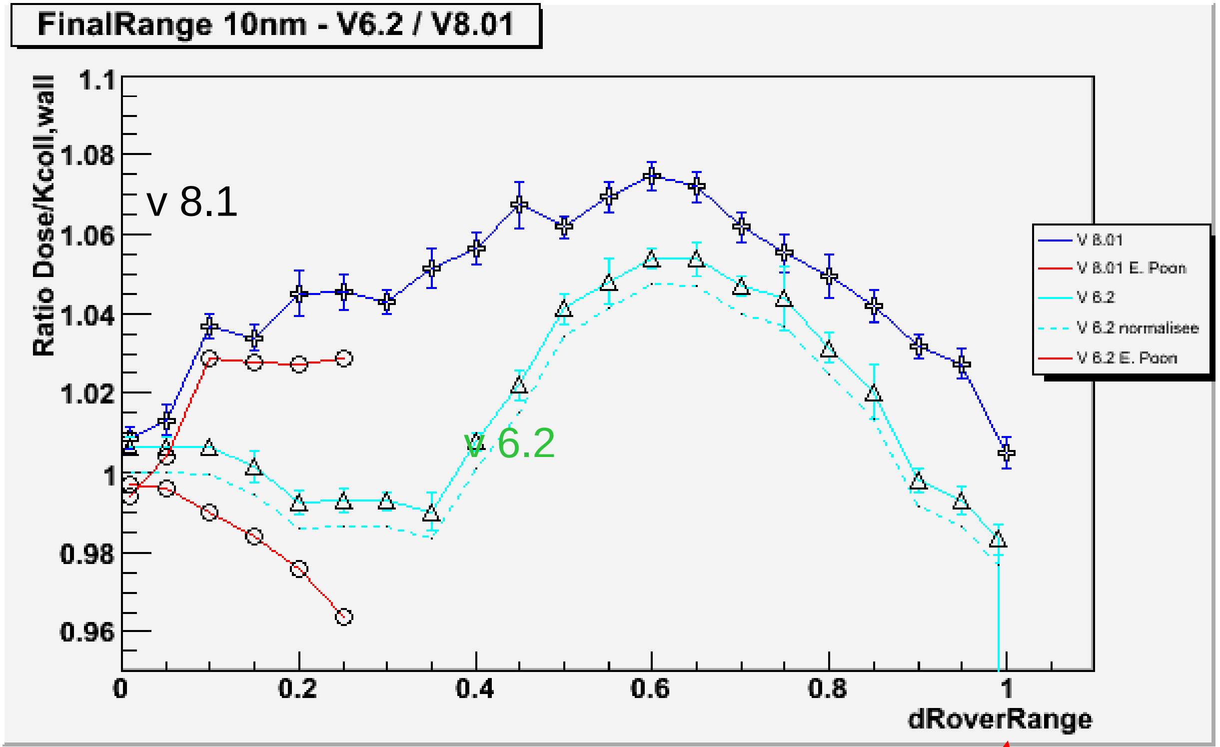
Work done under Continuous Slow Down Approximation (CSDA)

Geant4 v 6.2 vs 8.01

First step : reproduce 6.2 results and test 8.01 release

v 6.2 : RangeFactor = 0.2
v 8.1 : RangeFactor = 0.02

~ 4.10^{8} events per point



v 6.2 : aberrant point for dRoverRange = 1

Electron transport algorithm in Geant4 : e^- step limitation from physics

There are 4 step limitation constraints :

Ionization and brems production threshold (*aka Cut*) ❶

Continuous energy loss

max fractional energy loss per step. Step/Range < *dRoverRange*

down to a certain limit : *finalRange* ❷

Multiple scattering

limit defined at first step and reevaluated after a boundary, to allow back scattering of low energy e^-

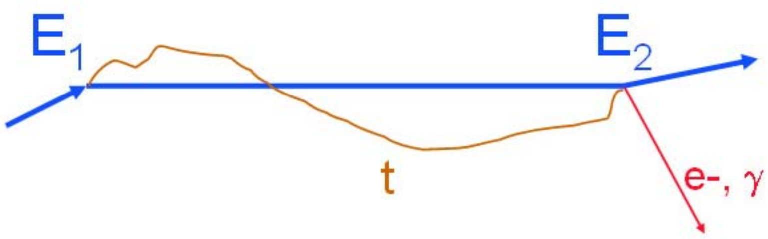
step = *RangeFactor* $*$ max(range,λ) ❸ (λ : transport mean free path)

geometry : force more than 1 step in any volume : *GeomFactor* ❹

Electron transport algorithm in Geant4 : end of a step

multiple scattering ⇨ true path length t computation
compute mean energy loss along t : $<\Delta E>$
add energy loss fluctuation : $dE = f(<\Delta E>)$

multiple scattering again ⇨ lateral displacement and deflection
secondary generation, if any : e- or γ , energy T_{kin}



Energy balance

$$E_1 - E_2 = <\Delta E> + dE + T_{kin}$$

Evolution of the electron transport algorithm since version 8.0

The main evolutions concern :

Mean energy loss and energy fluctuation computation

$$E_1 - E_2 = \langle \Delta E \rangle + dE + T_{kin}$$

Step limitations constraints for multiple scattering process

new default values for *RangeFactor* and *GeomFactor*

Single scattering while crossing boundaries

Mean energy loss computation <ΔE> alone

Mean energy loss computation algorithm :

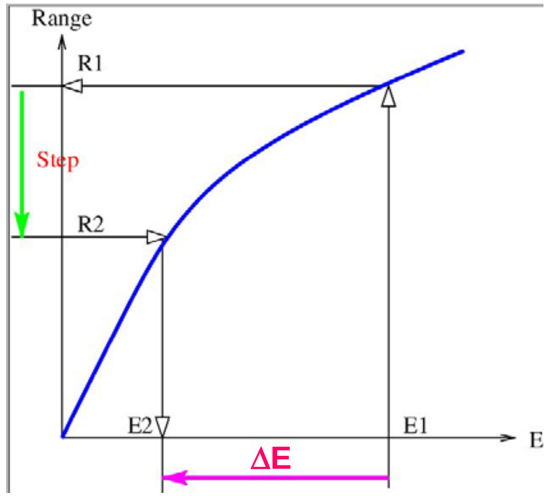
<ΔE> is computed from Range and inverse Range tables :

$$\langle \Delta E \rangle = E(R_1) - E(R_2)$$

For small steps a linear approximation is used :

$$\langle \Delta E \rangle = (dE/dx)*step$$

under the constraint : step/Range < *linLossLimit*



Problem : the default *linLossLimit* (0.05) value was too big

Test case : fluct and msc are switched off

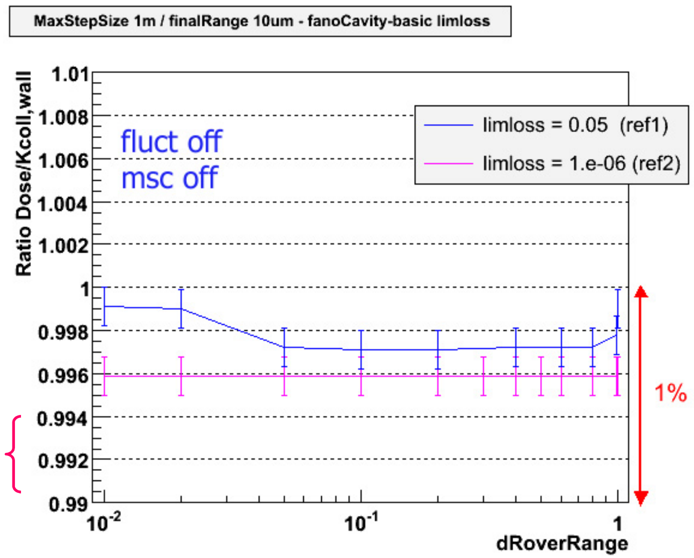
⇨ e- transport determinist and only governed by dRoverRange

