Geant4 release 9.4

Geant4 Electromagnetic Physics

Training course "Monte Carlo simulation for Micro- and Nanodosimetry"

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On behalf of Geant4 electromagnetic working groups

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  - Multiple scattering
- Geant4 cuts
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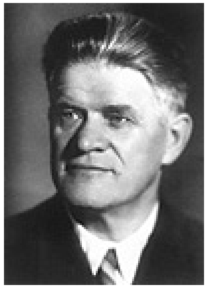
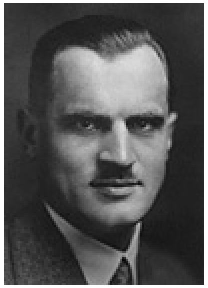
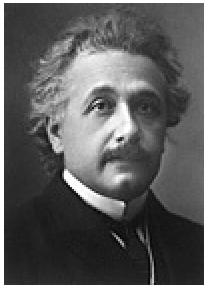
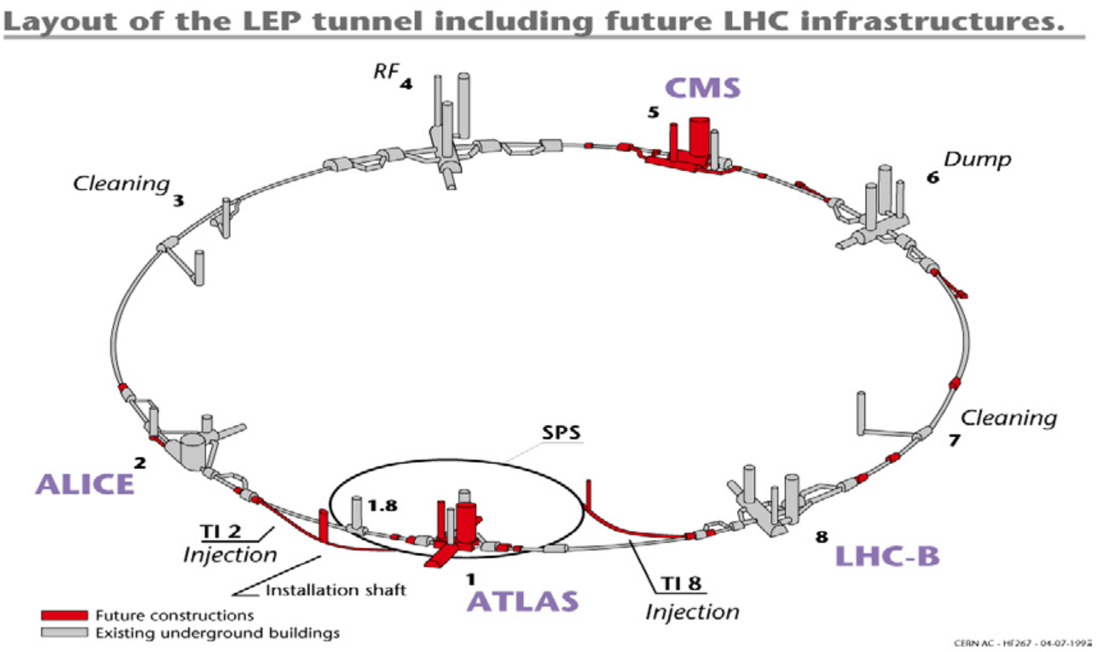
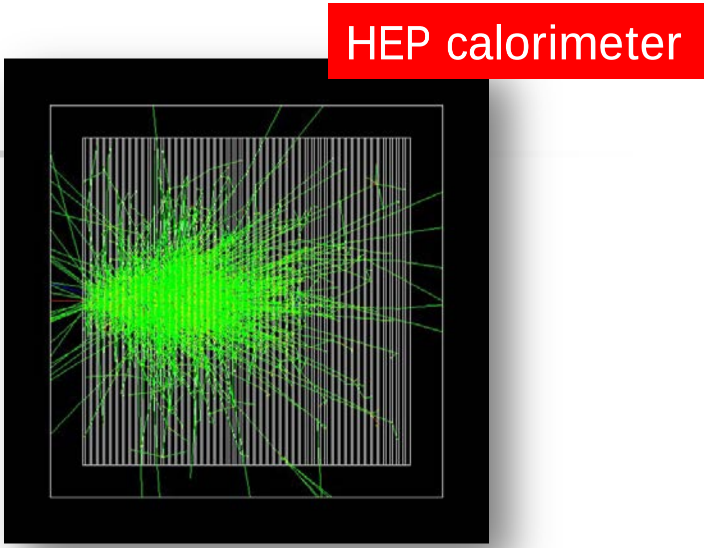




