Electromagnetic Physics 2
Improvements & validation

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on behalf of the

Geant4 Standard EM and Low Energy EM Physics Working groups

Geant4 EM packages

- ***Standard***
  - γ, e up to 100 TeV
  - hadrons up to 100 TeV
  - ions up to 100 TeV
- ***Muons***
  - up to 1 PeV
  - Energy loss propagator
- ***Xrays***
  - X-ray and optical photon production processes
- ***High-energy***
  - Processes at high energy (E>10GeV)
  - Physics for exotic particles
- ***Polarisation***
  - Simulation of polarized beams
- ***Optical***
  - Optical photon interactions

- **Low-energy**
  - **Livermore library γ, e- from 10 eV up to 1 GeV**
  - **Livermore library based polarized processes**
  - **PENELOPE code rewrite , γ, e- , e+ from 250 eV up to 1 GeV**
  - **hadrons and ions up to 1 GeV**
  - **Microdosimetry models (Geant4-DNA project) from 7 eV to 10 MeV**
  - **Atomic deexcitation**

- Adjoint

  New sub-library for reverse Monte Carlo simulation from the detector of interest back to source of radiation

- **Utils – general EM interfaces**

EM Physics in Examples

I. Compton scattering

II. Multiple scattering

III. Proton energy loss (Bragg peak)

I. Compton Scattering

Example of gamma process/models

Compton scattering

The Compton effect describes the scattering off quasi-free atomic electrons :

$$\gamma + e \to \gamma' + e'$$

Each atomic electron acts as an independent cible; Compton effect is called incoherent scattering. Thus:

$$\text{cross section per atom} = Z \times \text{cross section per electron}$$

The inverse Compton scattering also exists: an energetic electron collides with a low energy photon which is blue-shifted to higher energy. This process is of importance in astrophysics.

Compton scattering is related to (e^+, e^-) annihilation by crossing symmetry.

Klein-Nishina Compton Model

energy spectrum

Under the same assumption,the unpolarized differential cross section per atom is given by the Klein-Nishina formula [Klein29] :

$$\frac{d\sigma}{dk'} = \frac{\pi\, r_e^2}{mc^2}\,\frac{Z}{\kappa^2}\left[\epsilon + \frac{1}{\epsilon} - \frac{2}{\kappa}\left(\frac{1-\epsilon}{\epsilon}\right) + \frac{1}{\kappa^2}\left(\frac{1-\epsilon}{\epsilon}\right)^2\right] \qquad (1)$$

where

k' energy of the scattered photon ; $\epsilon = k'/k$

r_e classical electron radius

κ k/mc^2

k is total electron energy

Low-energy Limit of Compton Scattering

low energy limit

In fact, when $k \leq 100\ keV$ the binding energy of the atomic electron must be taken into account by a corrective factor to the Klein-Nishina cross section:

$$\frac{d\sigma}{dk'} = \left[\frac{d\sigma}{dk'}\right]_{KN} \times S(k, k')$$

See for instance [Cullen97] or [Salvat96] for derivation(s) and discussion of the *scattering function* S(k,k').

As a consequence, at very low energy, the total cross section goes to 0 like k^2. It also suppresses the forward scattering.

At X-rays energies the scattering function has little effect on the Klein-Nishina energy spectrum formula 1. In addition the Compton scattering is not the dominant process in this energy region.

Standard Model of Compton Scattering

total cross section per atom in GEANT4

The total cross section has been parametrized [GEANT3] :

$$\sigma(Z,\kappa) = \left[P_1(Z) \frac{\log(1+2\kappa)}{\kappa} + \frac{P_2(Z) + P_3(Z)\kappa + P_4(Z)\kappa^2}{1 + a\kappa + b\kappa^2 + c\kappa^3} \right]$$

where:

$$\begin{aligned} \kappa &= k/mc^2 \\ P_i(Z) &= Z(d_i + e_i Z + f_i Z^2) \end{aligned}$$

The fit was made over evaluated data points (NIST) for:

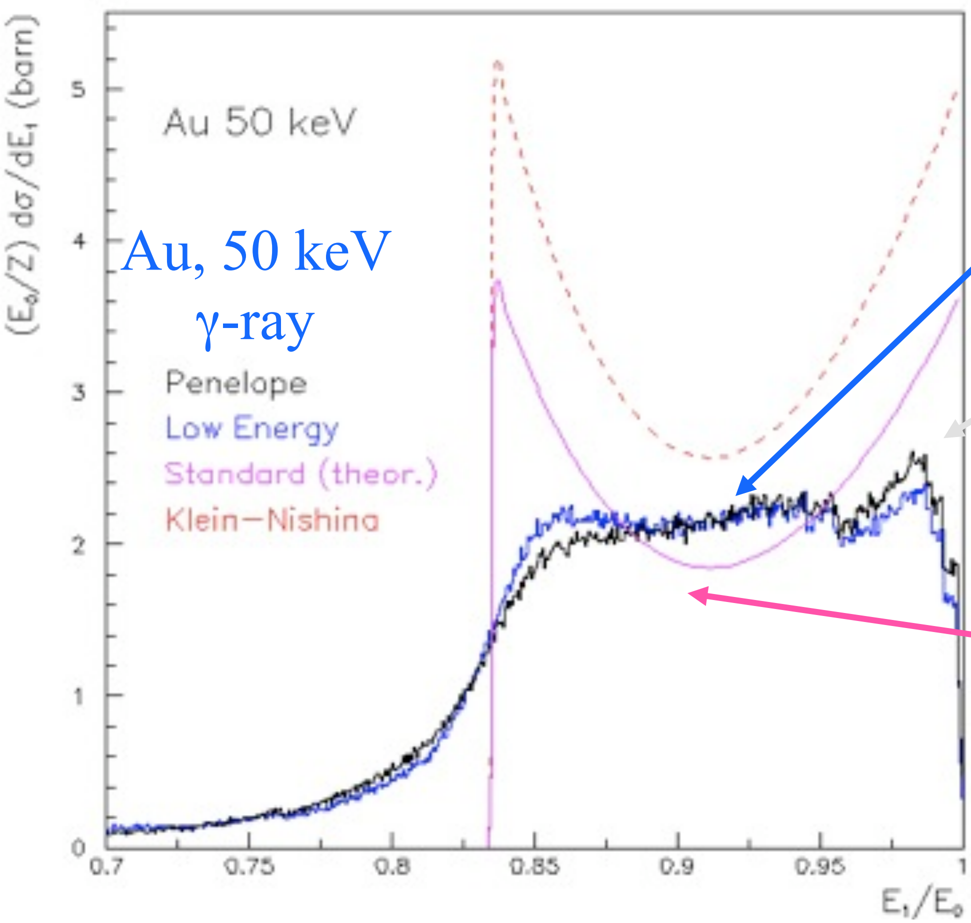
$$1 \le Z \le 100 \qquad ; \qquad k \in [1\ \text{keV}, 100\ \text{GeV}]$$

The accuracy of the fit is estimated to be:

$$\frac{\Delta\sigma}{\sigma} = \begin{cases} \approx 10\% & \text{for } k \quad \simeq 1\ \text{keV} - 20\ \text{keV} \\ \le 5-6\% & \text{for } k \quad > 20\ \text{keV} \end{cases}$$

Doppler broadening in Compton scattering

Compton scattering: electrons bound and not at rest (as assumed for Klein-Nishina) → change of angular distribution, reduction of XS



Au, 50 keV γ-ray

Penelope model includes it (via **analytical** approach)

Livermore model also deals with Doppler broadening (**EGS database** approach)

Good agreement Penelope-Livermore

Standard model **includes cross section** suppression, but samples final state according to Klein-Nishina

Courtesy of L. Pandola

When/how to Use Low-energy Models?

