Geant 4

Electromagnetic Physics

G. Santin*, P. Nieminen

giovanni.santin@esa.int

ESA/ESTEC Space Environments and Effects Analysis Section

**RHEA System, based at ESTEC*

Geant4 Space Users' Forum

ESTEC

20 Jan 2003

Outline

Geant4

- Geant4 Standard EM processes
  - Charged particles and photons
  - How-To: some Physics List details
- Geant4 "Low Energy" EM processes
  - Charged particles and photons
  - Hadron EM processes
  - How-To

- Derived from talks by
  - Michel Maire, LAPP Annecy
  - P.Nieminen, ESA-ESTEC
  - M.G.Pia, Univ.&INFN Genova

Geant4 processes

- "Process" in Geant4
  - a C++ class describing how and when a physical interaction takes place along a particle track
- Final state generation independent from
  - Cross sections
  - Tracking
- The process interface (G4VProcess) is
  - Common to all processes
  - Very stable
- Building the "Physics List", the user can
  - Choose the list of particles and processes used in the application
    - Mandatory and critical user's task
  - Modify existing processes
  - Add new processes
- Physics lists require sometimes tricky details
  - Examples distributed with the release

Standard EM processes

Geant 4

- The primary is assumed to have ≥ 1 keV
  - Atomic electrons are "quasi-free"
    - Binding energy neglected (except photoelectric)
  - Atomic nucleus "fixed"
    - Recoil momentum neglected
  - Matter described as
    - Homogeneous
    - Isotropic
    - Amorphous

Overview of the processes: charged particles

- Common to all
  - Ionization
  - Coulomb scattering from nuclei
  - Cherenkov
  - Scintillation
  - Transition radiation
- Muons
  - e^+/e^- pair production
  - Bremsstrahlung
  - Nuclear interaction
- Electrons and positrons
  - Bremsstrahlung
  - e^+ annihilation
- Photons
  - Gamma conversion (~10 MeV →)
  - Incoherent scattering (~10 keV → ~10 MeV)
  - Photoelectric effect (← ~10 keV)
  - Coherent scattering (← ~100 keV)
- Optical photons (see P.Gumplinger)
  - Reflection and refraction
  - Absorption
  - Rayleigh scattering

Ionisation

- Basic mechanism: Inelastic collisions with the atomic electrons of the material, ejecting off an electron from the atom
  - Small energy transfer in individual collisions
  - Large number of collisions

  } macroscopic average energy loss

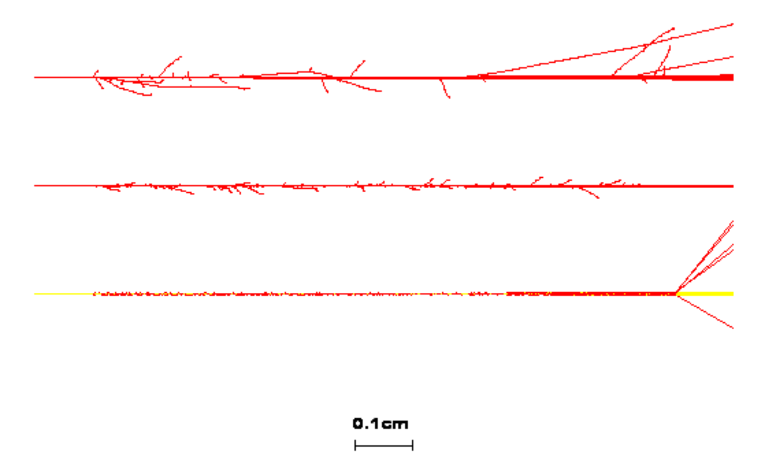
  \+ fluctuations

- Depending on the amount of matter
  - Energy loss can be strongly asymmetric (→ Landau tail)

Ionization in Geant4

Geant 4

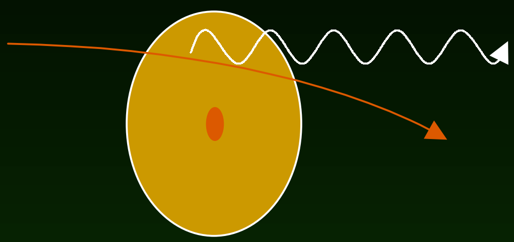
- The cross section depends on the electron cut
  - Below the threshold, soft δ-rays are only counted as continuous energy loss
  - High energy knock-on electrons are produced and tracked
- Both continuous energy loss (below the production cut) and δ-ray energy spectrum
  - obtained integrating the differential cross section for the ejection of an electron
- Different processes for different particles
  - *e.g.* e^+/e^-
    - Möller or Bhabha cross sections
    - Integration → Berger-Seltzer dE/dx formula
  - Muons
    - Integration → Bethe-Bloch formula
- 200 MeV electrons, protons, alpha
  - 1 cm Aluminum

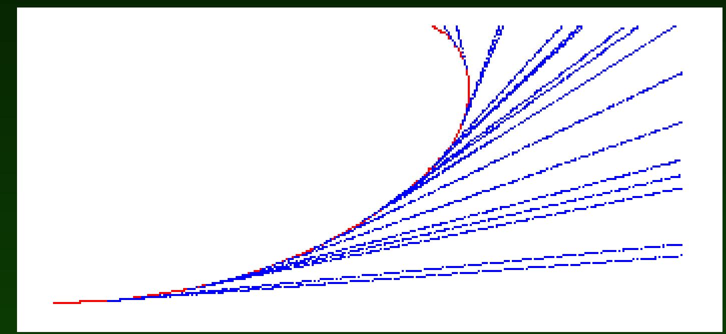


Geant 4

Bremsstrahlung

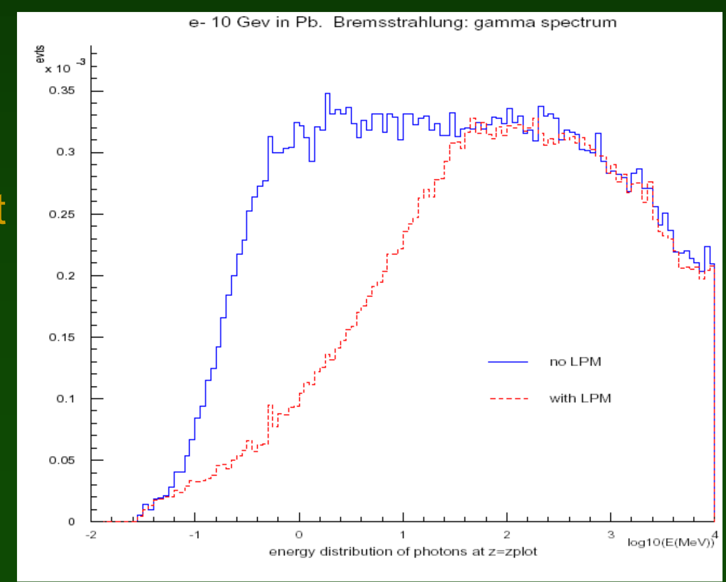
- Fast moving charged particles are decelerated in the atoms Coulomb field. A fraction of their kinetic energy is emitted in form of real photons
  - Probability ~$1/M^2$ (M = mass of the incident particle) and ~Z^2 (Z = atomic number of the material)





- High energy photons created and tracked above a given threshold k_{cut}

- Bethe-Heitler formula, corrected and extended
  - Screening, atomic electrons, polarization,…
  - Landau-Pomeranchuk-Migdal suppression effect