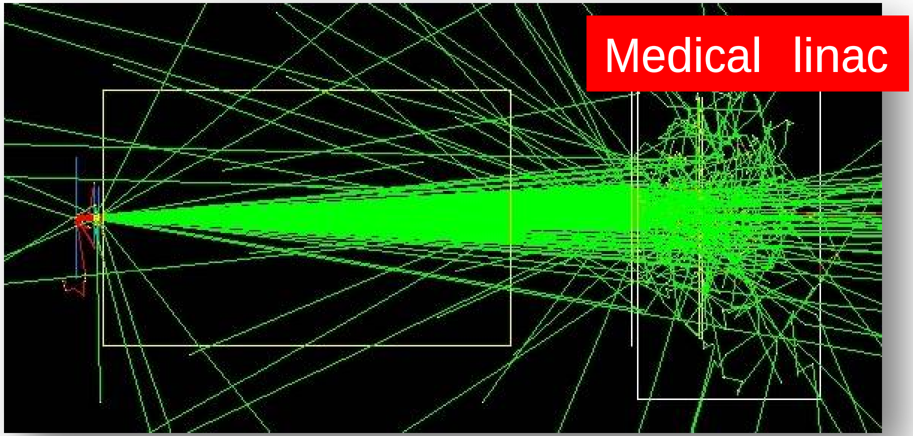
Electromagnetic (EM) physics overview



Gamma and electron transport

- Photon processes
  - γ conversion into e+e- pair
  - Compton scattering
  - Photoelectric effect
  - Rayleigh scattering
  - *Gamma-nuclear interaction in hadronic sub-package CHIPS*
- Electron and positron processes
  - Ionization
  - Coulomb scattering
  - Bremsstrahlung
  - *Nuclear interaction in hadronic sub-package CHIPS*
  - Positron annihilation
- Suitable for HEP & many other Geant4 applications with electron and gamma beams





Located in $G4INSTALL/sources/processes/electromagnetic

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
- X-rays
  - 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 250 eV up to 1 GeV
  - Livermore library based polarized processes
  - PENELOPE code rewrite , γ, e- , e+ from 250 eV up to 1 GeV (2001 version & 2008 version in 9.5)
  - hadrons and ions up to 1 GeV
  - atomic de-excitation (fluorescence + Auger)
- DNA
  - microdosimetry models for radiobiology (Geant4-DNA project) from 0.025 eV to 10 MeV
- Adjoint
  - New sub-library for reverse Monte Carlo simulation from the detector of interest back to source of radiation
- Utils : general EM interfaces

Software design

- Since Geant4 9.3beta (June, 2009) the design is uniform for all EM packages
  - Allowing a coherent approach for high-energy and low-energy applications
- A physical interaction or process is described by a process class
  - Naming scheme : « G4ProcessName »
  - For example: G4Compton for photon Compton scattering
  - Assigned to Geant4 particle types
  - Inherit from G4VEmProcess base class
- A physical process can be simulated according to several models, each model being described by a model class
  - Naming scheme : « G4ModelNameProcessNameModel »
  - For example: G4LivermoreComptonModel
  - Models can be assigned to certain energy ranges and G4Regions
  - Inherit from G4VEmModel base class
- Model classes provide the computation of
  - Cross section and stopping power
  - Sample selection of atom in compound
  - Final state (kinematics, production of secondaries…)

How to invoke EM Physics in Geant4 ?

Physics lists

- A Physics list is the mandatory user class making the general interface between the physics the user needs and the Geant4 kernel
  - It should include the list of particles
  - The G4ProcessManager of each particle maintains a list of processes

- Geant4 provides several configurations of EM physics lists called constructors
(G4VPhysicsConstructor) in the physics_list library of Geant4

- These constructors can be included into a modular Physics list in a user application (G4VModularPhysicsList)

EM Physics List constructors for High Energy Physics

- Used by Geant4 validation suites
  - Are robust due to intensive tests by Geant4 team
  - well known precision and limitations
- May be used in any application domain

Constructor	Components	Comments
G4EmStandardPhysics	Default (QGSP_BERT, FTFP_BERT...)	ATLAS, and other HEP productions, other applications
G4EmStandardPhysics_option1	Fast due to simple step limitation, cuts used by photon processes (QGSP_BERT_EMV)	CMS and LHCb production, good for crystals not good for sampling calorimeters
G4EmStandardPhysics_option2	Experimental: WentzelVI model of multiple scattering (QBBC, ...)	Used for testing of new models

Combined EM Physics List constructors

- For today focus more to precision than to maximum simulation speed
- Ion stopping model based on the ICRU'73 data
- Strong step limitation from ionisation and multiple scattering per particle type
- Recommended for hadron/ion therapy, space applications

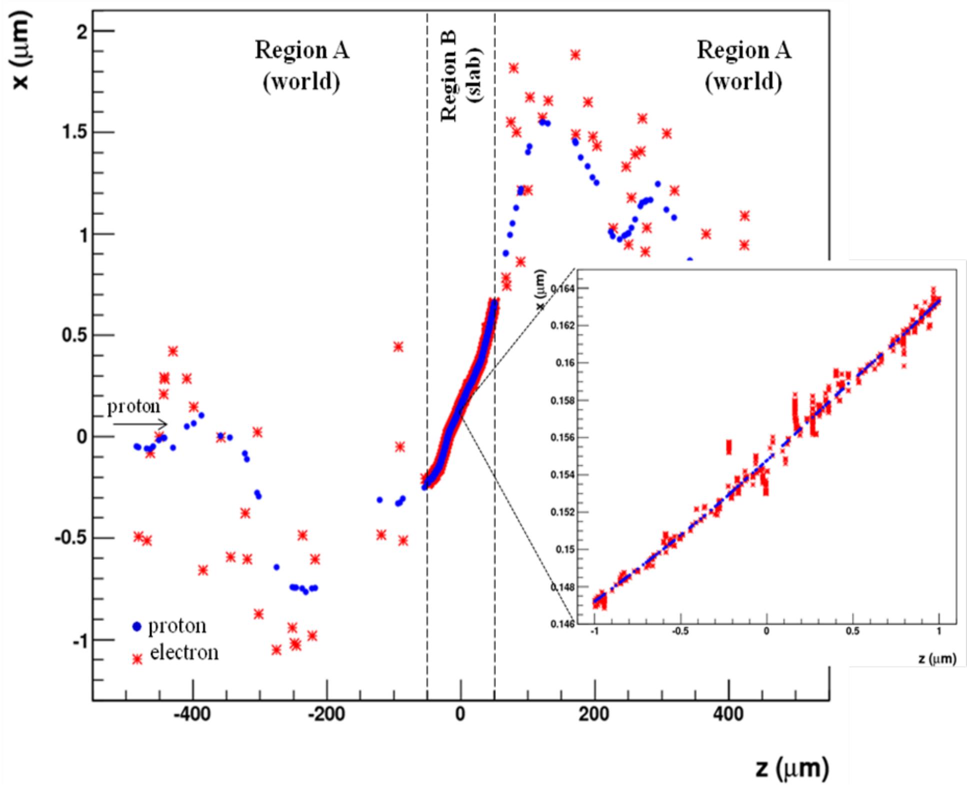
Constructor	Components	Comments
G4EmStandardPhysics_option3	Urban MSC model (QGSP_BIC_EMY, Shielding)	Proton/ion therapy
G4EmLivermorePhysics	GoudsmithSaunderson MSC model Livermore models for γ, e^- below 1 GeV, Standard models above 1 GeV	Livermore low-energy electron and gamma transport
G4EmPenelopePhysics	GoudsmithSaunderson MSC model Livermore models for γ, $e^\pm$ below 1 GeV, Standard models above 1 GeV	Penelope low-energy $e^\pm$ and gamma transport