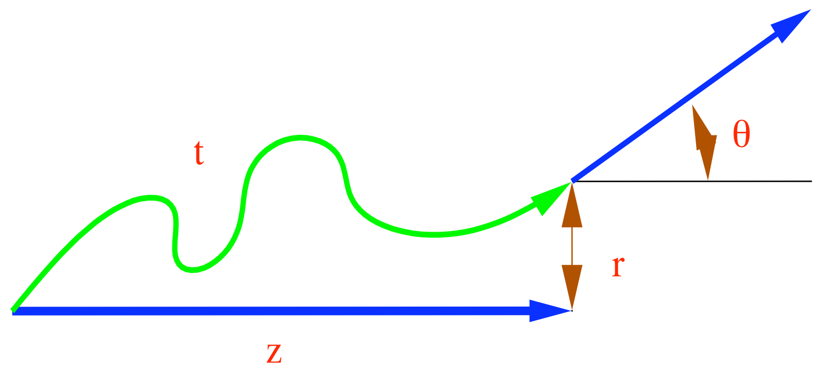
- **Use** Penelope or Livermore models (as an *alternative* to Standard models) when you:
  - need precise treatment of EM showers and interactions at low-energy (keV scale)
  - are interested in atomic effects, as fluorescence x-rays, Doppler broadening, etc.
  - can afford a more CPU-intensive simulation
  - want to cross-check an other simulation (with a different model)
  - Use Penelope models for low-energy positrons (no Livermore models available)
- For EM physics above 1 MeV similar results as Standard EM models are usually obtained
  - some CPU performance penalty for low-energy models
- Optimisation of transition energy between Standard and Low-energy models is one of our goal for future
  - User contribution will help a lot

II. Multiple Scattering

Elastic (Rutherford) Scattering

Multiple Coulomb scattering (MSC)

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.



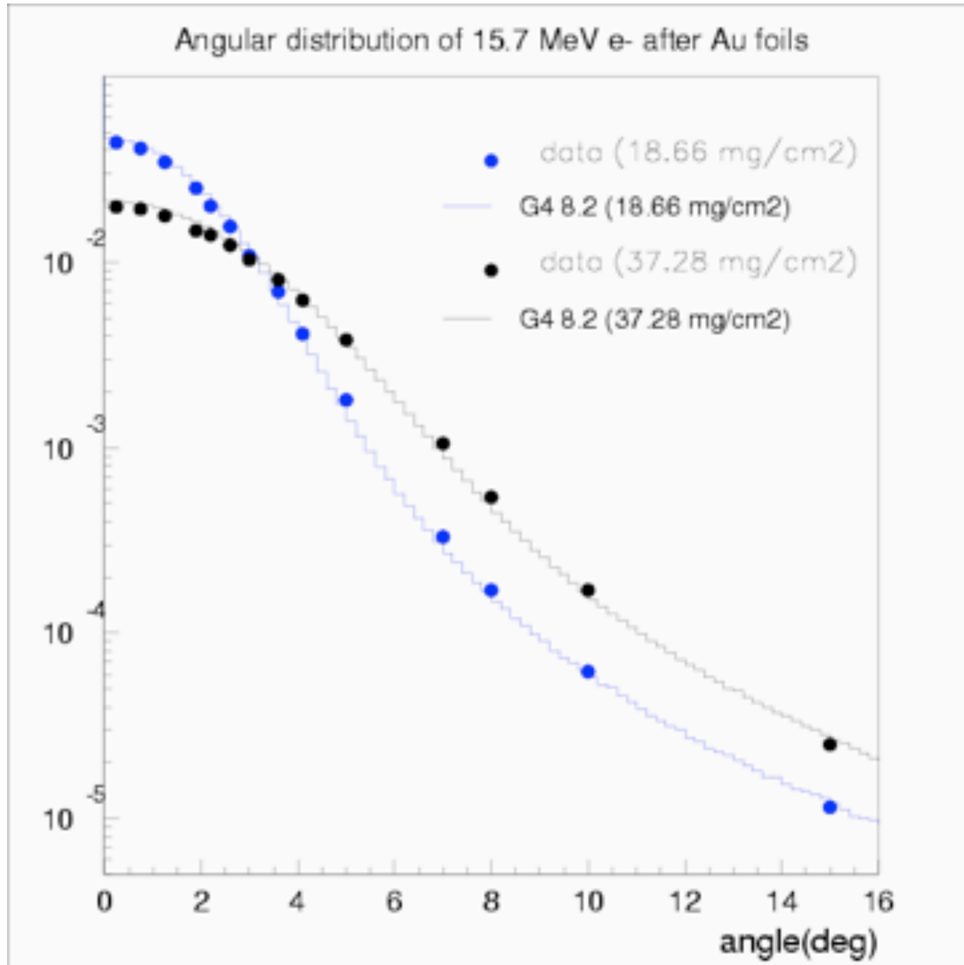
- longitudinal displacement z (or geometrical path length)
- lateral displacement r, Φ
- true (or corrected) path length t
- angular deflection θ, ϕ

Geant4 State of Art for 9.3

Model	Particle type	Energy limit	Specifics and applicability
Urban (Urban 2006)	any	-	Default model, (Lewis1950) approach, tuned to data, LHC production
Screened Nuclear Recoil (Mendenhall and Weller 2005)	p, ions	< 100 MeV/A	Theory based, providing simulation of nuclear recoil for sampling of radiation damage, focused on precise simulation of effects for space app.
Goudsmit-Saunderson (new, O.Kadri 2009)	e^+, e^-	< 1 GeV	Theory based cross sections (1950 Goudsmit and Saunderson), EPSEPA code developed by Penelope group , final state using EGSnrc method (Kawrakov et al. 1998), precise electron transport
Coulomb Scattering (new, 2008)	any	-	Theory based (Wentzel 1927) single scattering model, uses nuclear form-factors (Butkevich et al. 2002), focused on muons and hadrons
WentzelVI (new, 2008)	any	-	MSC for small angles, Coulomb Scattering (Wentzel 1927) for large angles, focused on simulation for muons and hadrons