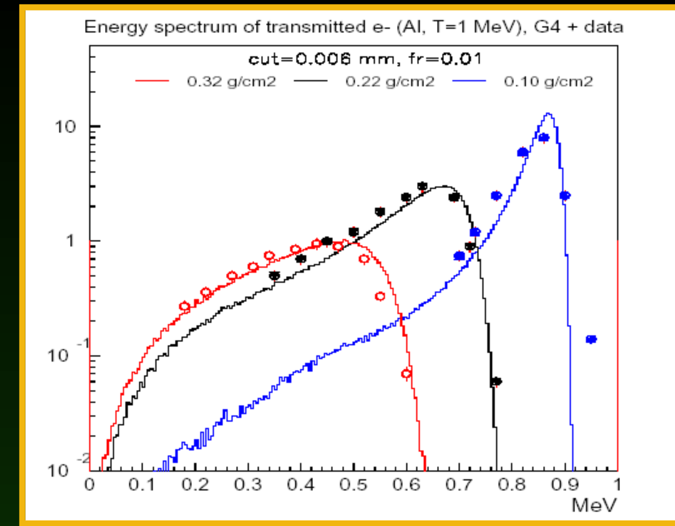


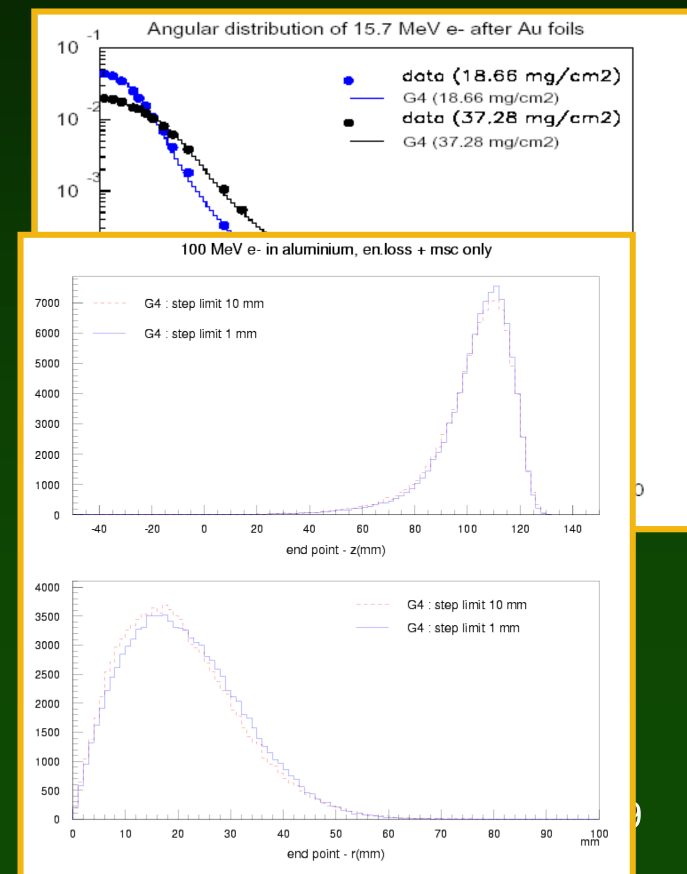
Multiple Scattering

- GEANT4 uses a new model (L.Urban) which simulates the scattering of the particle after a step, computes the mean path length correction and the mean lateral displacement
  - This model does not use the Moliere formalism

- New tuning in the 5.0 release
  - Good behavior both for high energy protons and low energy electrons
  - Backscattering well described

- Very weak dependence on the step limit
  - longitudinal (z) and tranverse (r) distances



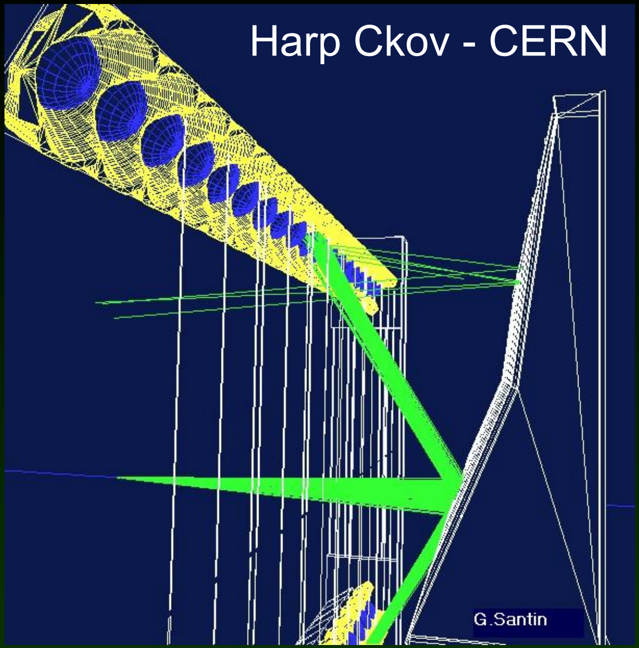


- Bibliography:

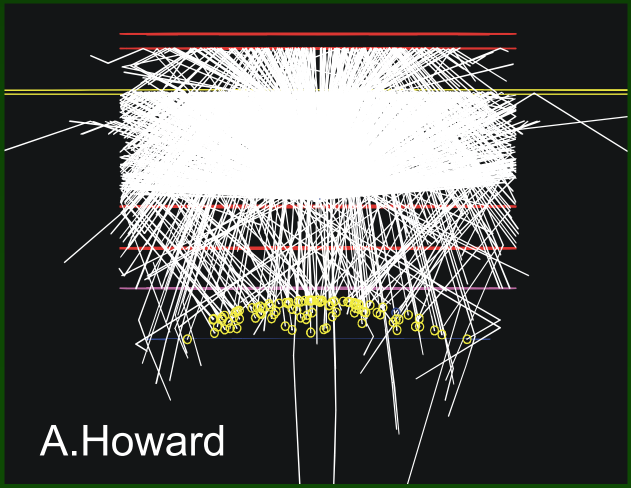
  - S. Goudsmit and J. L. Saunderson. *Phys. Rev. 57 (1940) 24.*
  - H. W. Lewis. *Phys. Rev. 78 (1950) 526.*
  - Reformulated in J. M. Fernandez-Varea *et al. NIM B73 (1993) 447.*

…some light!

- Cherenkov effect
  - See novice example "N06"



- Scintillation
  - New features in 5.0
    - Fast and slow components
    - Particle dependent excitation levels
    - Poisson for small mean number of photons
  - See P.Gumplinger
  - Extended example "Underground experiment", A.Howard



- Combined with Optical Processes
  - See talk by Peter Gumplinger

How to use these processes: Physics list implementation

Geant 4

- Code (here and later) taken from the

"Educated Guess Physics Lists" (see J.P.Wellisch)

```
#include "G4MultipleScattering.hh"
#include "G4eIonisation.hh"
#include "G4eBremsstrahlung.hh"
#include "G4eplusAnnihilation.hh"

class G4EMBuilder {
…
    G4MultipleScattering  theElectronMultipleScattering;
    G4eIonisation         theElectronIonisation;
    G4eBremsstrahlung     theElectronBremsStrahlung;

    G4MultipleScattering  thePositronMultipleScattering;
    G4eIonisation         thePositronIonisation;
    G4eBremsstrahlung     thePositronBremsStrahlung;
    G4eplusAnnihilation   theAnnihilation;
};
```

…implementation…

Geant 4

- Attach the processes to the particles

```
G4ProcessManager * pManager = 0;
  …
  pManager = G4Electron::Electron()->GetProcessManager();
  pManager->AddDiscreteProcess(&theElectronBremsStrahlung);
  pManager->AddProcess(&theElectronIonisation, ordInActive,2, 2);
  pManager->AddProcess(&theElectronMultipleScattering);
  pManager->SetProcessOrdering(&theElectronMultipleScattering, idxAlongStep,  1);
  pManager->SetProcessOrdering(&theElectronMultipleScattering, idxPostStep,  1);

  pManager = G4Positron::Positron()->GetProcessManager();
  pManager->AddDiscreteProcess(&thePositronBremsStrahlung);
  pManager->AddDiscreteProcess(&theAnnihilation);
  pManager->AddRestProcess(&theAnnihilation);
  pManager->AddProcess(&thePositronIonisation, ordInActive,2, 2);
  pManager->AddProcess(&thePositronMultipleScattering);
  pManager->SetProcessOrdering(&thePositronMultipleScattering, idxAlongStep,  1);
  pManager->SetProcessOrdering(&thePositronMultipleScattering, idxPostStep,  1);
```