User interfaces and helper classes

- G4EmCalculator – easy access to cross sections and stopping powers (TestEm0)
- G4EmProcessOptions – c++ interface to EM options alternative to UI commands
- G4EmSaturation – Birks effect
- G4ElectronIonPair – sampling of ionisation clusters in gaseous or silicon detectors
- G4EmConfigurator – add models per energy range and geometry region

Specialized models per G4Region: example of DNA physics

- Standard EM physics constructor as a base
- G4EmConfigurator is used to add DNA models
- DNA models are enabled only in the small G4Region for energy below 10 MeV
- CPU performance optimisation



Example: G4EmStandard Physics

```
G4ProcessManager* pmanager

   if ( particleName == "gamma"  ) {
     pmanager->AddDiscreteProcess(new G4PhotoElectricEffect);
     pmanager->AddDiscreteProcess(new G4ComptonScattering);
     pmanager->AddDiscreteProcess(new G4GammaConversion);
                                                        AlongStep
   } else if ( particleName == "e+" ) {           AtRest   PostStep
     pmanager->AddProcess(new G4eMultipleScattering, -1,   1, 1);
     pmanager->AddProcess(new G4eIonisation,         -1,   2, 2);
     pmanager->AddProcess(new G4eBremsstrahlung,     -1,   3, 3);
     pmanager->AddProcess(new G4eplusAnnihilation,    0,  -1, 4);
```

Only PostStep

3 stages

- Numbers are process order
  - G4Transportation is the 1st (order = 0) for AlongStep and PostStep
- "-1" means that the process is not active

Atomic de-excitation effects

- Atomic de-excitation initiated by other EM processes
  - Examples: photo-electric effect, ionisation by e- and ions (eg. PIXE)
  - Leave the atom in an excited state

- EADL data contain transition probabilities
  - radiative: fluorescence
  - non-radiative:
    - Auger e-: inital and final vacancies in different sub-shells
    - Coster-Kronig e-: identical sub-shells

- Atomic de-excitation simulation is now compatible with both Standard & LowE EM categories

Including atomic effects

- How to use fluorescence in Livermore & Penelope Physics ?
  - Fluorescence is automatically activated for gamma photo electric effect.

- How to include fluorescence, Auger emission in Standard EM (options 2 & 3 in 9.4) ?
  - Some UI commands are available (no more code edition necessary !)

```
/run/initialize
/process/em/fluo true
/process/em/auger true
/process/em/pixe true
```

- From the next release these commands will be universal for all reference Physics Lists

How to extract Physics ?

- Possible to retrieve Physics quantities using a G4EmCalculator object
- Physics List should be initialized
- Example for retrieving the total cross section of a process with name procName, for particle and material matName

```
#include "G4EmCalculator.hh"
...
G4EmCalculator emCalculator;

G4Material* material =
  G4NistManager::Instance()->FindOrBuildMaterial(matName);

G4double density = material->GetDensity();

G4double massSigma = emCalculator.ComputeCrossSectionPerVolume
    (energy,particle,procName,material)/density;

G4cout << G4BestUnit(massSigma, "Surface/Mass") << G4endl;
```

- A good example: $G4INSTALL/examples/extended/electromagnetic/TestEm14. Look in particular at the RunAction.cc class

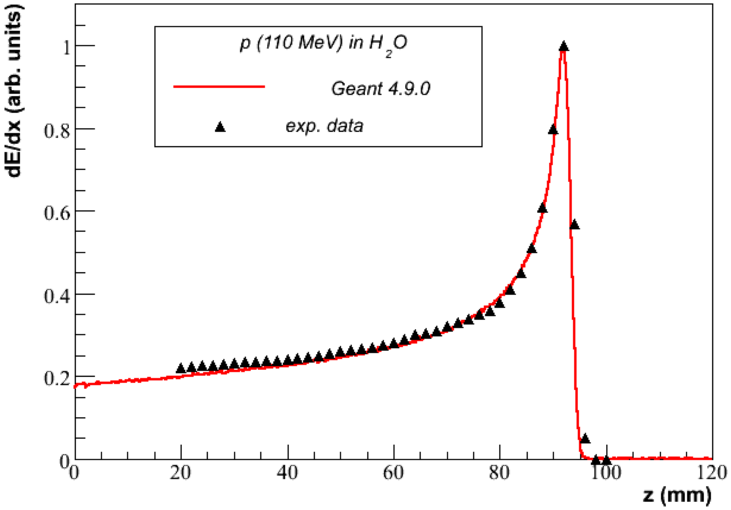
Details of selected standard models: Ionisation