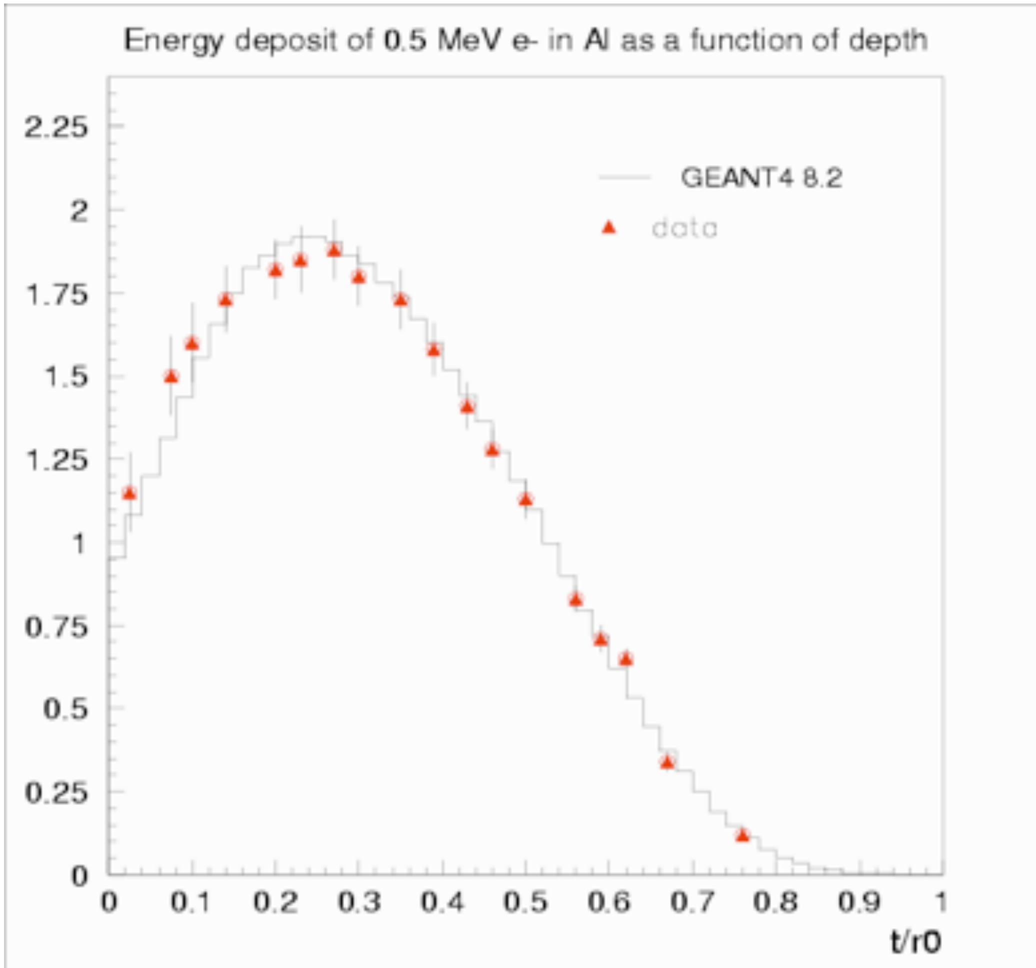
Geant4 Urban MSC model

- To get more complete information it is better to **start with theory** of Lewis which based on the transport equation of charged particles
- The Urban MSC model uses **phenomenological functions** to sample angular and spatial distributions after the simulation step
- The functions parameters are chosen to provide the **same** value of **moments** of the distribution as in Lewis theory
- See details in the Geant4 Physics Reference Manual and in EM web



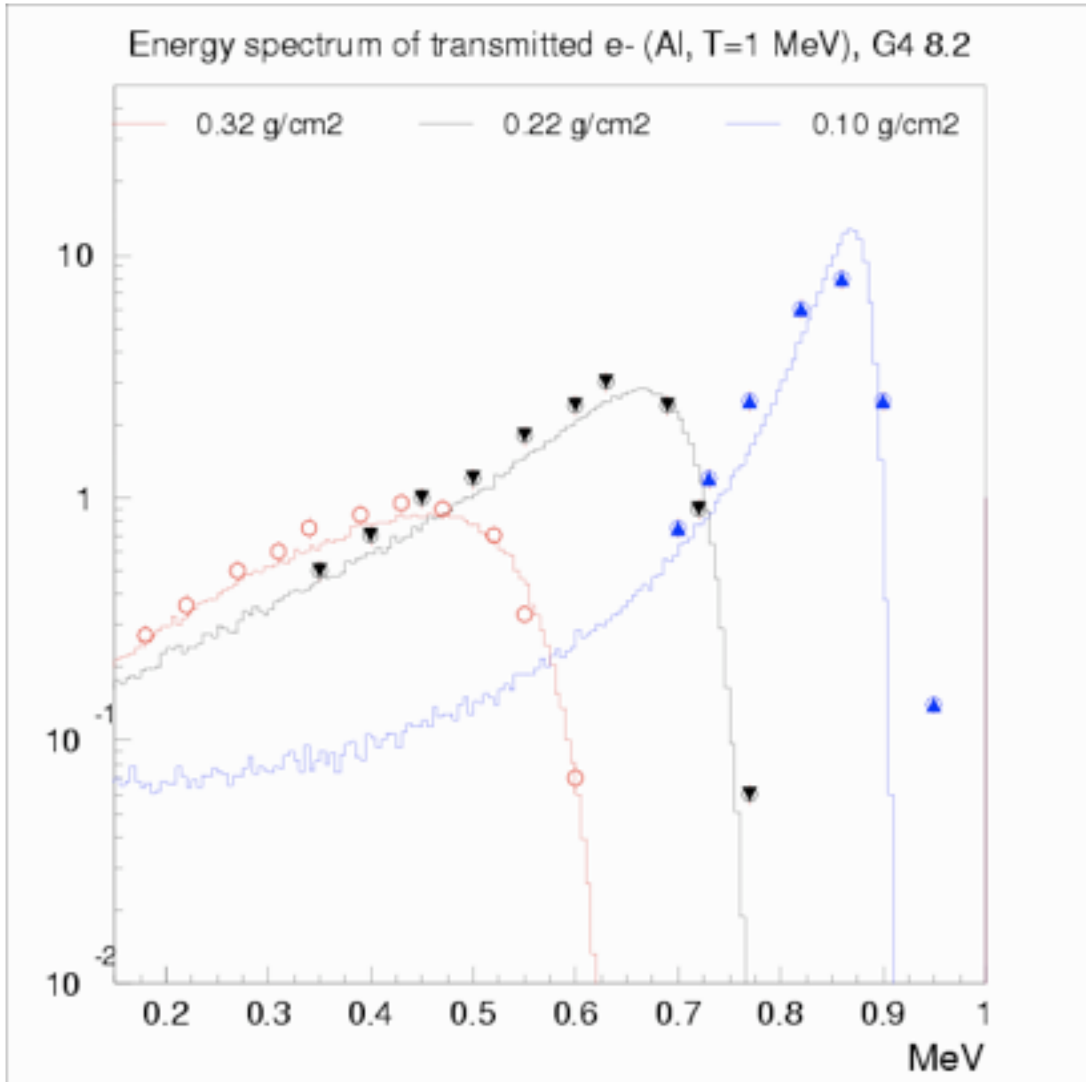
Step limitation from MSC : g4 7.1 → g4 8.3