- And the same for the other charged particles

Compton scattering

- Parameterization based on the Klein-Nishina formula, corrected for low energy distortions

$$\sigma(Z, E_\gamma) = \left[P_1(Z) \frac{\log(1+2X)}{X} + \frac{P_2(Z) + P_3(Z)X + P_4(Z)X^2}{1 + aX + bX^2 + cX^3} \right].$$

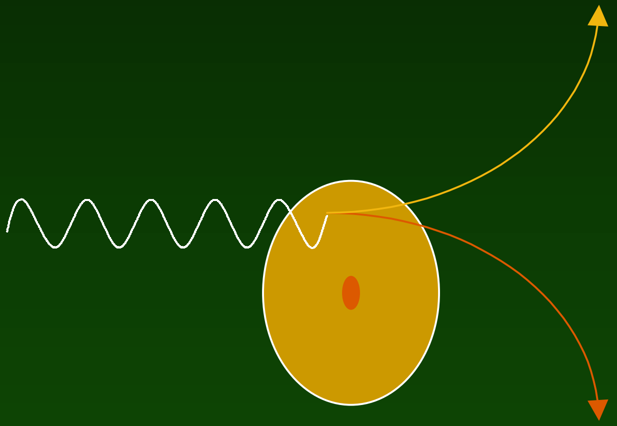
  – Fit over 511 data points
  – $1 \leq Z \leq 100$
  – 10 keV ≤ k ≤ 100 GeV

- The accuracy of the fit is estimated to be
  – $d\sigma/\sigma$ =
    - ~ 10 % for k ~10 keV → 20 keV
    - ~ 5-6 % for k > 20 keV

Gamma conversion in (e^+,e^-) pair

- Transformation of a photon in a (e^+,e^-) pair in the Coulomb field of an atom (for momentum conservation)
  - Dominant process for $E\gamma \geq$ few tens of MeV

- Differential cross section: Bethe-Heitler formula corrected and extended for various effects
  - Screening of nucleus field
  - Pair creation in the field of atomic electrons
  - Correction to the Born approximation
  - LPM suppression mechanism
  - …



- In Geant4: parameterized and fitted against data (Hubbel *et al.* 1980)
  - $1 \leq Z \leq 100$, $E\gamma$: 1.5 MeV → 100 GeV
  - $d\sigma/\sigma \leq 5$ % (with a mean value of 2.2 %)

How to use the photon processes

Geant 4

- Create…

```
#include "G4PhotoElectricEffect.hh"
#include "G4ComptonScattering.hh"
#include "G4GammaConversion.hh"

class G4EMBuilder {
…
    G4PhotoElectricEffect  thePhotoEffect;
    G4ComptonScattering    theComptonEffect;
    G4GammaConversion      thePairProduction;
…
};
```

- And attach the processes to the “gamma” particle

```
pManager = G4Gamma::Gamma()->GetProcessManager();
pManager->AddDiscreteProcess(&thePhotoEffect);
pManager->AddDiscreteProcess(&theComptonEffect);
pManager->AddDiscreteProcess(&thePairProduction);
```

Low Energy EM processes

Geant 4

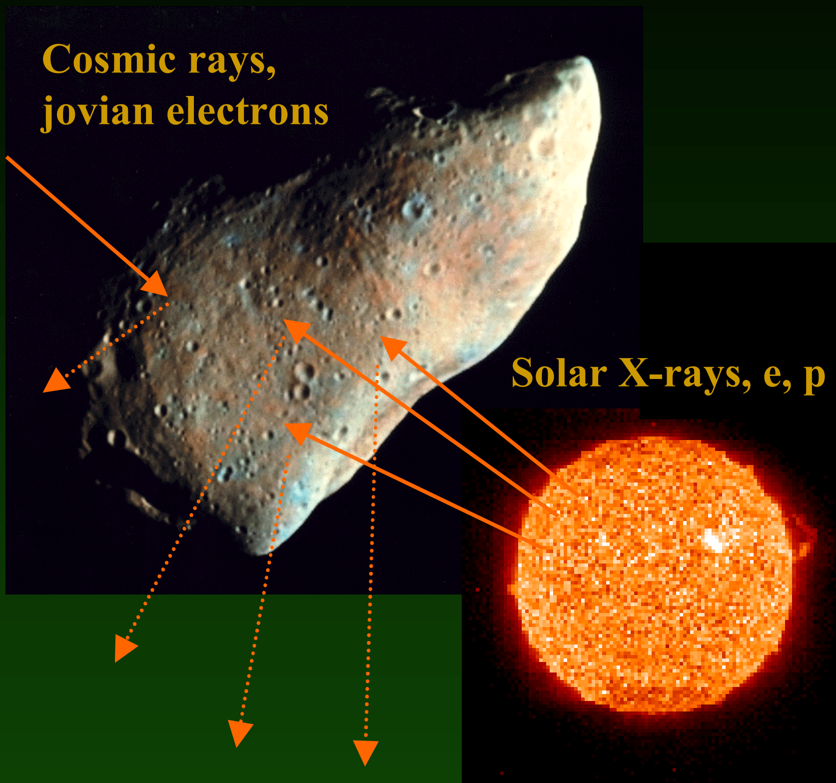
- A package in the Geant4 electromagnetic package
  - *geant4/source/processes/electromagnetic/lowenergy/*
- A set of processes extending the coverage of electromagnetic interactions in Geant4 down to "*low*" energy
  - 250 eV *(in principle even below this limit)* for electrons and photons
  - down to the approximately the ionization potential of the interacting material for hadrons and ions
- A set of processes based on detailed models
  - shell structure of the atom
  - precise angular distributions
- Complementary to the "standard" electromagnetic package

Electron and photon processes: energy cut-offs

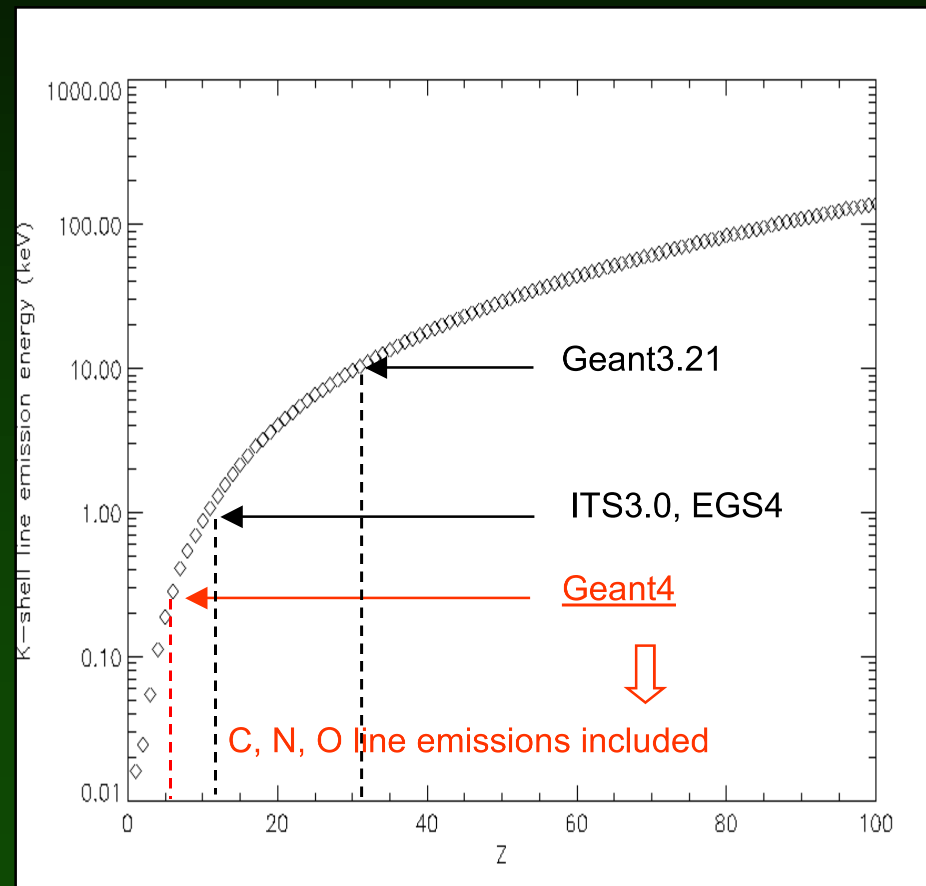
• Geant3.21	10 keV
• EGS4, ITS3.0	1 keV
• Geant4 “standard models”	
– Photoelectric effect	10 keV
– Compton effect	10 keV
– Bremsstrahlung	1 keV
– Ionisation (δ-rays)	1 keV
– Multiple scattering	1 keV
• <u>Geant4 low-energy models</u>	<u>250 eV</u>