Hadron and ion ionisation

- 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
  - ICRU'49 and NIST databases

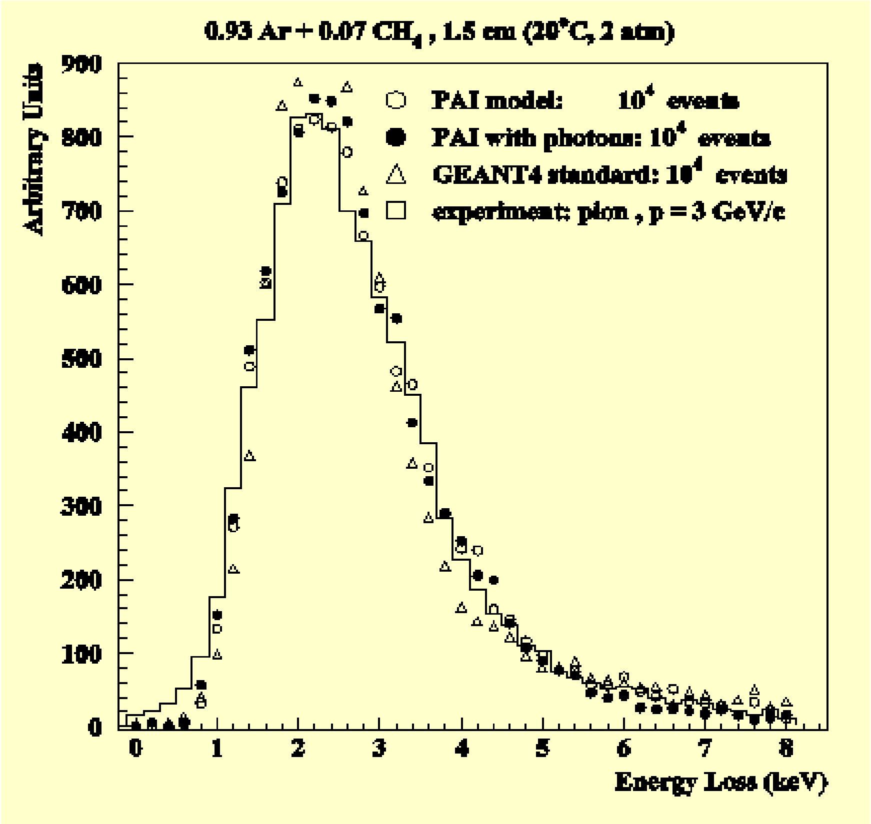


Simulation of a step of a charged particle

- The Bethe-Bloch formula (or low-energy parameterision) provides value of mean energy loss
- Values of mean dE/dx, range and cross section of δ-electron production are pre-computed at initialisation stage of Geant4 and stored in G4PhysicsTables
- Spline interpolation method is used in the run time for fast interpolation at each simulation step to get mean energy loss
- Sampling of energy loss fluctuation is performed
  - The interface to a fluctuation model G4VEmFluctuationModel
- The cross section of δ-electron production is used to sample production above the threshold T_{cut} PostStep
- If de-excitation is active then fluorescence and Auger electron production is sampled AlongStep

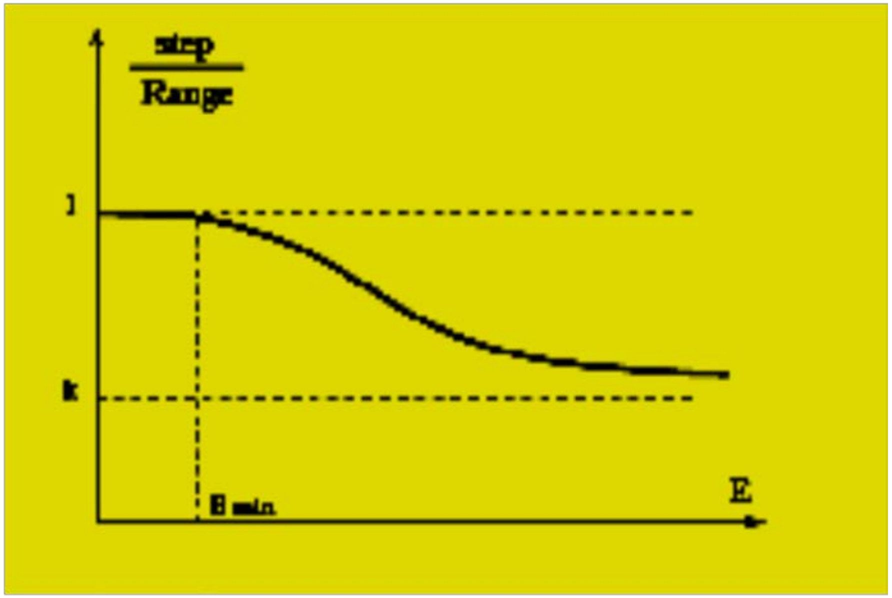
Geant4 models of energy loss fluctuations