- **Step limit defined at first step and reevaluated after a boundary**
  - **applied only if range > safety**
- **StepLimit = F_R •max (range, λ)**
  - **λ is transport cross section**
  - **new default Range Factor F_R = 0.04 (instead of 0.2)**
    - **strong constraint only for low energy particles**
- **step limit min becomes material dependant, via λ :**
  - **StepLimitMin = max (0.04 λ, 5 nm)**
- Low-energy electron transport is very essential for HEP simulation
  - Determined response of HEP calorimeters

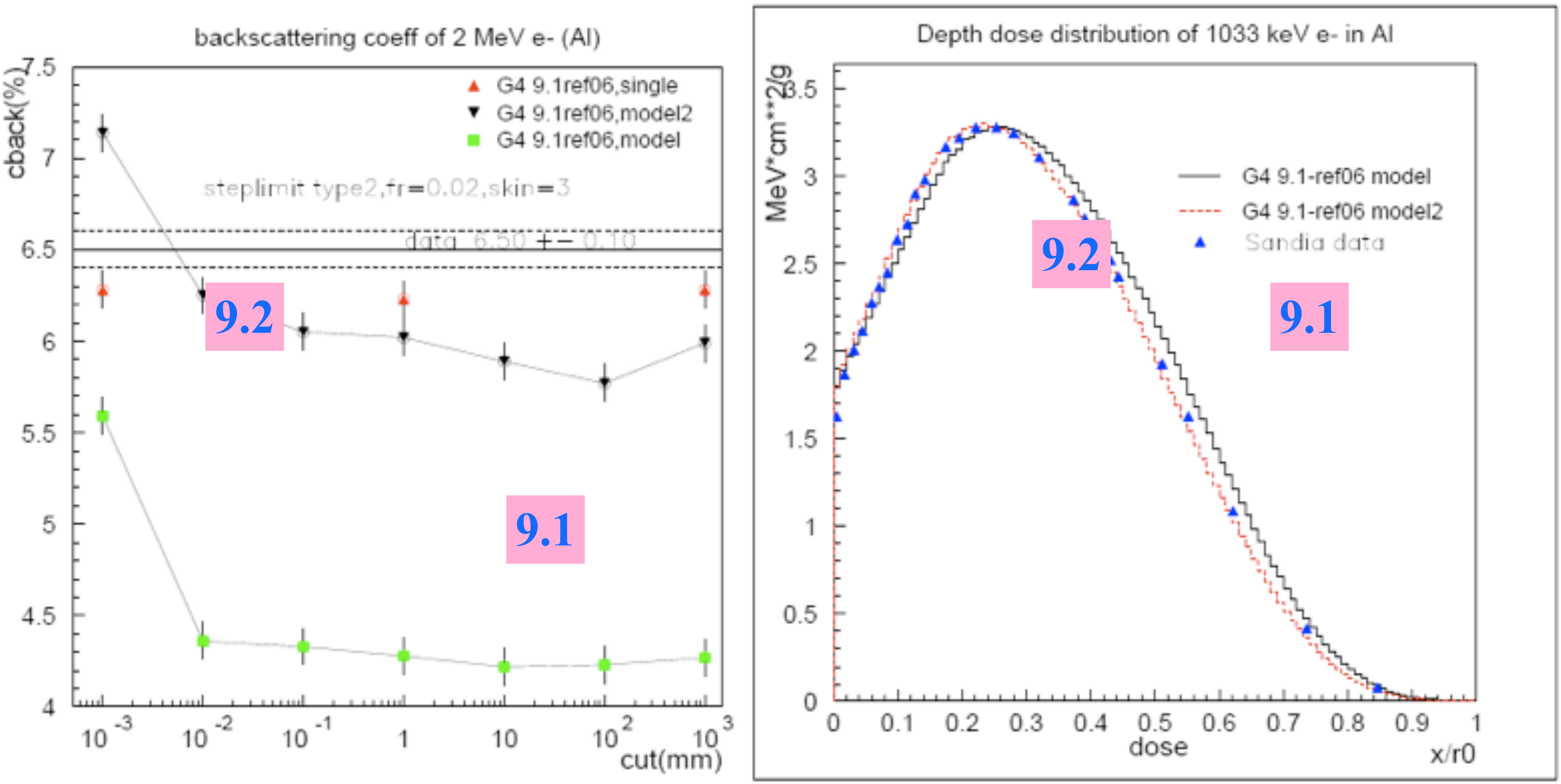


Sampling of MSC : g4 7.1 → g4 8.3

- **Reevaluate safety radius before to perform lateral displacement**
  - **d < safety (*safety is often underestimated*)**
- **Correlate final direction with lateral displacement**
  - **u · d = f (λ) taken from Lewis theory**
- **Single Coulomb scattering at boundaries**
  - **1 very small step (~ λ elastic) before boundary crossing**
  - **apply approximate single Coulomb scattering in this step**