(for a fixed value of finalRange = 10 μm)

⇨ new default : *linLossLimit* = 1.e-06

complete stability

but shift ~ 4 per mille



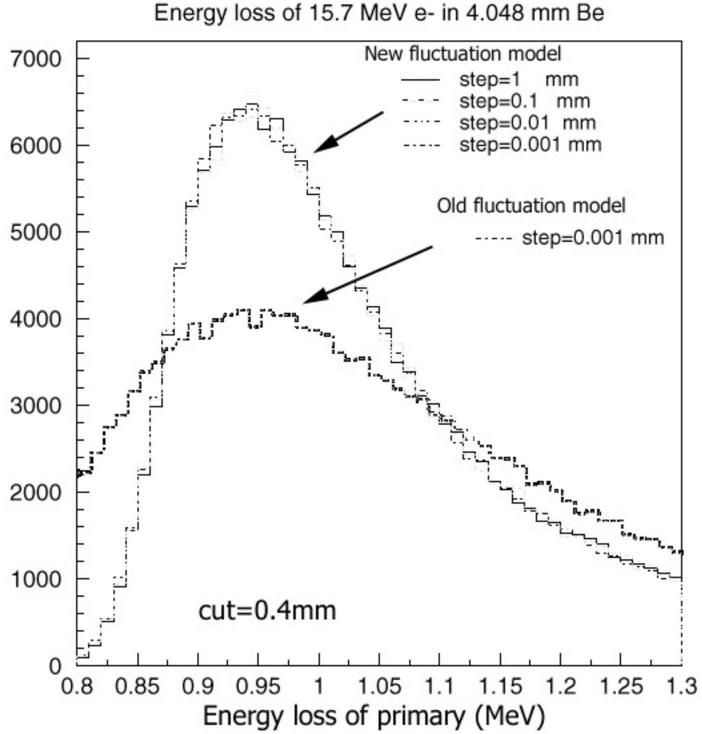
Energy loss fluctuation computation dE alone

In simulation, we cannot use Laudau distribution which assumes no δ-rays production

⇨ double counting

Geant has its own model of fluctuations which is cut and material dependent

(L. Urban, NIM A362(1995) 416)



Problem :

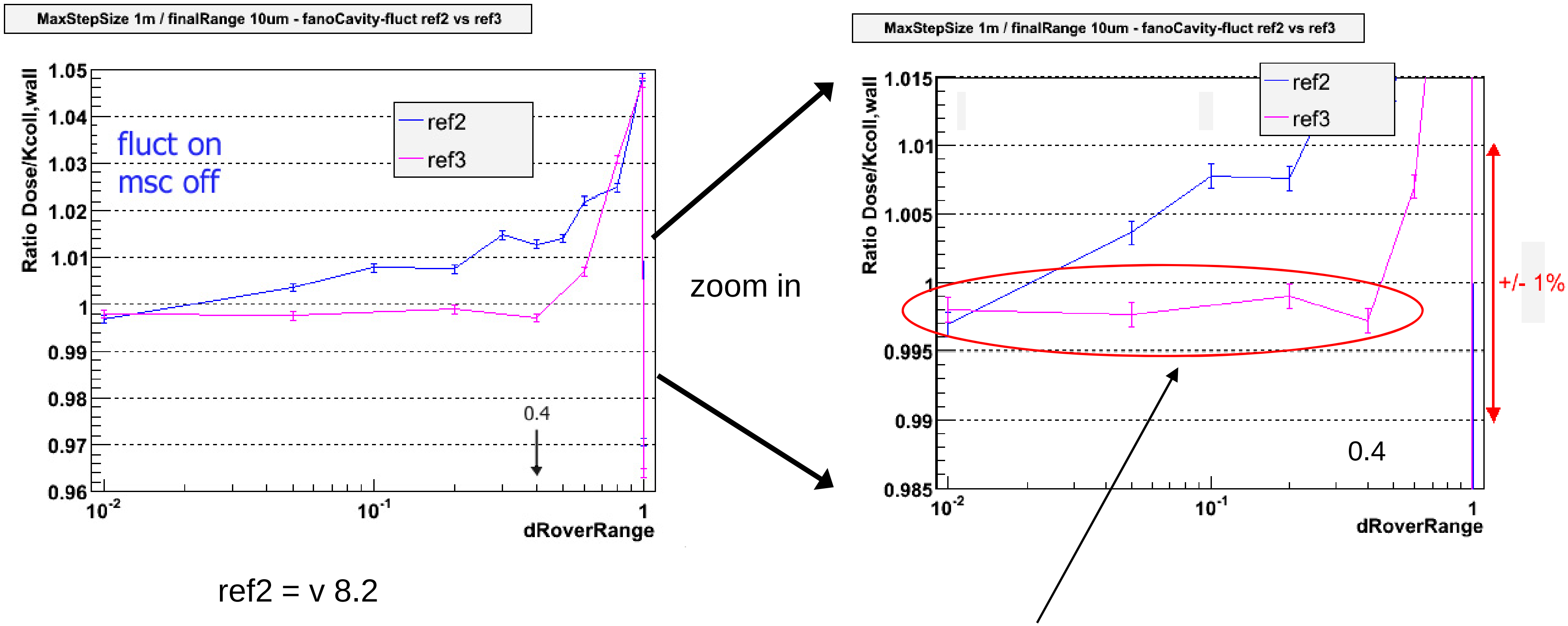
the model was deficient for small energy loss : small steps or in gas

⇨ enhanced model in Geant4 8.2 ref3

(Geant4 Physics Reference Manual, April 2007)

Energy loss fluctuation computation dE alone

Fano cavity response (multiple scattering is switched off)



ref2 = v 8.2

⇨ Stability ~ 3 per mille

Step limitations constraints for multiple scattering

Step limitations

RangeFactor : 0.2 → 0.02, applied to the whole track (v8.0, January 2006)

GeomFactor : 1→3

Multiple scattering final state

single Coulomb scattering near boundaries (ref3, April 2007)

few very small steps (~λ elastic) while crossing boundaries over a thickness defined by *skin**λ

apply approximate single Coulomb scattering

better evaluation of lateral displacement : reevaluate safety radius before to perform lateral displacement

⇨ displ < safety (*safety was often underestimated*)

correlate final direction (u) with lateral displacement (d)