- 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 cross section data
  - **Energy transfers are sampled with production of secondary e^- or γ**
  - **Very slow model, should be applied for sensitive region of detector**



Step limitation by ionization processes

- To guarantee precision of computation step should be limited
- Step limit S is defined by stepping function
- It takes into account particle range R and two parameters k and ρ:



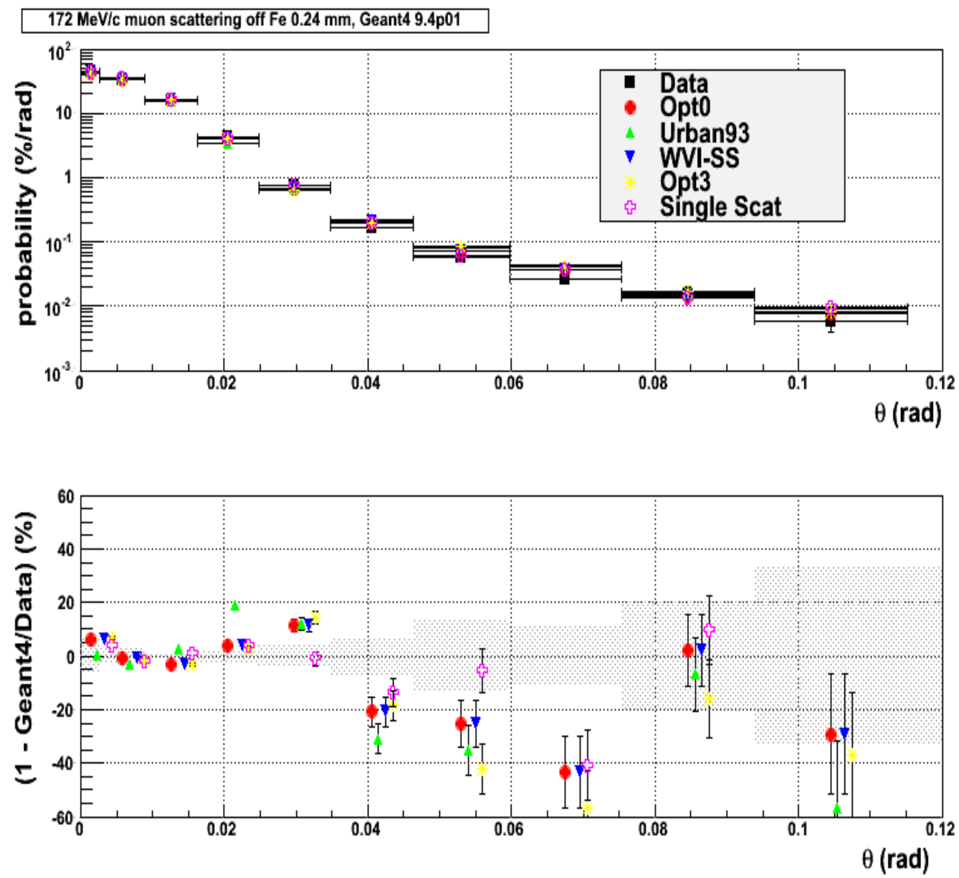
$$S/R = k + \rho/R \cdot (1-k) \cdot (2 - \rho/R)$$

- /process/eLoss/StepFunction 0.1 50 um

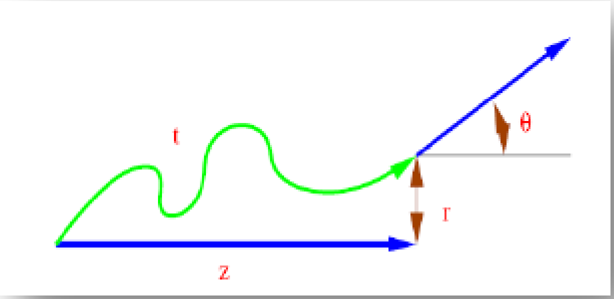
Details of selected standard models: Multiple scattering

Multiple Coulomb Scattering (MSC)

- Charged particles traversing a finite thickness of matter suffer elastic Coulomb scattering
- The cumulative effect of these small angle scatterings is a net deflection from the original particle direction
- MSC implementation determine accuracy and CPU performance of simulation



MSC algorithm



- Legend
  - True path length : t
  - Longitudinal or geometrical displacement : z
  - Lateral displacement : r
  - Angular deflection : (θ, φ)

- The algorithm performs several steps for the simulation of MSC which are essentially the same for many « condensed » simulations
  - The physics processes and the geometry select the step length; MSC performs the t ↔ z transformation only
  - The transport along the initial direction is not MSC's business
  - Sampling of scattering angle (θ, φ)
  - Computing of lateral displacement and relocation of particle

MSC models

Model	Particle type	Energy limit	Specifics and applicability
Urban (Urban 2006)	Any	-	Default model, (Lewis 1950) approach, tuned to data, used for LHC production.
Screened Nuclear Recoil (Mendenhall and Weller 2005)	p, ions	< 100 MeV/A	Theory based process, providing simulation of nuclear recoil for sampling of radiation damage, focused on precise simulation of effects for space app.
Goudsmit-Saunderson (Kadri 2009)	e^+, e^-	< 1 GeV	Theory based cross sections (Goudsmit and Saunderson 1950). EPSEPA code developed by Penelope group, final state using EGSnrc method (Kawrakov et al. 1998), precise electron transport
Coulomb scattering (2008)	any	-	Theory based (Wentzel 1927) single scattering model, uses nuclear form-factors (Butkevich et al. 2002), focused on muons and hadrons
WentzelVI (2009)	any	-	MSC for small angles, Coulomb Scattering (Wentzel 1927) for large angles, focused on simulation for muons and hadrons.
Ion Coulomb scattering (2010)	ions	-	Model based on Wentzel formula + relativistic effects + screening effects for projectile & target. From the work of P. G. Rancoita, C. Consolandi and V. Ivantchenko.