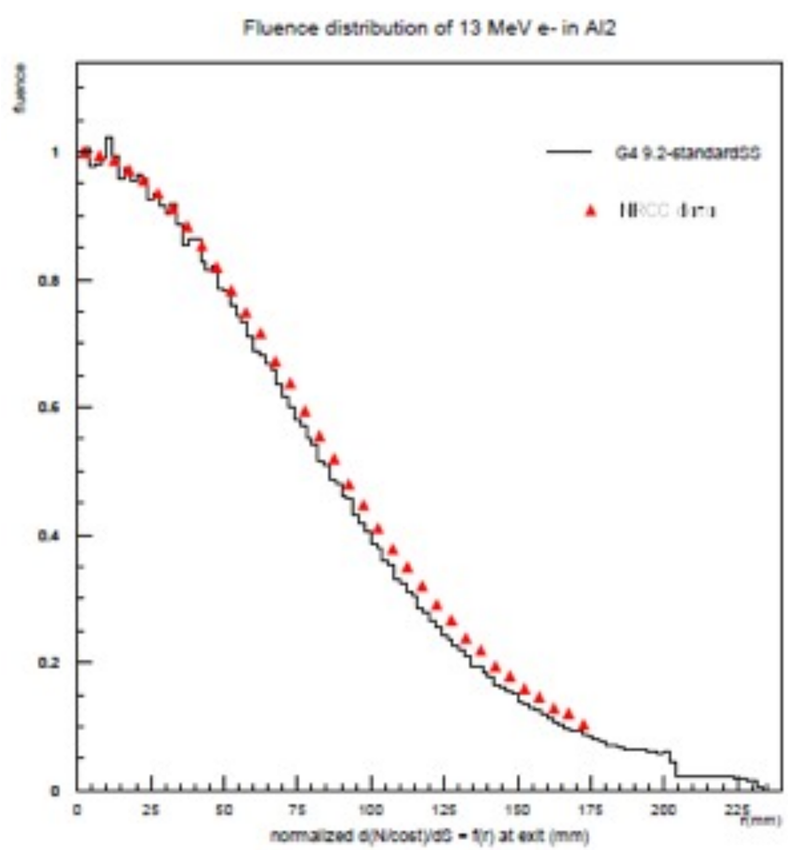


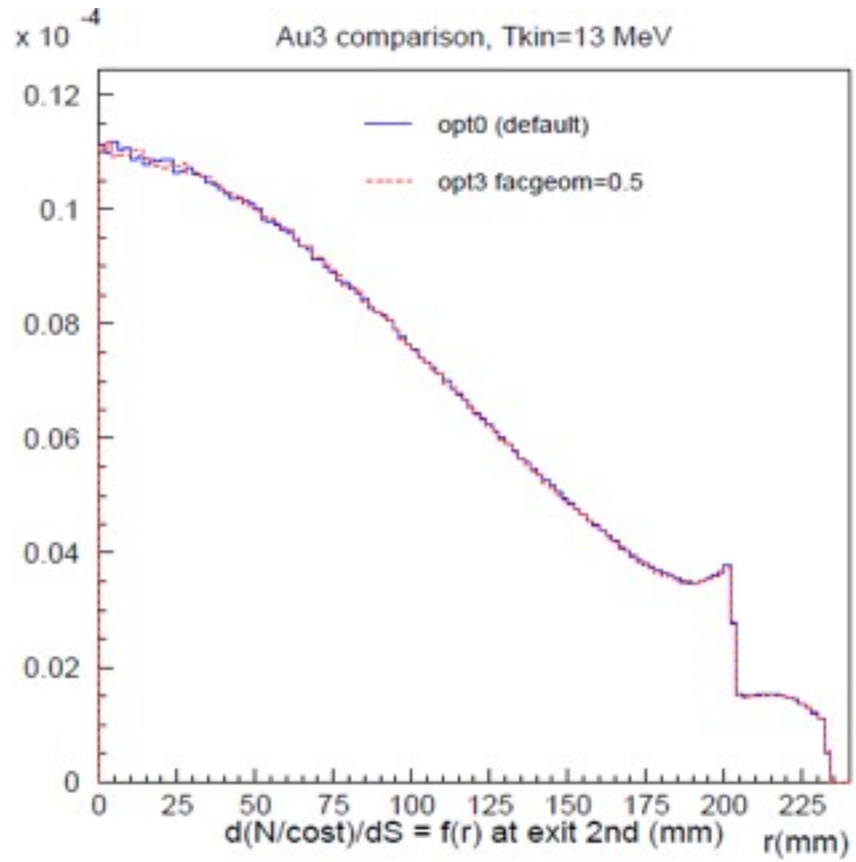
Evolution of multiple scattering model



Electron Benchmark (J.Perl et al.)

- New electron MSC benchmark results B.A.Faddegon, I.Kawrakov, Yu.Kubyshin, J.Perl, J.Sampau, L.Urban Phys.Med.Biol. 54 (2009) 6151
- Detailed data for electron scattering at 13 – 20 MeV
- New examples *electronScattering* are released (traditional scoring versus G4Scorer facility)





MSC Options for g4 9.3

- To avoid user confusions new processes per particle type have been introduced:
  - G4eMultipleScattering for $e^{\pm}$
  - G4MuMultipleScattering for $\mu^{\pm}$
  - G4hMultipleScattering for hadrons and ions
- *G4MultipleScattering* process marked as an obsolete
- Urban models
  - G4UrbanMscModel92 – use in default and Opt1 PhysLists for e+-
  - G4UrbanMscModel93 – in all other PhysLists e+-
  - G4UrbanMscModel90 – use as a default for muons, hadrons, ions
- Alternative multiple and single scattering models are available for users
  - How to use is shown in extended examples

1st hands-on

- Task 3c
  - Exercise 10:
    - » Activate/De-activate multiple scattering
  - Exercise 3.11 :
    - » Change parameters of electromagnetic processes

III. Ionisation for protons

Example of process/models

Mean Restricted Energy Loss

The mean rate of the energy lost by the incident particle due to the soft δ-rays is :

$$\frac{dE_{soft}(E, T_{cut})}{dx} = n_{at} \cdot \int_0^{T_{cut}} \frac{d\sigma(Z, E, T)}{dT} T \, dT \qquad (13)$$

n_{at} : nb of atoms per volume in the matter.

The total cross-section per atom for the ejection of an electron of energy $T > T_{cut}$ is :

$$\sigma(Z, E, T_{cut}) = \int_{T_{cut}}^{T_{max}} \frac{d\sigma(Z, E, T)}{dT} \, dT \qquad (14)$$

where T_{max} is the maximum energy transferable to the free electron.

Energy-Range relation

Mean total pathlength of a charged particle of kinetic energy E :

$$R(E) = \int_{\epsilon=0}^{\epsilon=E} \left[\frac{d\epsilon}{dx}\right]^{-1} d\epsilon$$

In GEANT4 the energy-range relation is extensively used :

- to control the stepping of charged particles
- to compute the energy loss of charged particles
- to control the production of secondaries (cut in range)