X-Ray Surveys of Solar System Bodies

Geant 4



Courtesy SOHO EIT



Induced X-ray line emission: indicator of target composition (~100 μm surface layer)

Features of electrons and photon models

Geant 4

- Validity range from 250 eV to 100 GeV
- Elements Z=1 to 100
- Based on evaluated databases for cross sections and generation of final state:
  - **EADL** (Evaluated Atomic Data Library),
  - **EEDL** (Evaluated Electrons Data Library),
  - **EPDL97** (Evaluated Photons Data Library)

evaluated data libraries from LLNL, courtesy Dr. Red Cullen.

A version of libraries especially formatted for use with Geant4 available from Geant4 distribution source.

Calculation of cross sections

Geant 4

- Interpolation from the data libraries

$$\log(\sigma(E)) = \frac{\log(\sigma_1)\log(E_2/E) + \log(\sigma_2)\log(E/E_1)}{\log(E_2/E_1)}$$

E_1 and E_2 are the closest lower and higher energy for which data (σ_1 and σ_2) are available

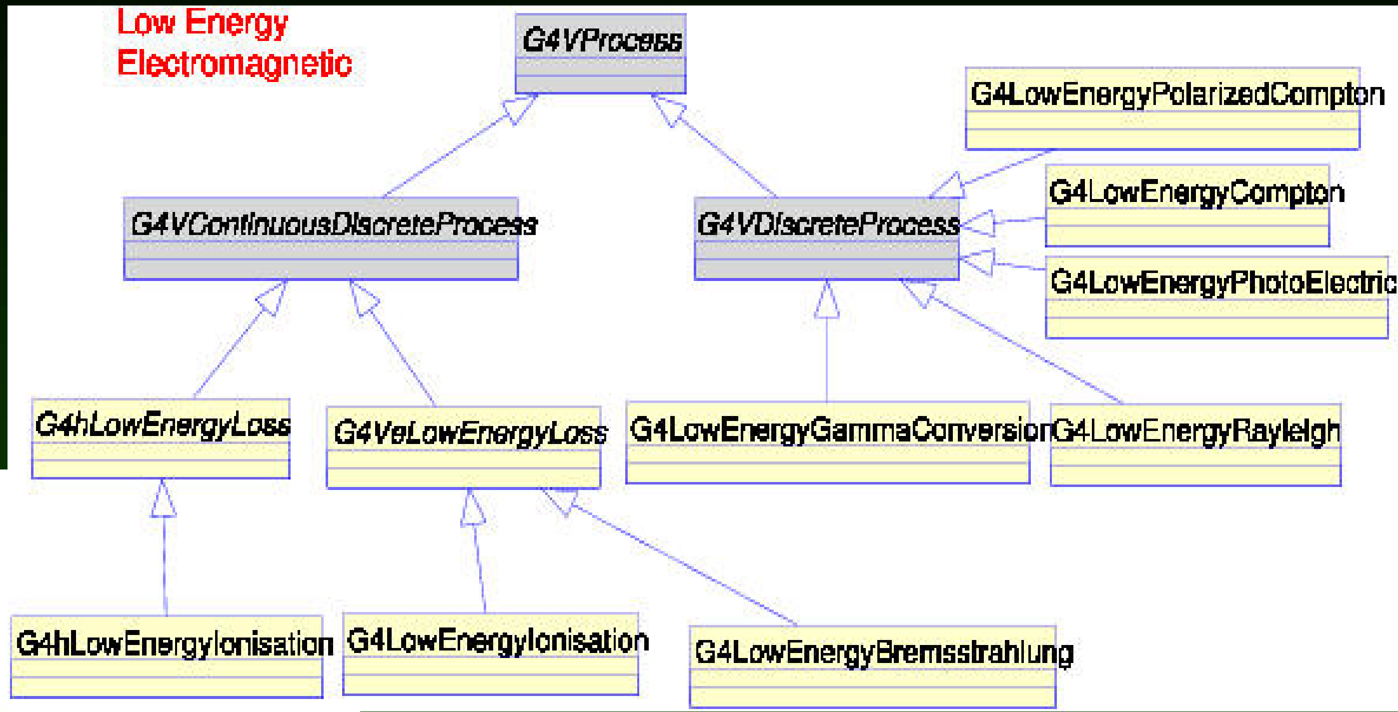
- Mean free path for a process, at energy E:

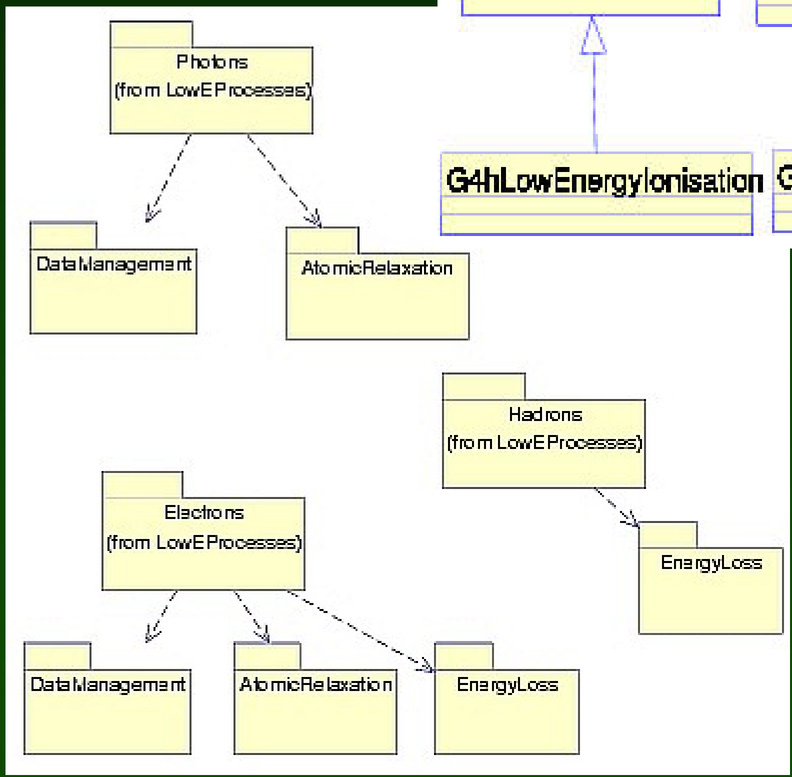
$$\lambda = \frac{1}{\sum_i \sigma_i(E) \cdot n_i}$$

n_i = atomic density of the i^{th} element contributing to the material composition