MSC classes

- Processes per particle type are available
  - G4eMultipleScattering for e+/e-
  - G4MuMultipleScattering for μ+/μ-
  - G4hMultipleScattering for hadrons and ions
- L. Urban models
  - G4UrbanMscModel93 : used by default in G4eMultipleScattering
  - G4UrbanMscModel90 : used for muons in G4MuMultipleScattering, and for hadrons & ions in G4hMultipleScattering
- Alternative single and multiple scattering models are available to users
  - see extended examples...

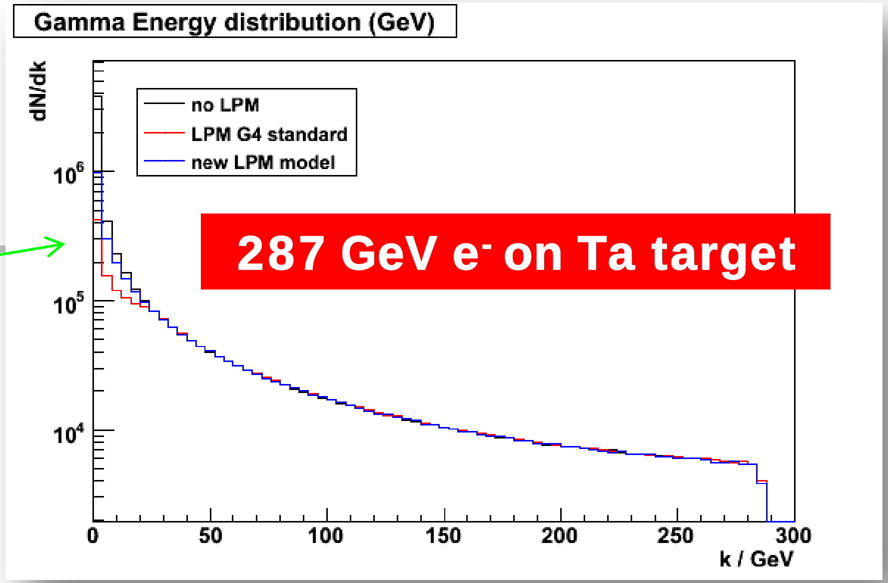
Step limitation for charged particle transport

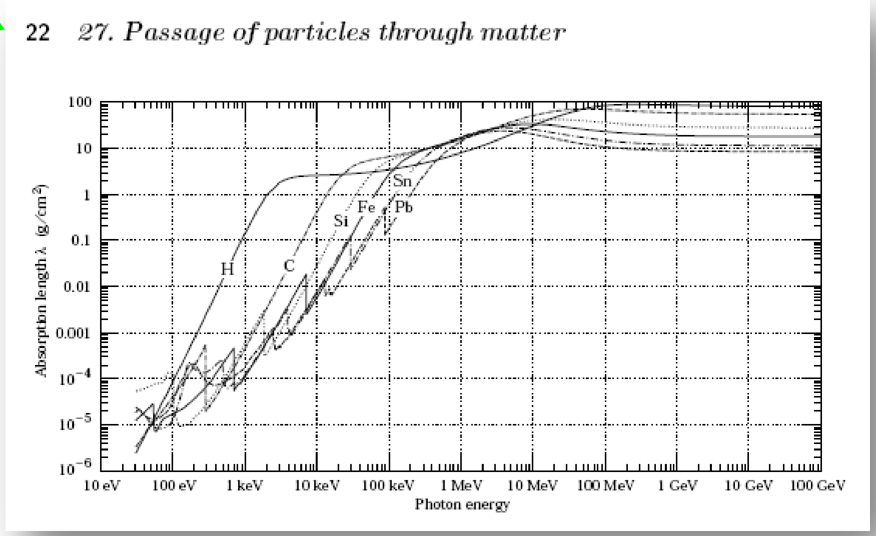
- Step of a charged particle may be limited by several Geant4 processes:
  - Ionisation – discussed in previous slide
  - Multiple scattering – strong step limitation new geometry boundary
  - Delta-electron production and bremsstrahlung – cut dependent
  - User defined step limit
- Simulation results strongly depend on step limit method

GEANT4 CUTS

Bremsstrahlung

- Bremsstrahlung spectrum grows to low energy as 1/k
  - k is the gamma energy
- Low energy gammas have very small absorption length





- Simulation of all low-energy gammas is non-effective
- Cuts/production threshold are used in all Monte Carlo codes
- Gamma emission below production threshold is taken into account as a continuous energy loss
- Similar approach is used for the ionisation process where spectrum of δ-electrons is proportional to $1/T^2$

Cut and production thresholds for energy loss processes

- User defines cut in range expressed in units of length
- Using this range Geant4 kernel compute production threshold T_{cut} for each material during initialization
- For a typical process (G4hIonisation, G4eIonisation, …), the production threshold T_{cut} subdivides the continuous and discrete parts of energy loss:
  - Mean rate of energy lost due to soft energy transfers
  - Total XS for discrete δ-electron production above T_{cut}

$$\frac{dE(E,T_{cut})}{dx} = n_{at} \int_0^{T_{cut}} T \frac{d\sigma(Z,E,T)}{dT} dT$$