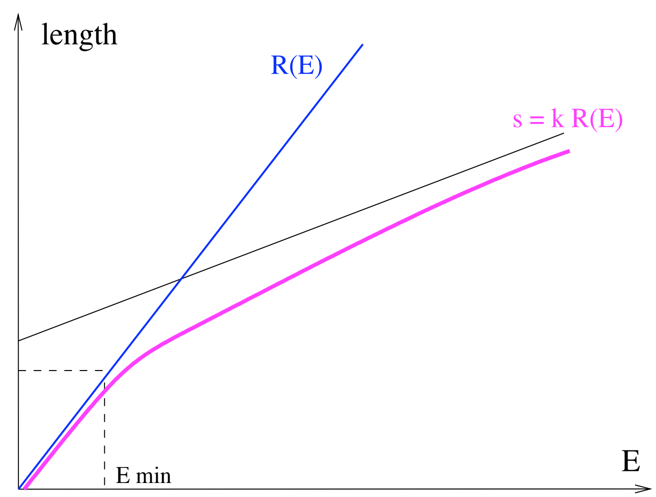
Step limitation by ionization processes

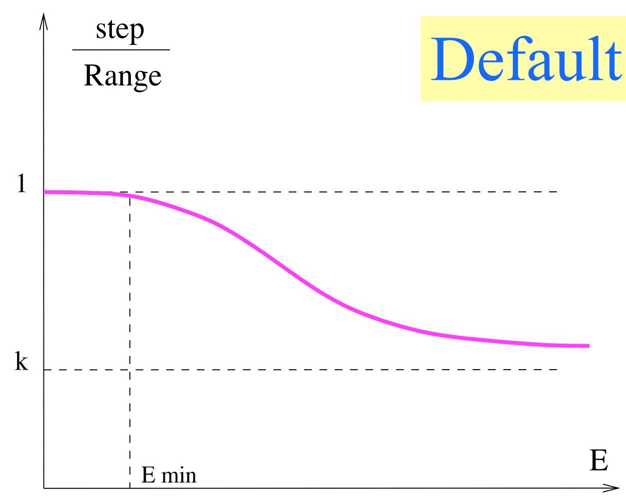
control the stepping of charged particles

The continuous energy loss imposes a limit on the stepsize.

The cross sections depend of the energy. The step size must be small enough so that the energy difference along the step is a small fraction of the particle energy.

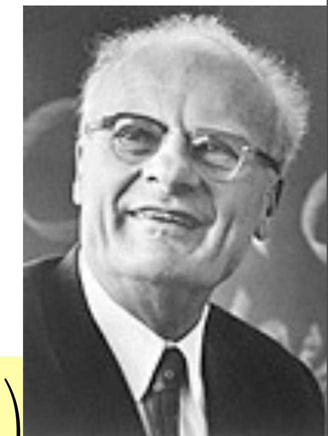
This constraint must be relaxed when $E \rightarrow 0$: the allowed step smoothly approaches the stopping range of the particle.





Default k = 0.2

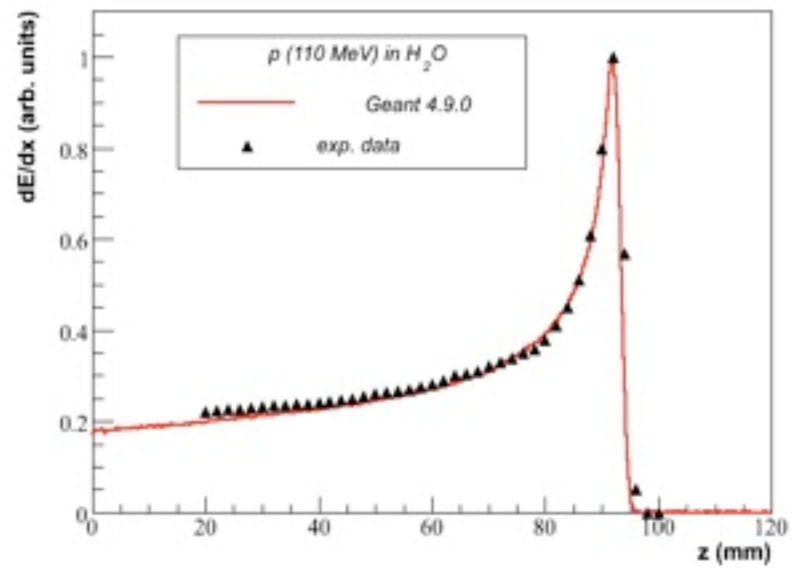
Hadron and Ion Ionisation



- ❑ Coulomb scattering
- ❑ Ionization
- ❑ Bethe-Bloch formula with corrections used for E>2 MeV

$$-\frac{dE}{dx} = 4\pi N_e r_0^2 \frac{z^2}{\beta^2}\left(\ln\frac{2m_e c^2\beta^2\gamma^2}{I} - \frac{\beta^2}{2}\left(1-\frac{T_c}{T_{max}}\right) - \frac{C}{Z} + \frac{G-\delta-F}{2} + zL_1 + z^2 L_2\right)$$

- C – shell correction
- G – Mott correction
- δ – density correction
- F – finite size correction
- L_1- Barkas correction
- L_2- Bloch correction
- Nuclear stopping
- Ion effective charge



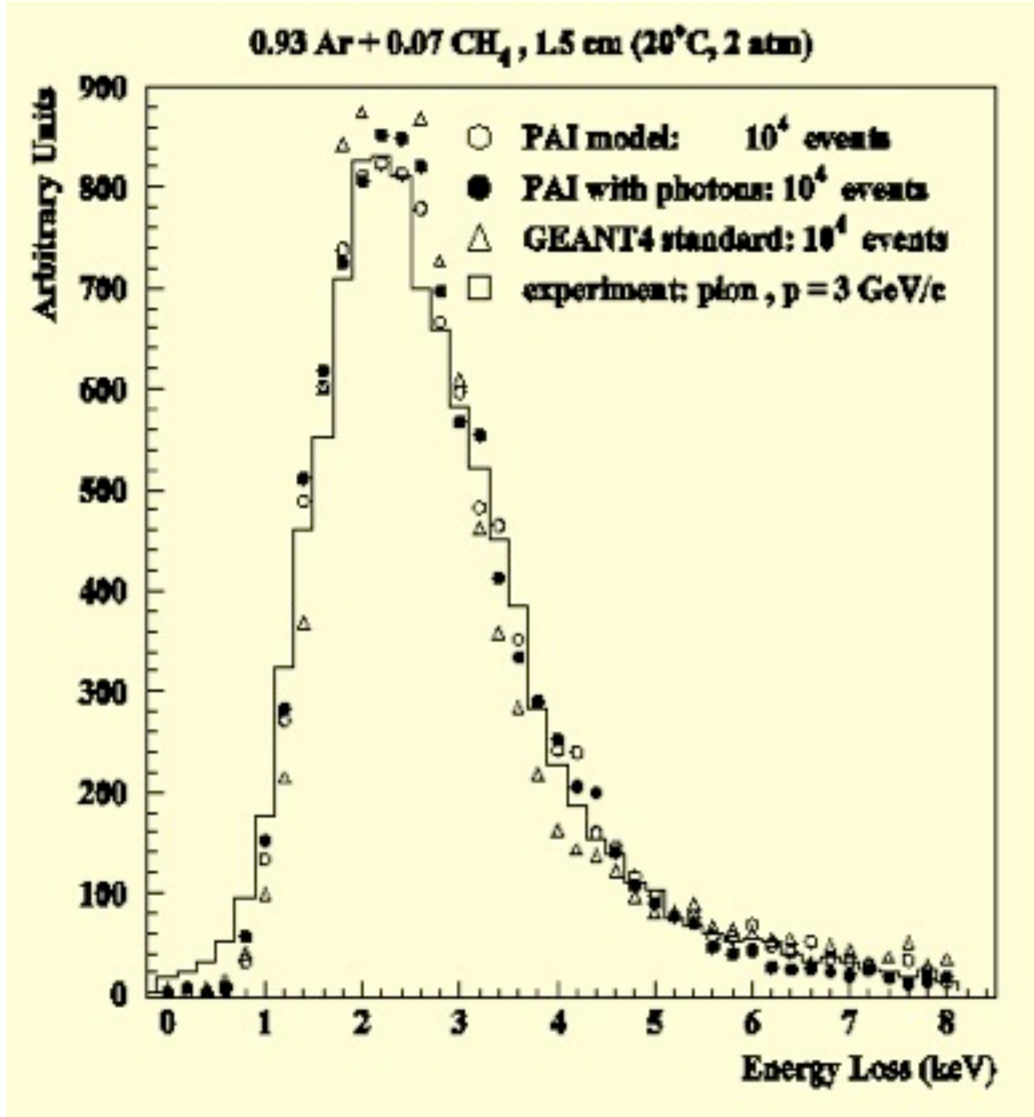
- ❑ Bragg peak parameterizations for E< 2 MeV
  - ❑ ICRU'49 and NIST databases