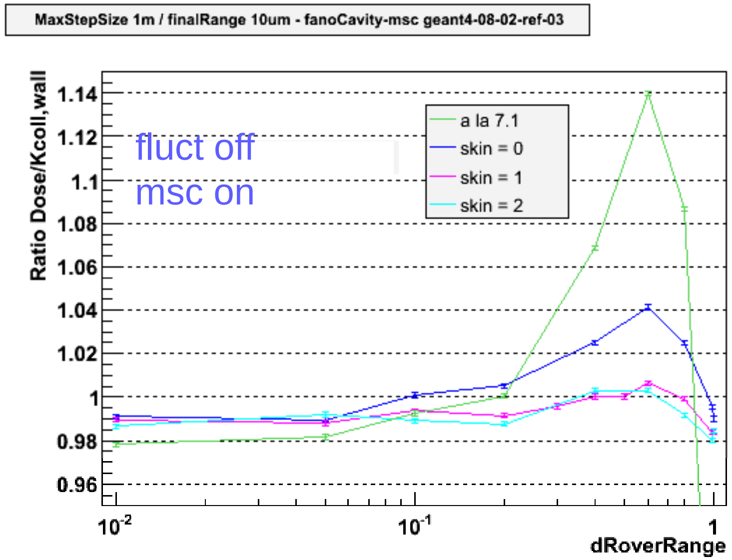
⇨ u.d = f (λ) taken from Lewis theory

angular distribution : both central part and tail slightly modified

Step limitations constraints - multiple scattering alone

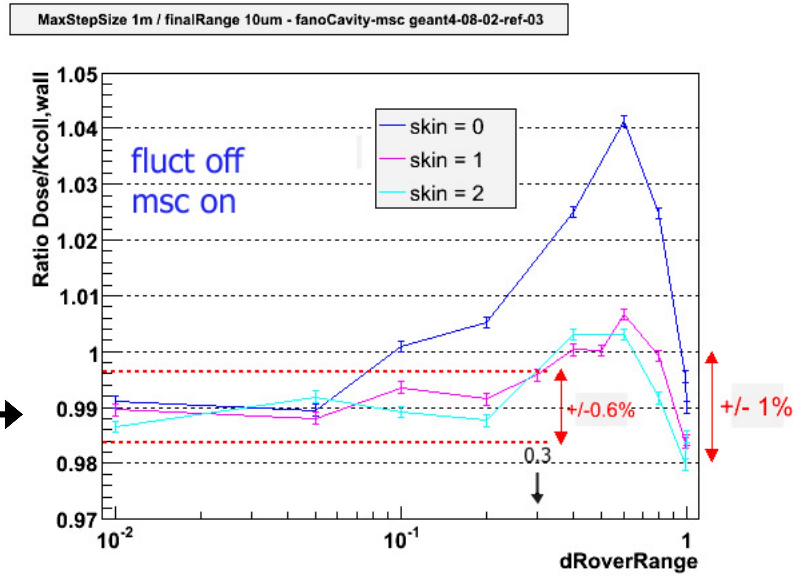
Fano cavity response (fluctuation is switched off)

Comparison with release 7.1



zoom in

Release 8.2



'a la 7.1' : RangeFactor = 0.2

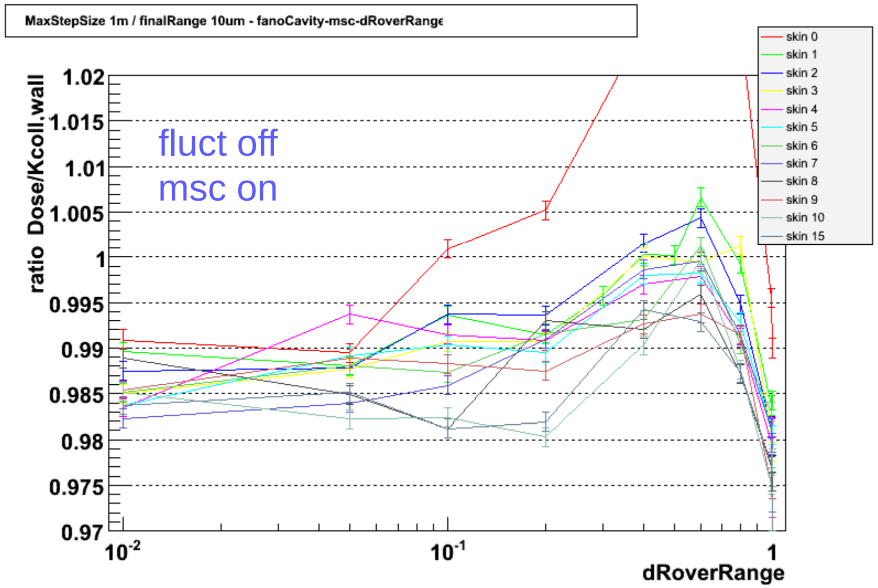
skin = 0 :
- no single scattering at boundary
- no computation to linear distance to boundary

stability within ~ 0.6 %
but shift ~1%

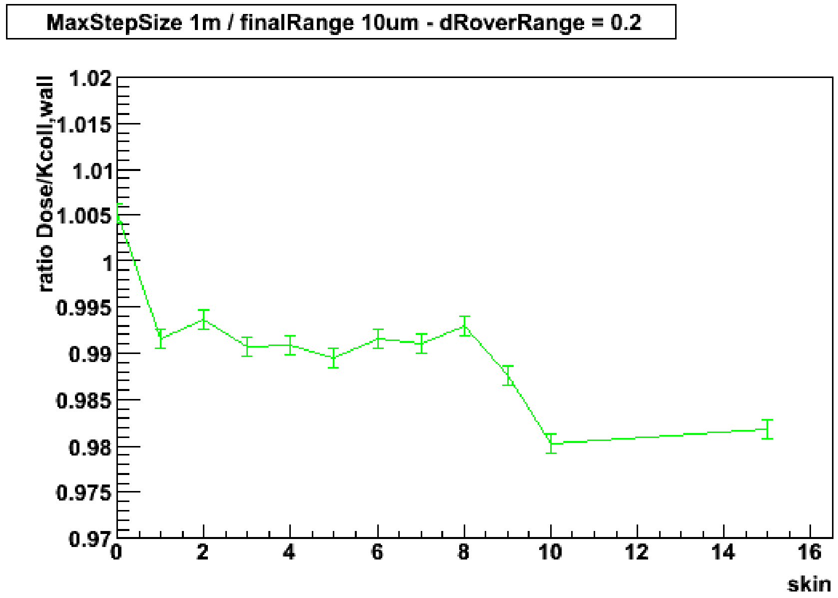
Step limitations constraints - multiple scattering alone

Fano cavity response (fluctuation is switched off)

for *Skin* = 0 to 10



vs *Skin* for dRoverRange=0.2



limit skin value : ~ 4-5

Geant4 release 8-2-ref3 and Fano cavity

All modifications presented in this talk are implemented in release 8-2-ref3

Global effect are shown here :

Default parameter value :