OOAD technology as a support to physics

Geant 4





Rigorous adoption of OO methods

➩ *openness to extension and evolution*

Extensive use of design patterns

Booch methodology

Overview of electron and photon physics

Geant 4

- Bremsstrahlung
- Ionisation

- Compton scattering
  - Polarised Compton
- Rayleigh scattering
- Photoelectric effect
- Pair production

- + atomic relaxation
  - fluorescence
  - Auger + Coster-Kronig effects

  following photoelectric effect and ionisation

LowE Photon processes

Geant 4

- LowE Compton scattering
  - Energy distribution of the scattered photon according to Klein-Nishina formula
    - multiplied by scattering functions *F*(*q*) from EPDL97 data library.
  - The effect of scattering function becomes significant at low energies
    - suppresses forward scattering
  - Angular distribution of the scattered photon and the recoil electron also based on EPDL97.
- LowE Rayleigh scattering
  - Angular distribution: $F(E,q)=[1+\cos^2(q)]\cdot F^2(q)$
  - where F(q) is the energy-dependent form factor obtained from EPDL97
  - Improved angular distribution available from Geant4 5.0 release, 13th December 2002

Geant 4

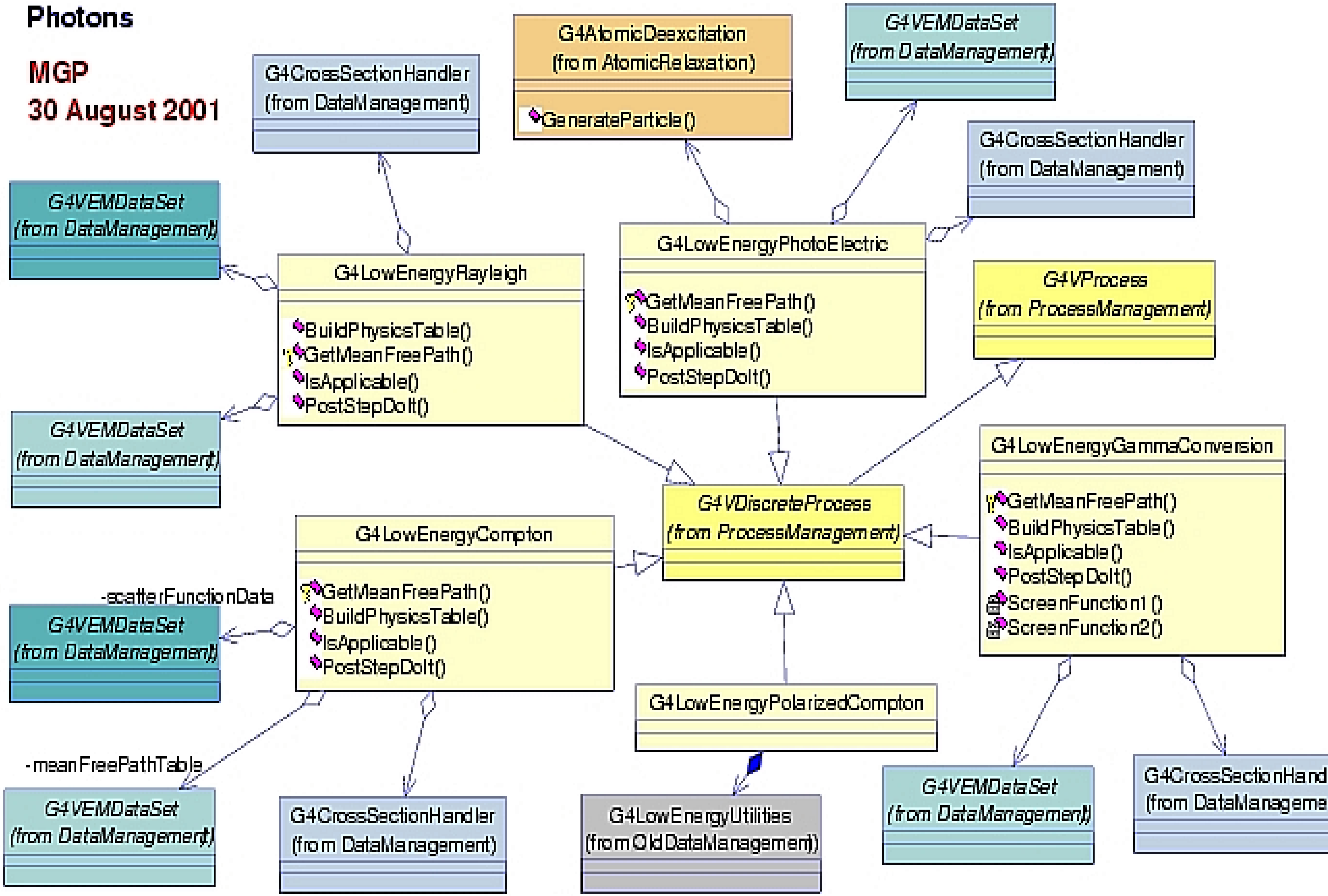
- LowE Photoelectric effect
  - Cross section
    - Integrated cross section (over the shells) from EPDL + interpolation
    - Shell from which the electron is emitted selected according to the detailed cross sections of the EPDL library
  - Final state generation
    - Direction of emitted electron = direction of incident photon
  - Deexcitation via the atomic relaxation sub-process
    - Initial vacancy + following chain of vacancies created (see later)

- LowE Gamma conversion into e^+/e^- pairs
  - Energy sampling from Bethe-Heitler cross sections with Coulomb correction
  - Energy and polar angle sampled w.r.t. the incoming photon using Tsai differential cross section
  - Azimuthal angle generated isotropically
  - e^- and e^+ assumed to have symmetric angular distribution