Simulation of a Step of a Charged Particle

- The Bethe-Bloch formula (or low-energy parameterision) provides value of mean energy loss
- The value of mean energy loss are pre-computed at initialisation stage of Geant4 and spline interpolation method is used in the run time
- At each simulation step of a charged particle the mean energy loss is computed and sampling of energy loss fluctuation is performed
  - The interface to a fluctuation class G4VEmFluctuationModel
- The cross section of δ-electron production above the threshold T_{cut} are also pre-computed
  - Final state generation PostStep is the step is limited by this process

Geant4 models of energy loss fluctuations

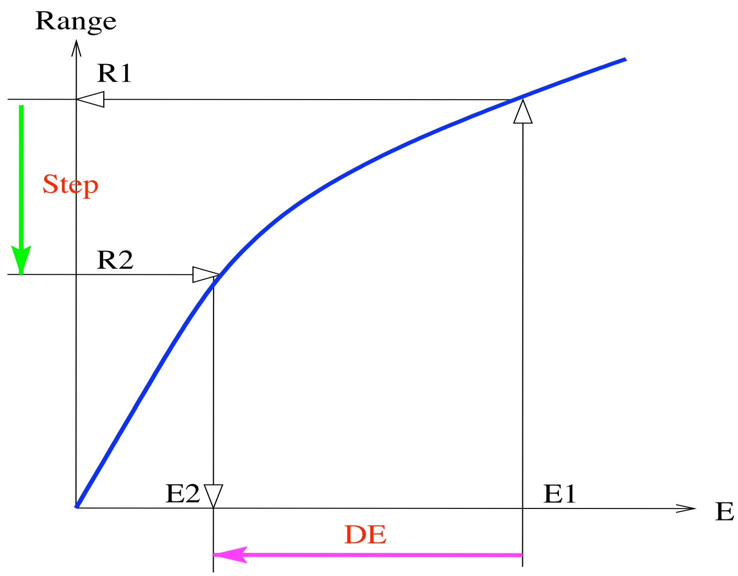
- Urban model based on a simple model of particle-atom interaction
  - **Atoms are assumed to have only two energy levels E_1 and E_2**
  - **Particle-atom interaction can be:**
    - **an excitation of the atom with energy loss $E = E_1 - E_2$**
    - **an ionization with energy loss distribution $g(E) \sim 1/E^2$**
- PAI model uses photo absorption data
  - **All energy transfers are sampled with production of secondary e^- or γ**
  - **Very slow model, should be applied for sensitive region of detector**



Interpolation of Data Tables

compute the mean energy loss of charged particles

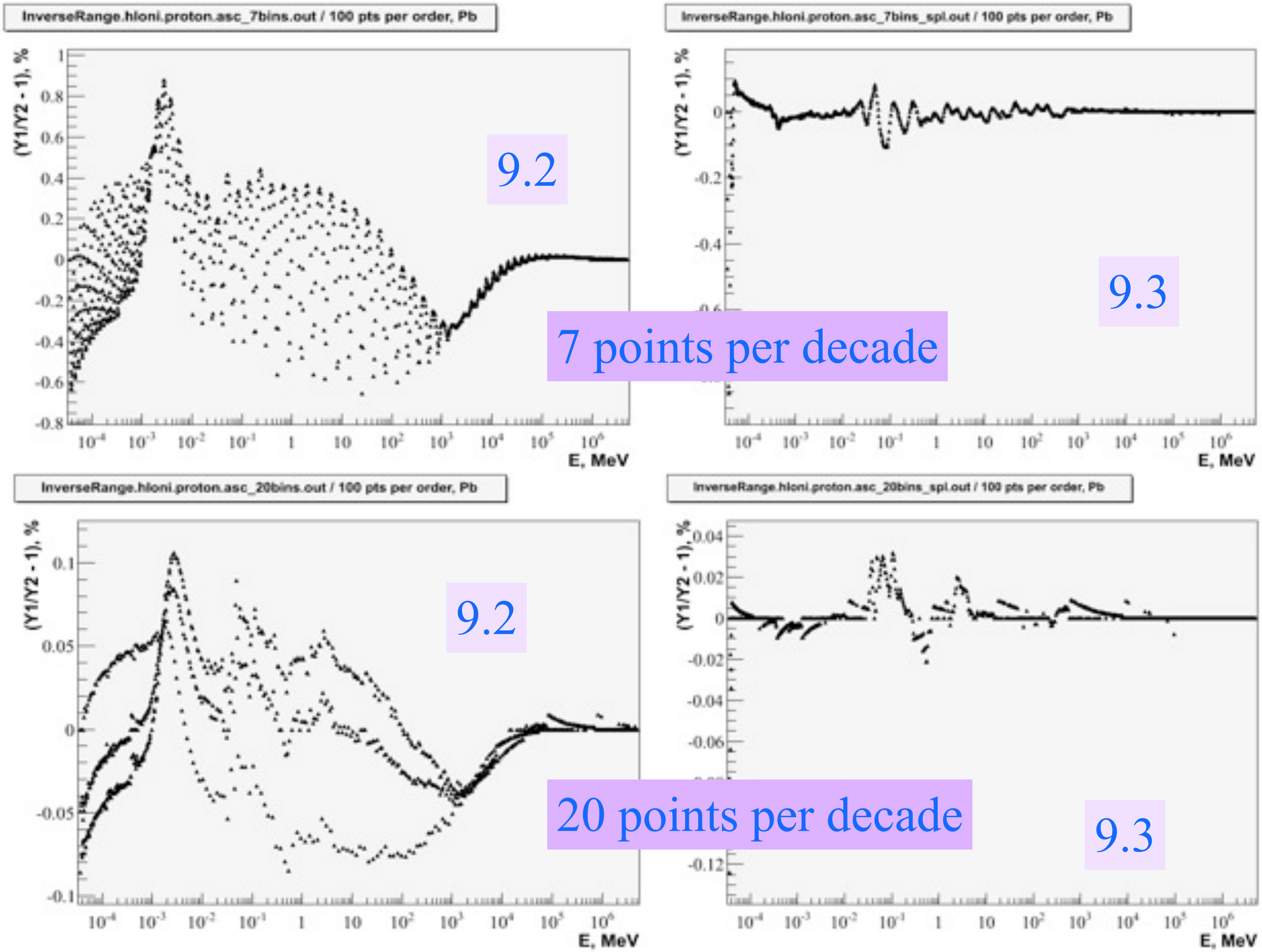
The computation of the mean energy loss on a given step is done from the Range and inverse Range tables.