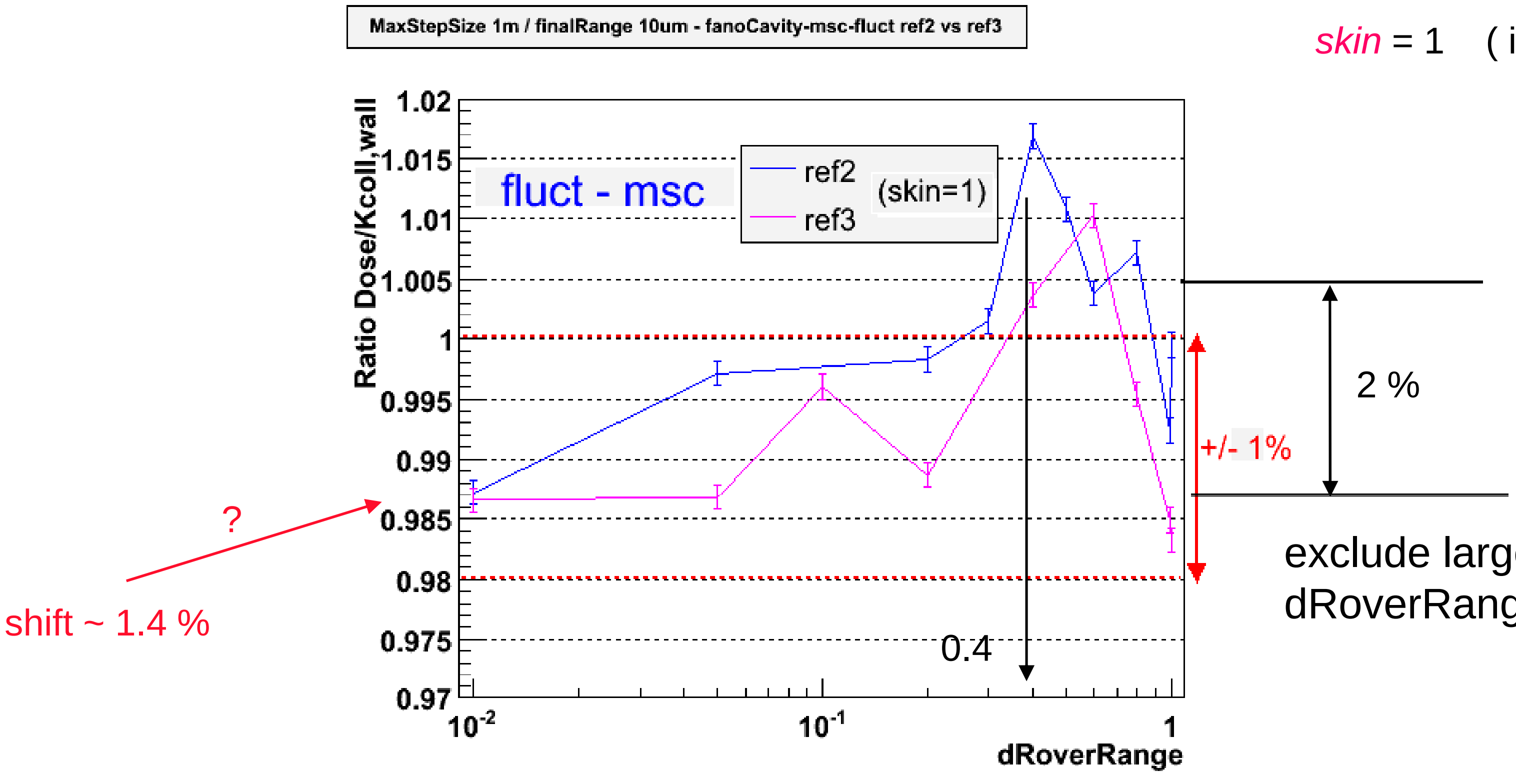
RangeFactor = 0.02

GeomFactor = 3

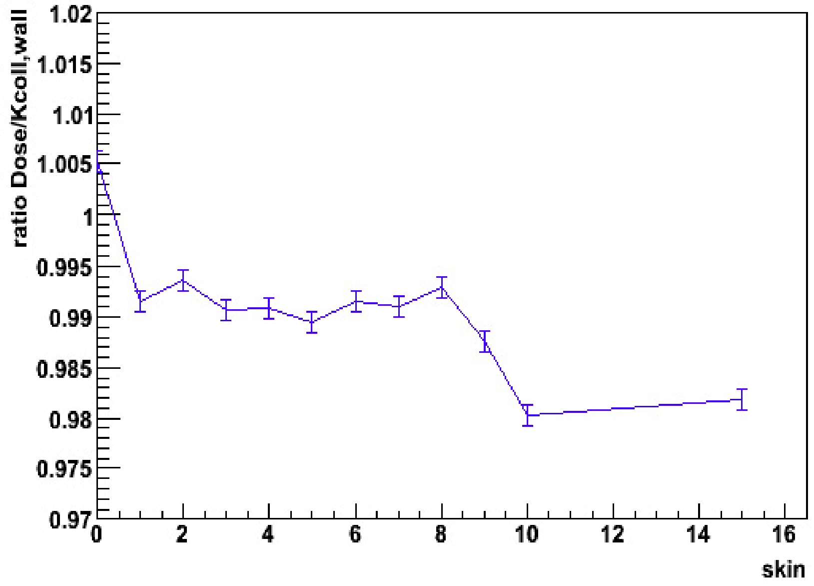
linLossLimit = 1.e-06

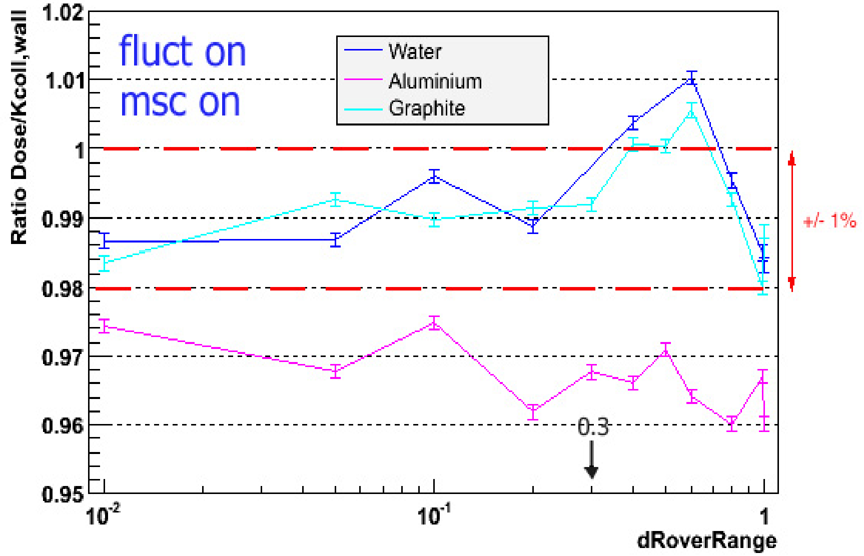
skin = 1 (in G4 9.0)

Release 8.2 vs 8-2-ref3



exclude large values of dRoverRange


ratio Dose/Kcoll,wall
1.02
1.015
1.01
1.005
1
0.995
0.99
0.985
0.98
0.975
0.97
0
2
4
6
8
10
12
14
16
skin


fluct on
msc on
Water
Aluminium
Graphite
Ratio Dose/Kcoll,wall
1.02
1.01
1
0.99
0.98
0.97
0.96
0.95
+/- 1%
0.3
10^{-2}
10^{-1}
1
dRoverRange

Summary

We analyzed the modifications of the Geant4 e- transport algorithms in the context of the Fano cavity setup.