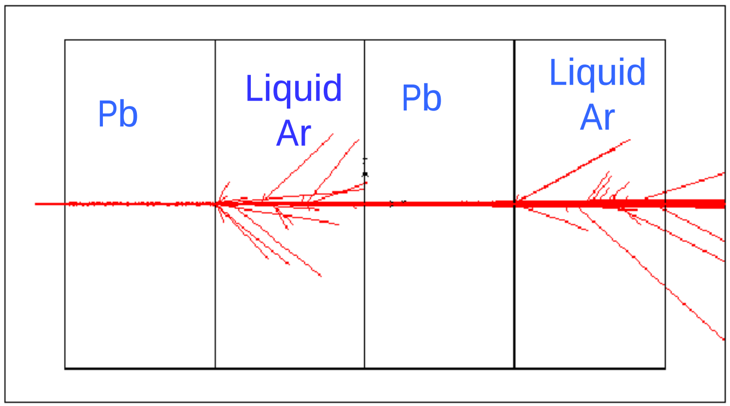
$$\sigma(Z,E,T_{cut}) = \int_{T_{cut}}^{T_{\max}} \frac{d\sigma(Z,E,T)}{dT} dT$$

- At each step energy deposition is sampled by a fluctuation model using the computed mean energy loss
- Optionally, energy loss may be modified :
  - for the generation of extra δ-electrons under the threshold when the track is in the vicinity of a geometrical boundary (sub-cutoff)
  - for the sampling of fluorescence and Auger–electrons emission
- 4-momentum balance is provided in all cases

Effect of production thresholds

500 MeV incident protons on EM Pb/LAr calorimeter

In Geant4



One sets the production threshold for delta rays as a <u>unique range</u>:

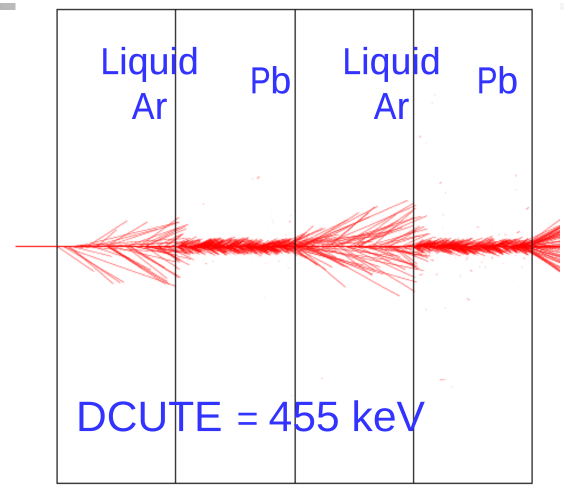
1.5 mm

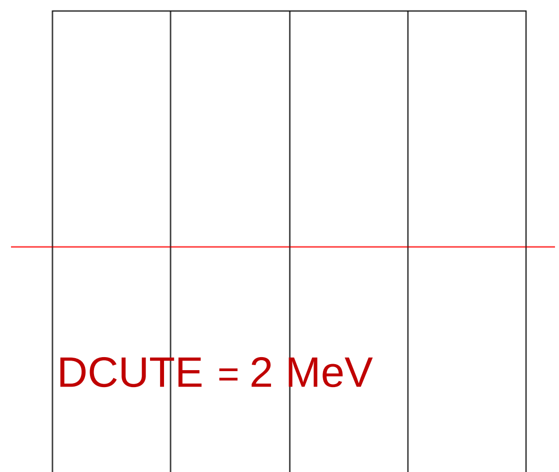
It is converted by Geant4 to energy:

T_c = 455 keV electron energy in liquid Ar

T_c = 2 MeV electron energy in Pb

In Geant3





one has to set the cut for delta-rays (DCUTE) as an <u>energy threshold</u>

<u>either</u> to the Liquid Argon value, thus producing many small unnecessary δ-rays in Pb,

<u>or</u> to the Pb value, thus killing the δ-rays production everywhere

What particles have cuts?

- Since Geant4 9.3 cuts are defined for
  - Gamma
  - Electron
  - Positron
  - Proton
- Cut for proton is used for all hadrons and ions by elastic scattering processes

Which processes use cuts ?

- It is not mandatory to use cuts
- Energy thresholds for gamma are used in Bremsstrahlung
- Energy thresholds for electrons are used in ionisation and e+e- pair production processes
- Energy threshold for positrons is used in the e+e- pair production process
- Energy thresholds for gamma and electrons are used optionally ("ApplyCuts" options) in all discrete processes
  - Photoelectric effect, Compton, gamma conversion
- Energy threshold for protons are used in processes of elastic scattering for hadrons and ions defining the threshold for kinetic energy of nuclear recoil

Comments

- Range cut approach was established for simulation of energy deposition inside solid or liquid media
  - Sampling and crystal calorimeters
  - Silicon tracking
- For specific user application, it may be revised, for example, by defining different cuts in range for electron and gamma
  - Gaseous detectors
  - Muon system
- Tracking cuts may be also used (saving some CPU) for simulation of penetration via shielding or for simulation in non-sensitive part of the apparatus
  - Astrophysics applications
- Do we need cuts for nano-dosimetry?