This is more accurate than $\Delta E = (dE/dx) * \text{stepLength}$. if step is long

dEdx, Range and inverse Range tables are computed initialization phase of Geant4 using production thresholds (cuts) per detector region

Proton Inverse Range in Lead



Where to find out information?

Manuals

- Geant4 User Guides

  http://geant4.web.cern.ch/geant4/support/userdocuments.shtml
  - User's Guide: For Application Developers
  - Physics Reference Manual
  - Software Reference Manual

- User support entry point in the web: http://geant4.web.cern.ch/geant4/support/index.shtml

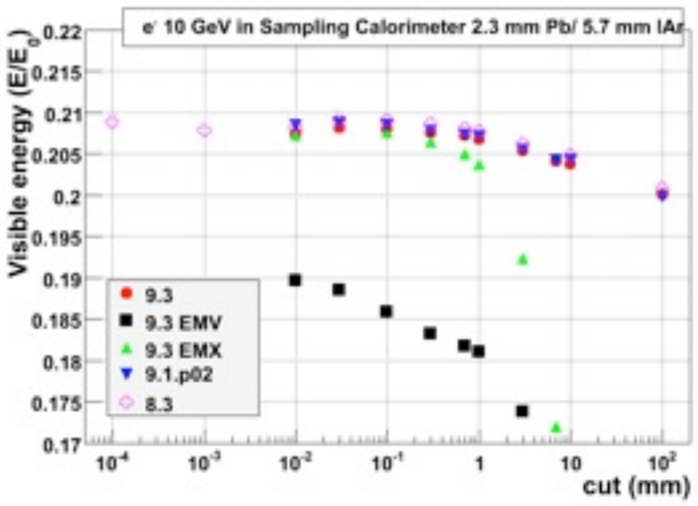
- Hyper News Forum “emprocesses” http://hypernews.slac.stanford.edu/HyperNews/geant4/cindex

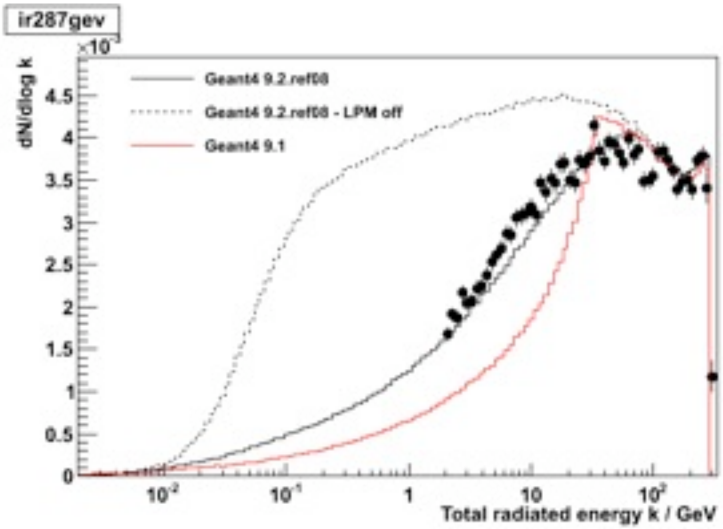
Documentation on EM physics

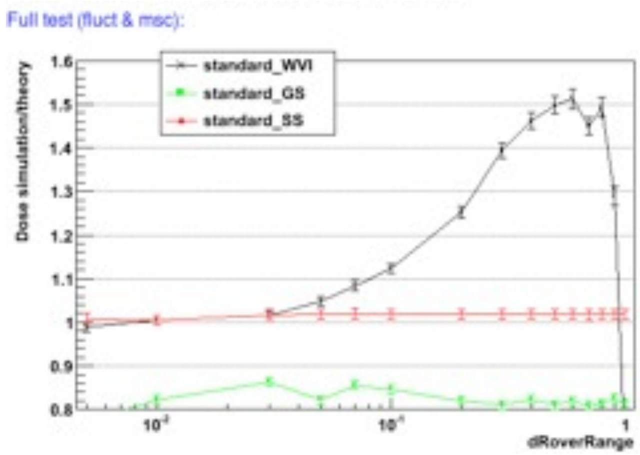
- The electromagnetic web pages::
  - EM Home page easily accessible from G4 web http://geant4.web.cern.ch/geant4/collaboration/EMindex.shtml
  - EM TWiki pages have been created *https://twiki.cern.ch/twiki/bin/view/Geant4/ElectromagneticPhysics*
  - Pages are maintained by common efforts of both EM groups
    » User contribution welcome

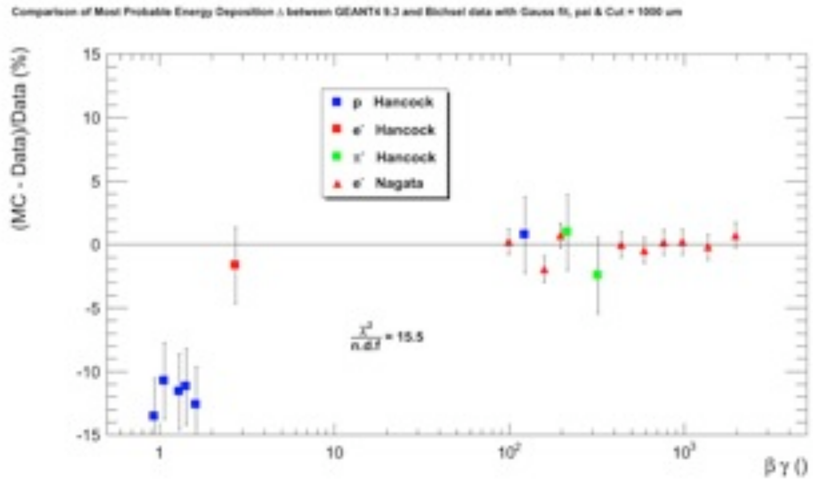
EM Validation Repository

- Web Interface at: http://www-zeuthen.desy.de/geant4/web/verification3.php









Thank you for your attention!

2nd Hands-on

- Task 3c
  - Exercise 3.12 :
    - » Energy response to gamma, electrons, muons
  - Exercise 3.13 :
    - » Bragg peak and electron energy profile