Stability of the mean energy loss computation has been slighty improved (~2 per mille)

Model of energy loss fluctuations has been changed for very small amount of matter. Stability ~3 per mille over a large range of step size limitation

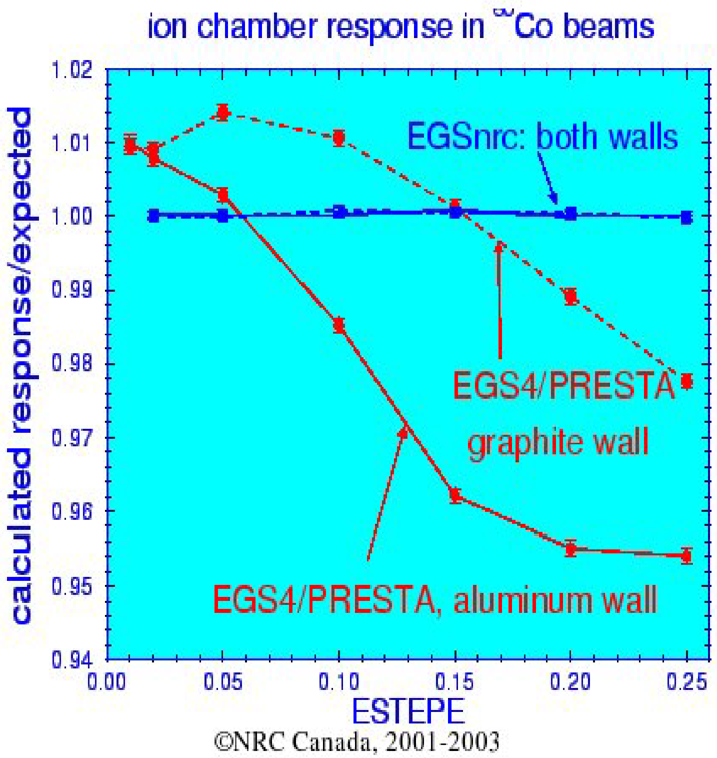
Multiple scattering model has been enhanced in various manners. Relevant features are :

strong constraints on step limitation

single Coulomb scattering near boundaries

⇨ stability ~1.5 % for dRoverRange < 0.3

EGS - Penelope



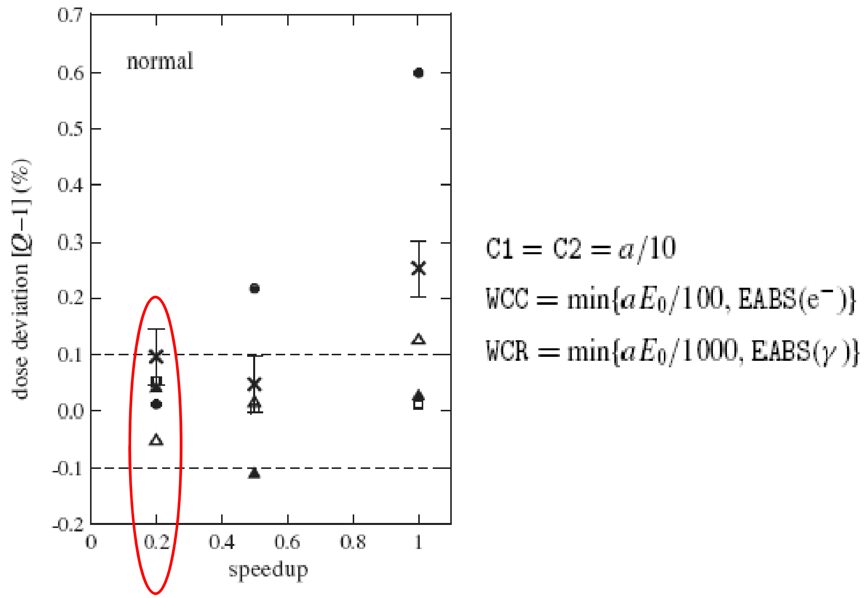


Figure 4. Deviation, in percentage, of the MC calculated dose with respect to the theoretical value as a function of the speedup parameter a. Initially, electrons travel normal to the gas–wall interface with the following kinetic energies: 10 keV (hollow squares), 100 keV (hollow triangles), 1 MeV (dots), 10 MeV (crosses) and 20 MeV (full triangles). All statistical standard uncertainties (1σ) are 0.05% (plotted for the 10 MeV data only) except for the 20 MeV cases for which it is 0.1%. The dashed lines enclose the region where simulation results are compatible with a zero deviation with a confidence level of 95% (68% for the 20 MeV data).

I.Kawrakow *Med.Phys. 27-3 (2000) 499*

J. Sempau et al. *Phys. Med. Bio. 51 (2006) 3533*

Additional comments

Need to be completed

understand the systematic shifts

study the effect of other paramaters

⇨ finalRange, stepMax, productionCut …

Recommanded parameter values and options will be different for bioMedical requirements (highest precision) and HEP-calorimetry usage

examples of Physics Lists

Fano cavity setup is included in our public test serie :

/geant4/examples/extended/medical/fanoCavity

see README

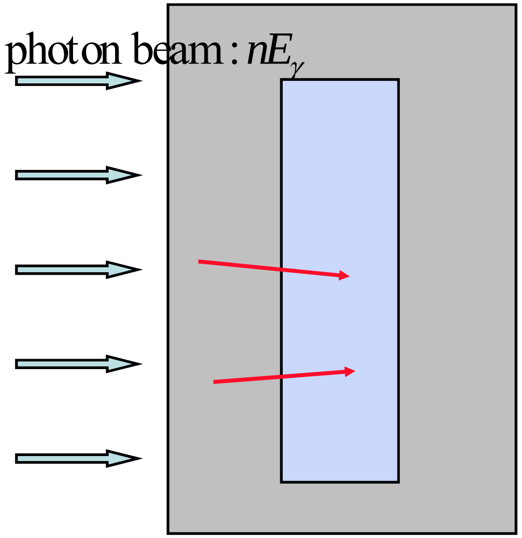
It is automatically executed by System Test Team before every release

Backup slides

Geant4 releases : v6 ⇨ v8

• v6.2	June 2004
• v7.0	January 2005
• v7.1	June 2005
• v8.0	January 2006
• v8.1	June 2006
• v8.2	January 2007
• v8.3	May 2007
• v9.0	June 2007 ?