Geant 4

Photons

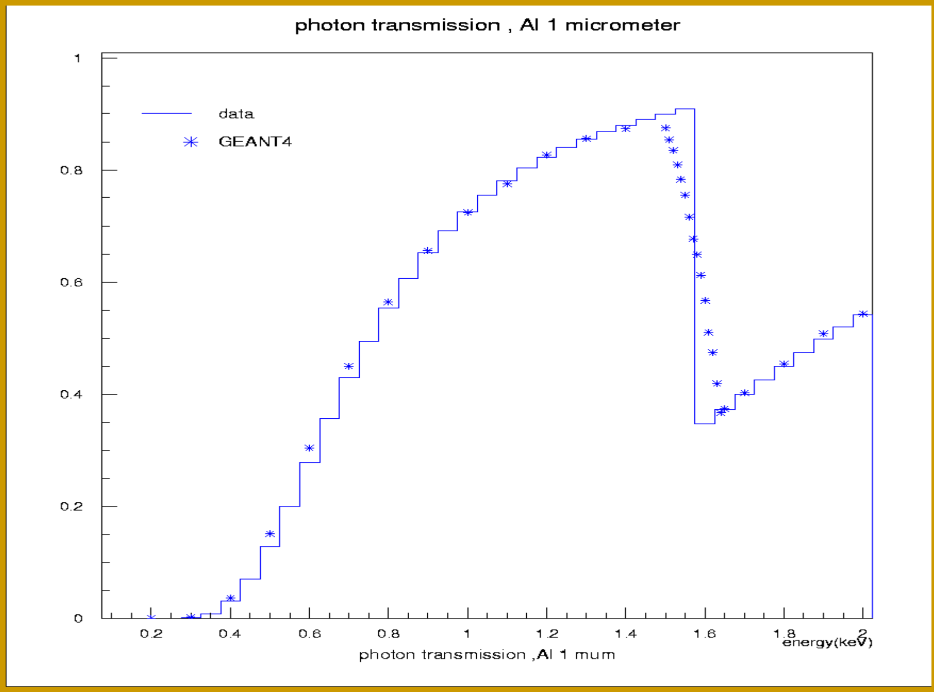
MGP
30 August 2001



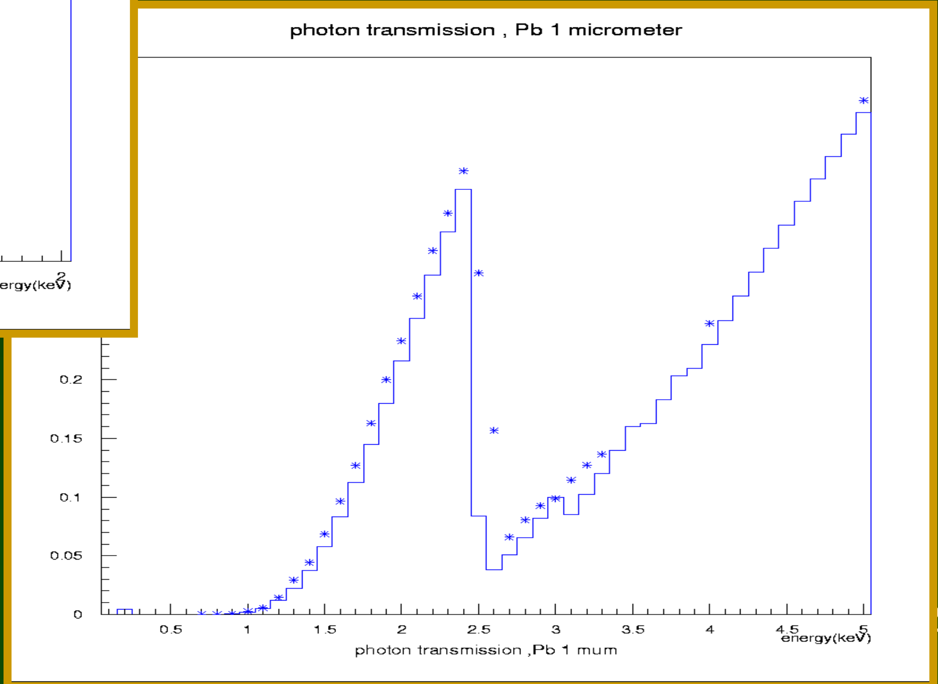
Geant 4

Results: photons

- Evidence of shell induced patterns
  - Photon transmission, 1 µm Al

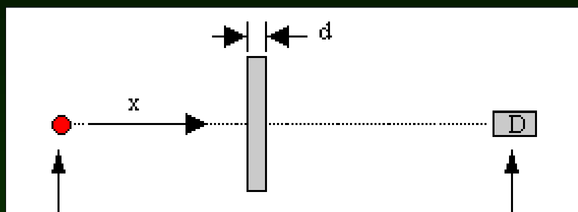


  - Photon transmission, 1 µm Pb



Results: photons

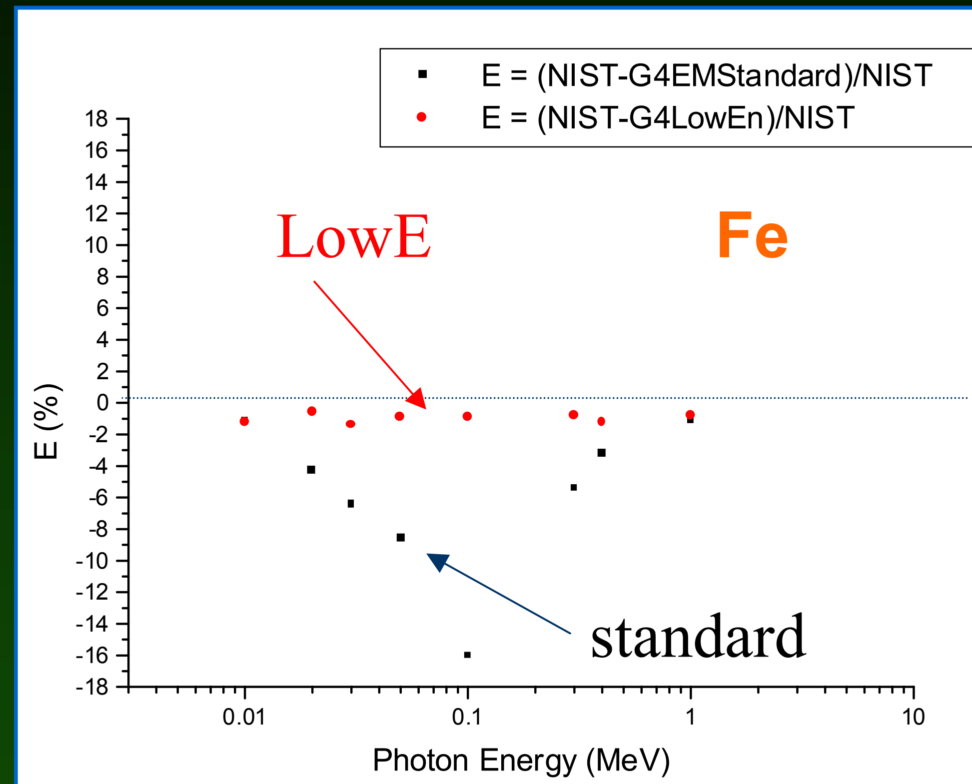
- Mass attenuation coefficient



Comparison against NIST data

Tests by IST - Natl. Inst. for Cancer Research, Genova (F. Foppiano et al.)

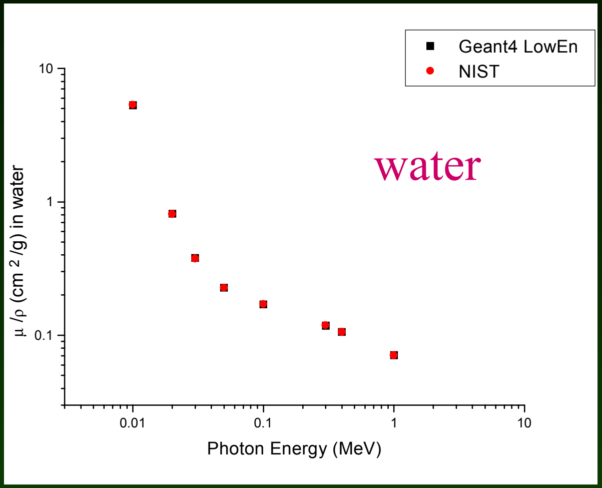
LowE accuracy ~ 1%

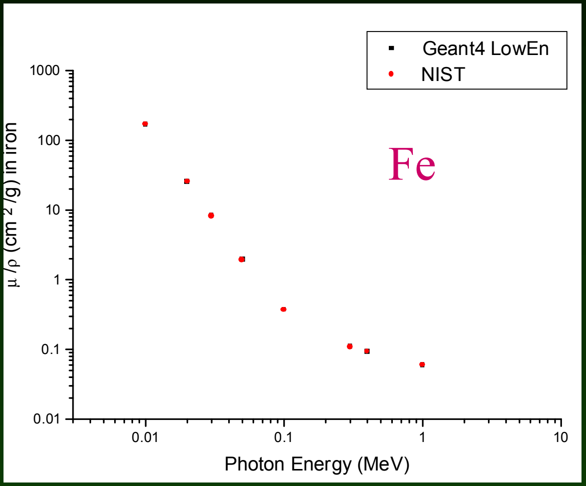


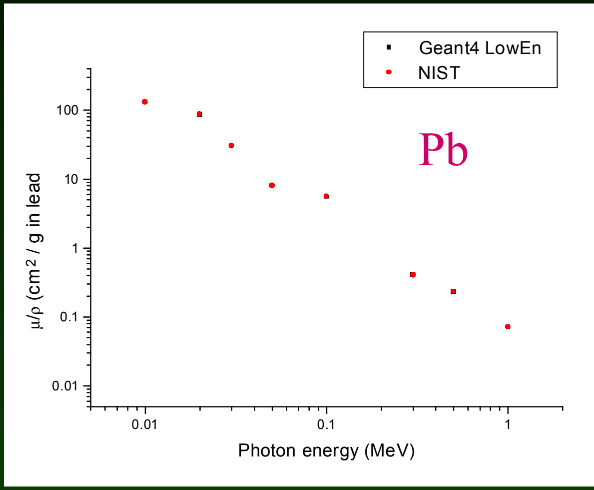
This test will be introduced into the Test & Analysis project for a systematic verification