How to define cut?

- Using UI interface to geant4 kernel:
  - /run/setCut 0.1 mm
  - /run/setCutForAGivenParticle e- 10 um
- Implementing virtual method SetCuts() of G4VUserPhysicsList
- In Geant4 examples several different implementations of cut definition in user code are shown
  - Including user defined UI commands
  - $G4INSTALL/examples/extended/electromagnetic

Cuts per G4Region

- Uniform cut in range providing balanced simulation of particle transport in media with different density
- Requirements for precision in different part of complex geometry may be very different
  - Micron precision in tracking devices millimeter precision in calorimeters
  - Unique value of the cut in range may be not effective and not practical

How to find help?

List of Main Geant4 Documents and Tools

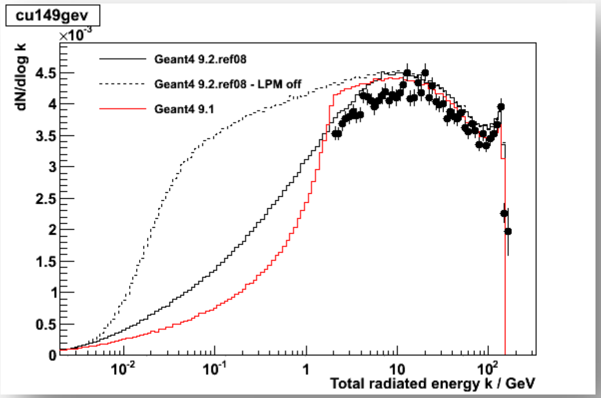
- User Documents
  - Application Developers' Guide
  - Installation Guide
  - Toolkit Developer Guide
  - Examples
  - Physics Reference Manual

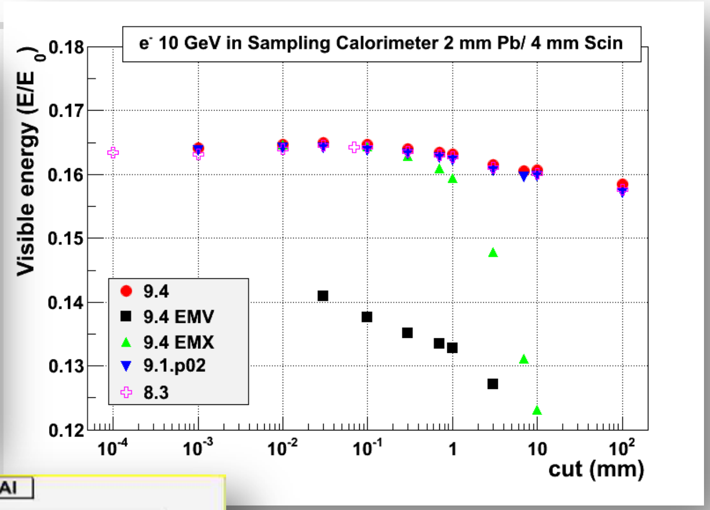
- User Aids
  - Linux Crossed Reference (LXR) source code browser
  - HyperNews User Forum
  - Bug report system

Suggestions

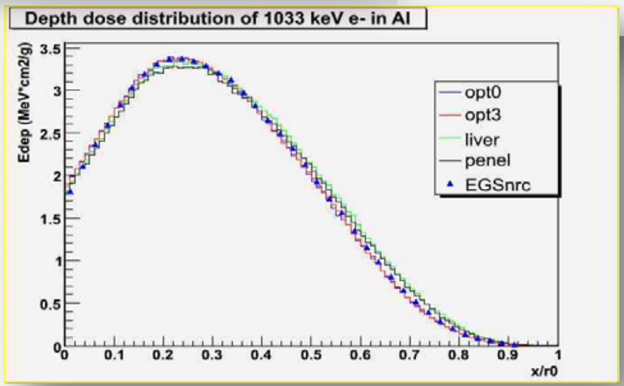
- The list of available EM processes and models is maintained by EM working groups in EM web pages
  - http://cern.ch/geant4/collaboration/working_groups/electromagnetic/index.shtml
- Geant4 extended and advanced examples show how to use EM processes and models
  - In $G4INSTALL/examples
- Visit Geant4 HyperNews forum "electromagnetic processes" for discussion
- Use Geant4 bug report system for problems
- User feedback is always welcome

Validation repository





- A web-based verification tool has been developed for easy comparison of EM physics results obtained with different Geant4 version, and with measurements



http://www-zeuthen.desy.de/geant4/web/

To learn more:

$G4INSTALL/examples/extended/electromagnetic

Check basic quantities	
Total cross sections, mean free paths …	TestEm0, Em13, Em14
Stopping power, particle range …	Em0, Em1, Em5, Em11, Em12
Final state : energy spectra, angular distributions	Em14
Energy loss fluctuations, fluorescence	Em18
Multiple Coulomb scattering	
as an isolated mechanism	Em15
as a result of particle transport	Em5
More global verifications	
Single layer: transmission, absorption, reflexion	Em5
Bragg curve, tallies	Em7
Depth dose distribution	Em11, Em12
Shower shapes, Moliere radius	Em2
Sampling calorimeters, energy flow	Em3
Crystal calorimeters	Em9
Other specialized programs	
High energy muon physics	Em17
Other rare, high energy processes	Em6
Synchrotron radiation	Em16
Transition radiation	Em8
Photo-absorption-ionization model	Em10

Refer to section on extended examples in App. User Guide.

Let us start exercises