Energy transfer coefficient

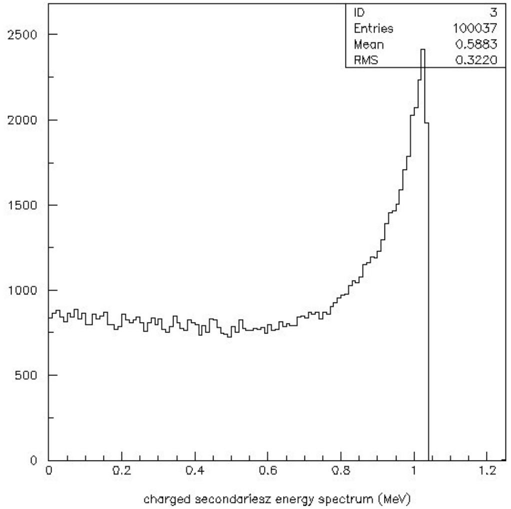


$$\mu_{tr}(E_\gamma) = \frac{1}{E_\gamma}\int_{T_{\min}}^{T_{\max}} \frac{d\sigma_{tot}}{dT} T\, dT = \sigma_{tot}(E_\gamma)\frac{\langle T\rangle}{E_\gamma}$$

σ_{tot} : total cross section per volume

T : kinetic energy of emited e^-

$$\left(\frac{\mu_{tr}(1.25\ \mathrm{MeV})}{\rho}\right)_{water} = 0.02998\ \mathrm{cm}^2/\mathrm{g}$$



From TestEm14:

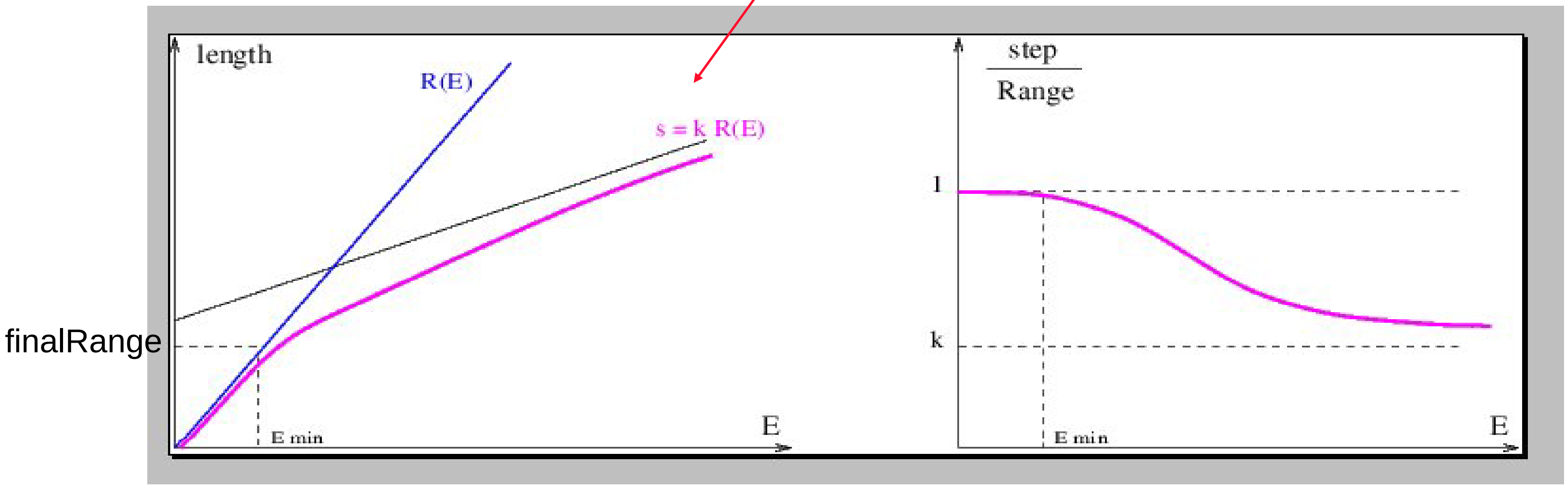
```
The run consists of 100000 gamma of 1.25 MeV through 100 m  of Water (density: 1 g/cm3 )

Process calls frequency --->  compt = 99961  conv = 37      phot = 2

MeanFreePath:  15.704 cm  +- 15.663 cm          massic: 15.704 g/cm2
CrossSection:  0.063678 cm^-1                   massic: 0.063678 cm2/g

mean energy of charged secondaries: 588.52 keV ---> mass_energy_transfer coef: 0.029981 cm2/g

Verification : crossSections from G4EmCalculator
        compt= 0.063447 cm2/g   conv= 2.0941e-05 cm2/g  phot= 2.2833e-06 cm2/g  total= 0.06347 cm2/g

User=8.3s Real=8.7s Sys=0.07s
```

Step limitation from continuous energy loss

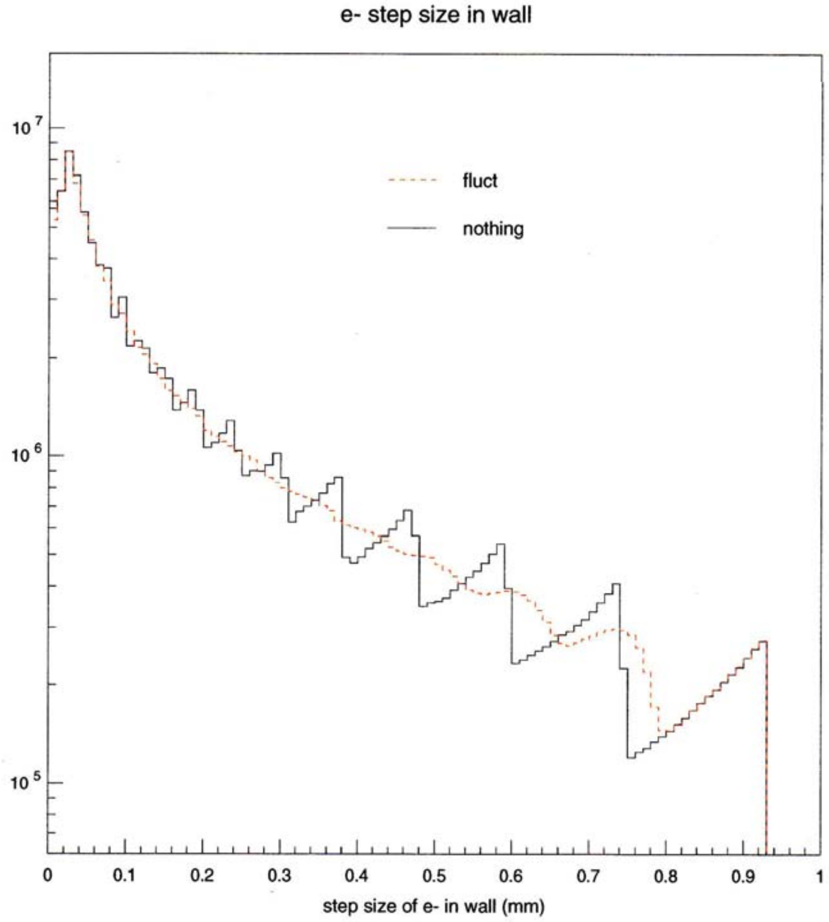
- The cross sections depend on the energy. The step size must be small enough to ensure a small fraction of energy loss along the step :