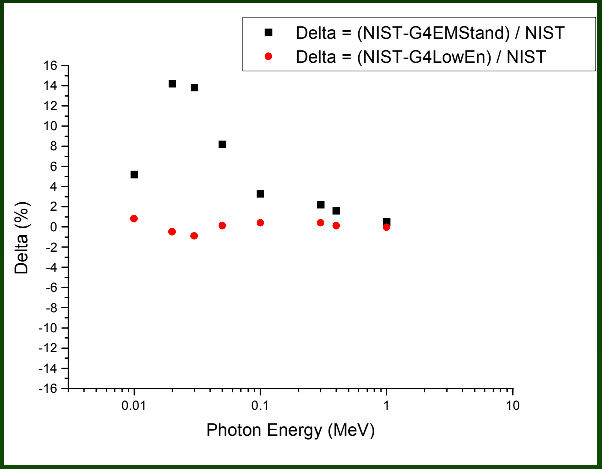
Results: Photon attenuation Geant4 VS NIST data

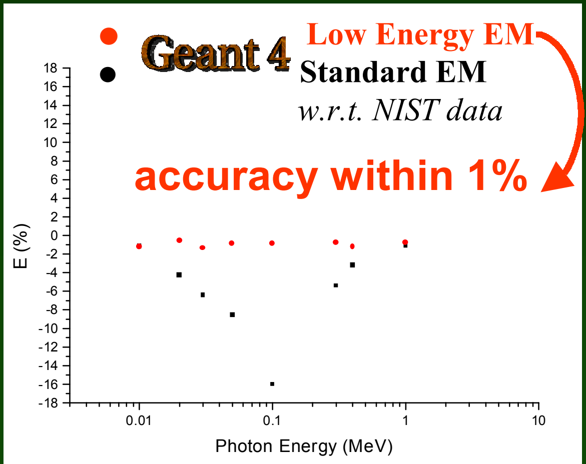
Test and validation by IST - Natl. Inst. for Cancer Research, Genova

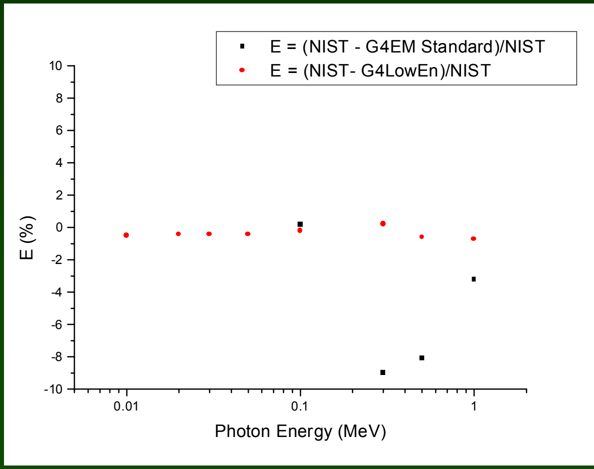












LowE Electron Bremsstrahlung

Geant 4

$$\frac{dE}{dx} = \sum_s \left(\sigma_s(T) \frac{\int_{0.1eV}^{T_C} t \frac{d\sigma}{dt} dt}{\int_{0.1eV}^{T_{MAX}} \frac{d\sigma}{dt} dt} \right)$$

Continuous energy loss

$$\sigma(T) = \sum_s \left(\sigma_s(T) \frac{\int_{T_C}^{T_{MAX}} \frac{d\sigma}{dt} dt}{\int_{0.1eV}^{T_{MAX}} \frac{d\sigma}{dt} dt} \right)$$

Gamma ray production

$$\frac{d\sigma}{dt} = \frac{F(x)}{x}, \quad x = \frac{t}{T}$$

F(*x*) obtained from EEDL. At high energies:

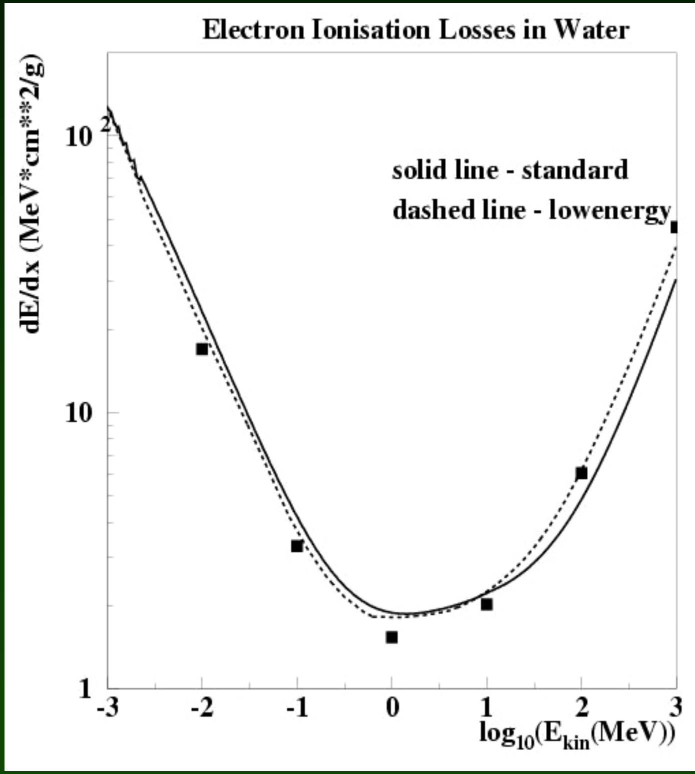
$$F(x) = 1 - x + 0.75x^2$$

Direction of the outgoing electron the same as that of the incoming one; angular distribution of emitted photons generated according to a simplified formula based on the Tsai cross section (expected to become isotropic in the low-E limit)

Geant 4

LowE Electron ionisation

- The δ-electron production threshold T_c is used to separate the continuous and discrete parts of the process
- Partial sub-shell cross sections σ_s obtained by interpolation of the evaluated cross section data in the EEDL library
  - New parameterisations of EEDL data library recently released
- Both the energy and the angle of emission of the scattered electron and the δ-ray are considered
- Interaction leaves the atom in an excited state; sampling for excitation is done both for continuous and discrete parts of the process
- The resulting atomic relaxation treated as follow-on separate process



LowE Electron ionisation - 2

$$\frac{dE}{dx} = \sum_s \left(\sigma_s(T) \frac{\int_{0.1eV}^{T_C} t \frac{d\sigma}{dt} dt}{\int_{0.1eV}^{T_{MAX}} \frac{d\sigma}{dt} dt} \right)$$

Continuous energy loss

$$\sigma(T) = \sum_s \left(\sigma_s(T) \frac{\int_{T_C}^{T_{MAX}} \frac{d\sigma}{dt} dt}{\int_{0.1eV}^{T_{MAX}} \frac{d\sigma}{dt} dt} \right)$$