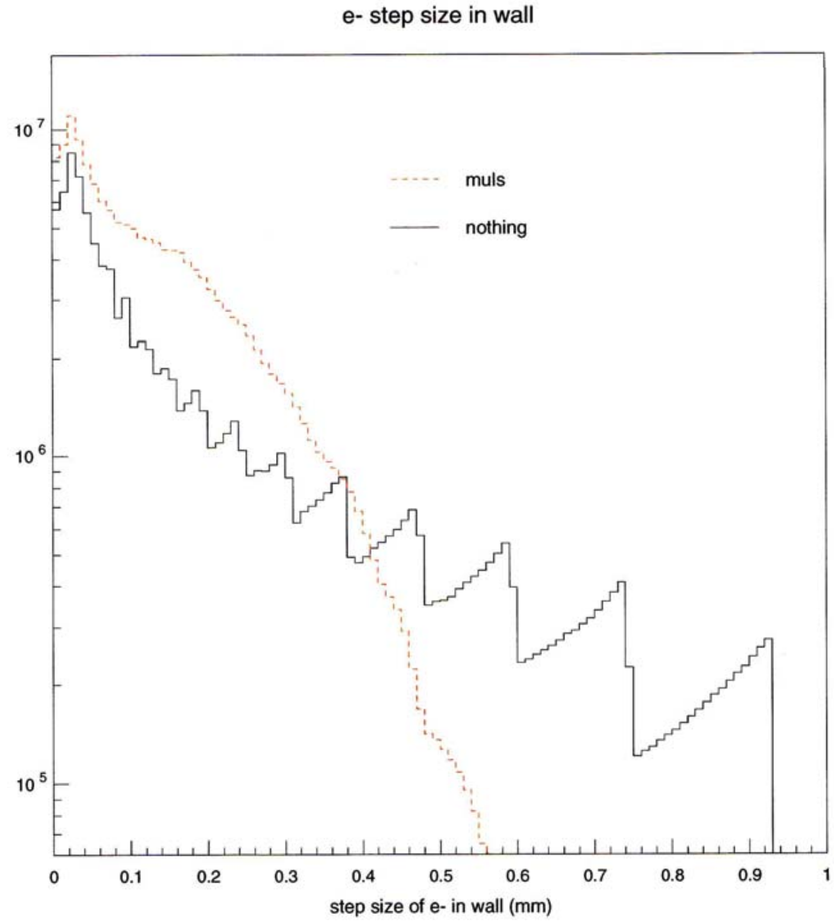
$$\frac{\text{step}}{\text{Range(E)}} \le \text{dRoverRange} \quad \begin{cases} 1 \text{ in G4 v6. and v7.} \\ 0.2 \text{ elsewhere} \end{cases}$$

- This constraint must be relaxed when E → 0

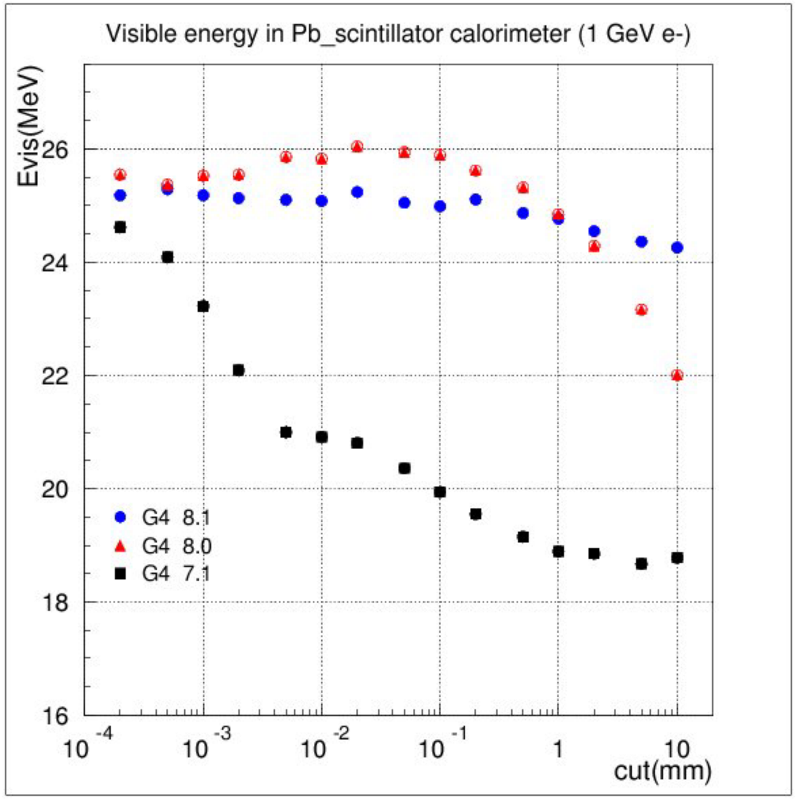


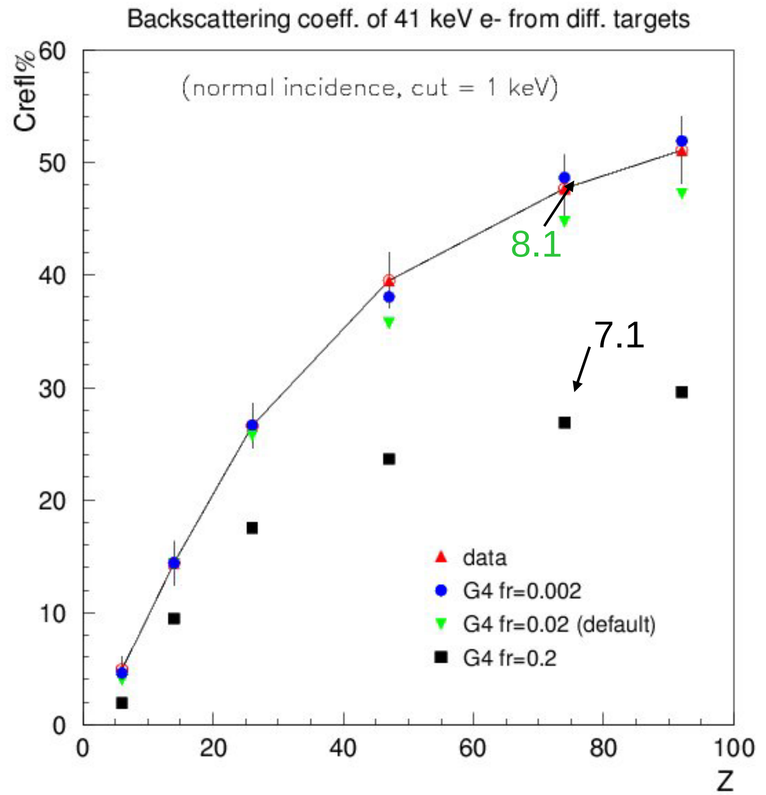
Step limitation competition



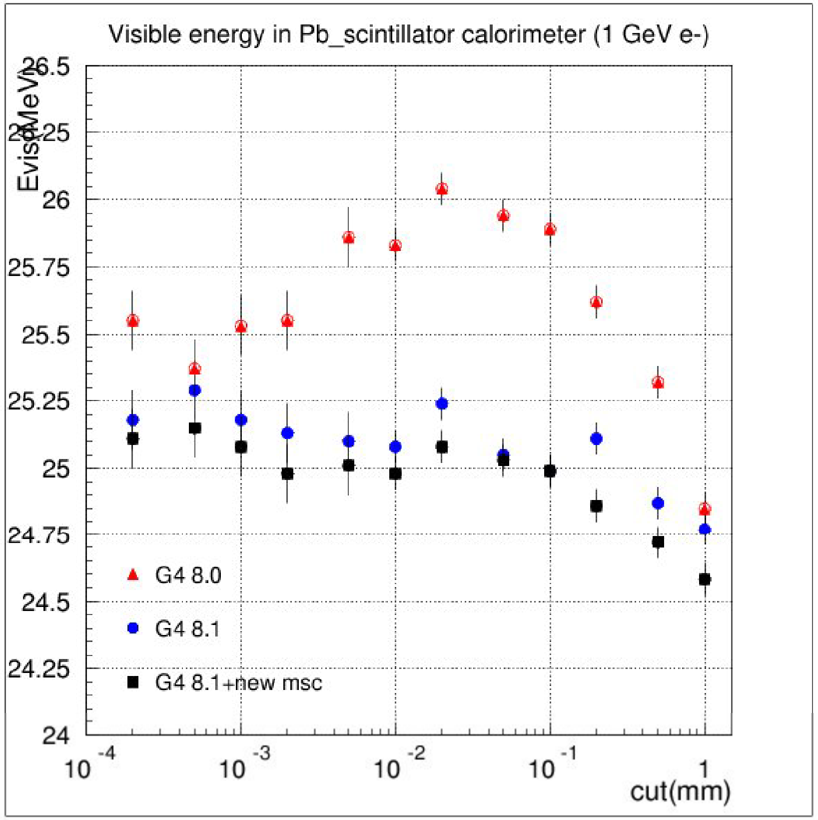


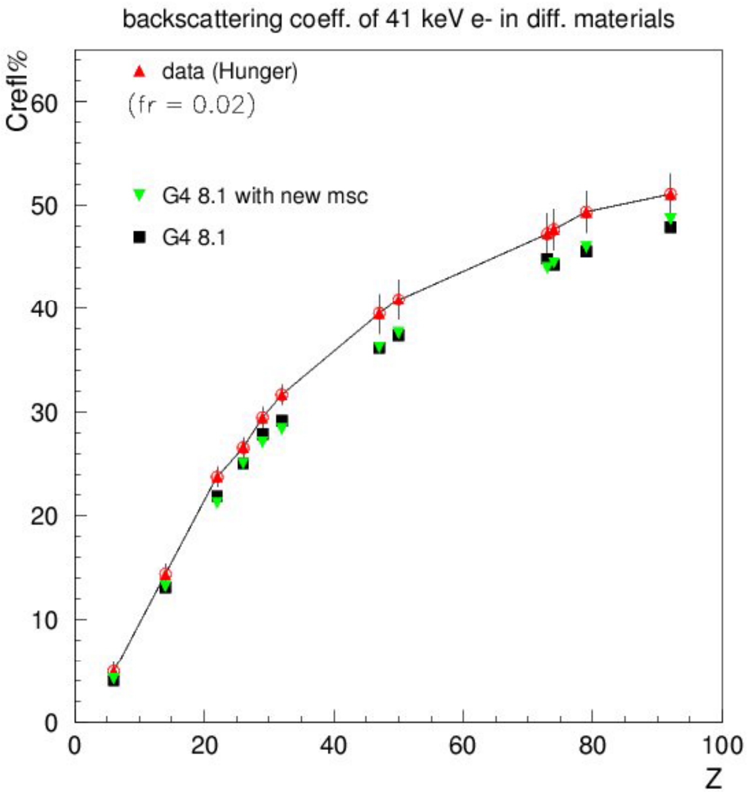
Sampling calorimeter : cut dependance





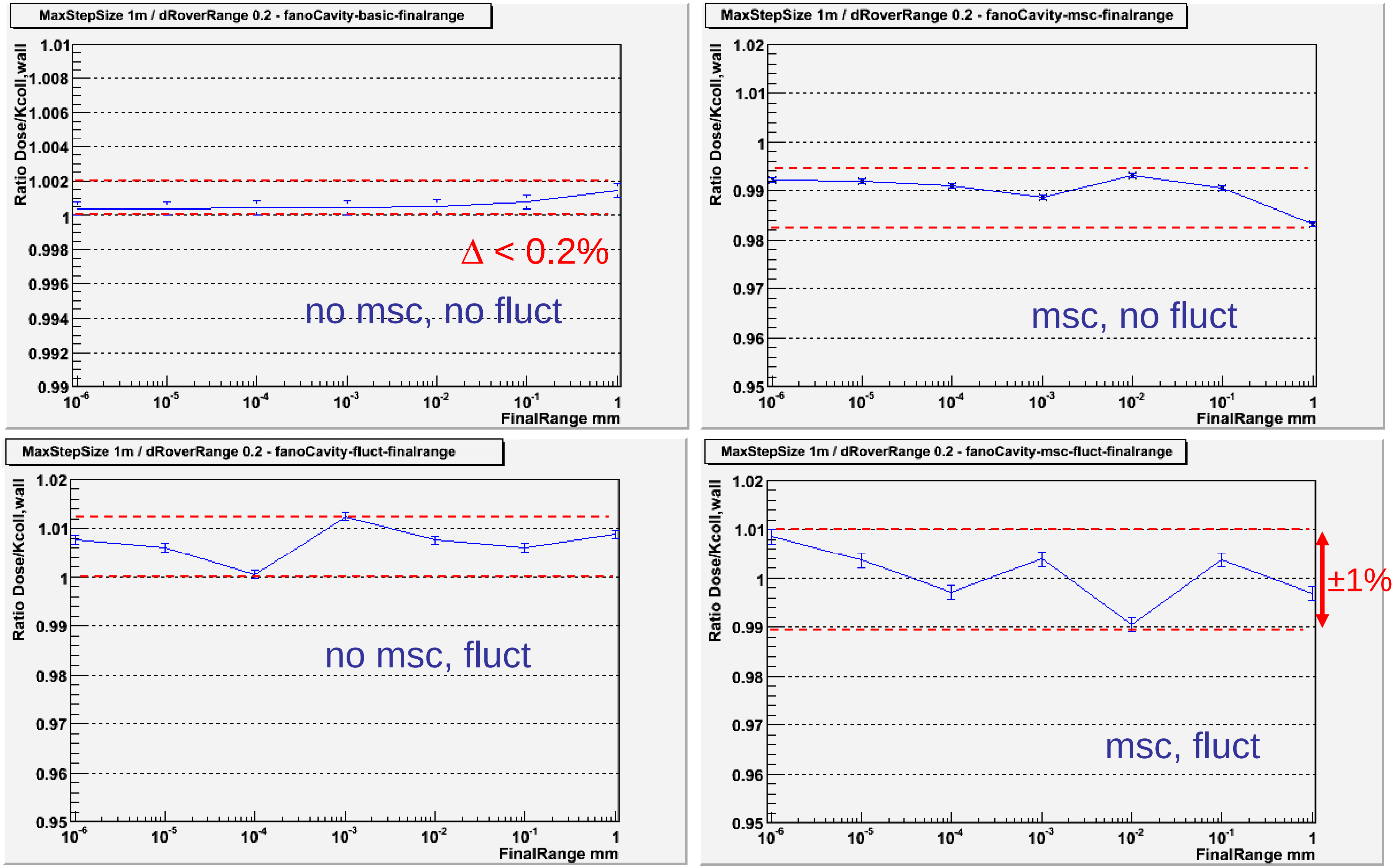
beyond 8.1 : single scattering and effective facrange





no big change, but slightly faster anyway

fanoCavity example : finalRange



Statistics : more than 10^6 electron entering the cavity