δ-electron production

$$\frac{d\sigma}{dt} = C \frac{P(x)}{x^2}, \qquad x = \frac{t + B_s}{T + B_s}$$

B_s is the binding energy of sub-shell s

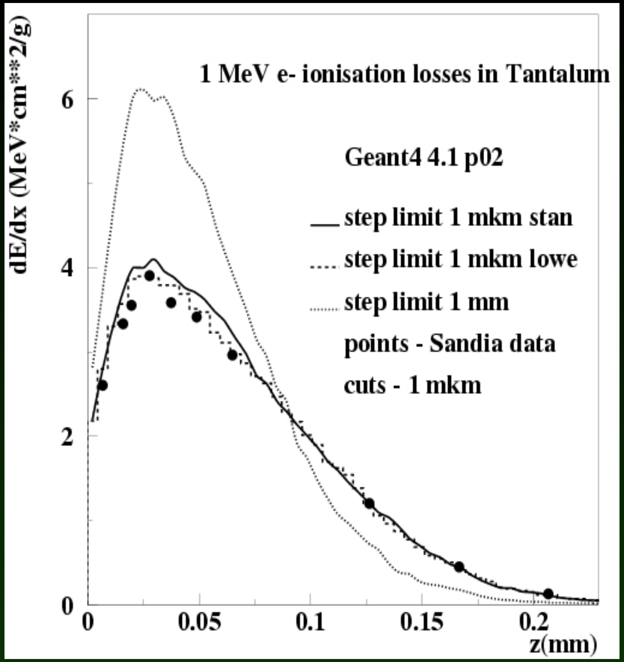
$$P(x) = 1 - gx + (1-g)x^2 + \frac{x^2}{1-x}\left(\frac{1}{1-x} - g\right) + \frac{A}{x}$$

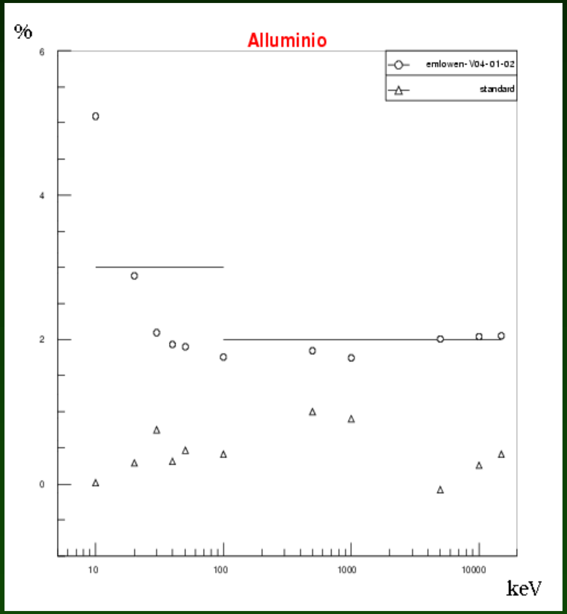
$$g = (2\gamma - 1)/\gamma^2$$

Value of coefficient A for each element is obtained from fit to EEDL data for energies available in the database

Results: electron dE/dx

- Ionisation energy loss in various materials
  - Compared to Sandia database
  - More systematic verification planned





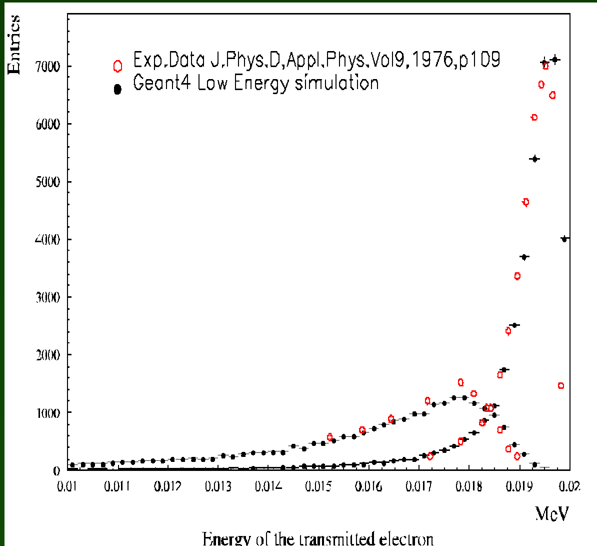
Range

In various simple and composite materials

Compared to NIST database

Transmitted electrons

- 20 keV electrons, 0.32 and 1.04 μm Al



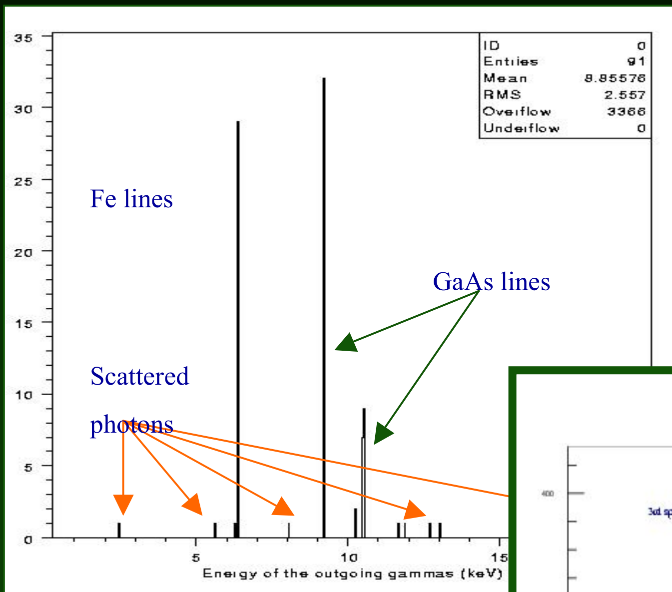
Atomic relaxation

Geant 4

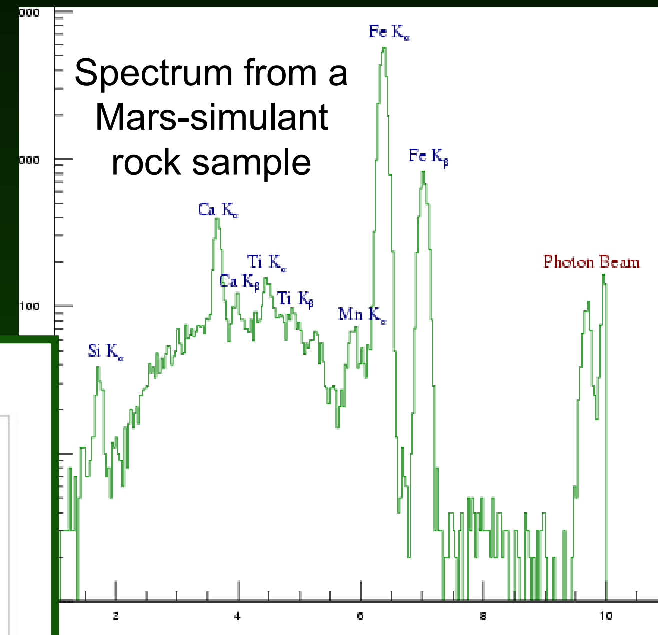
- Fluorescent transitions, Auger (and Coster-Kronig) effects implemented and released
- EADL data used to calculate the complete radiative and non-radiative spectrum of X-rays and electrons emitted
  - Transition probabilities available for $Z = 6 \rightarrow 100$
- K, L, M, N, and some O sub-shells considered
  - Transition probabilities for sub-shells O, P, and Q negligible (<0.1%) and smaller than the precision with which they are known
  - EADL quotes an uncertainty of 15 % on the transition probabilities
- For Z=1 to 5, a local energy deposit corresponding to the binding energy *B* of an electron in the ionized sub-shell simulated.
- For O, P, and Q sub-shells a photon emitted with energy *B*

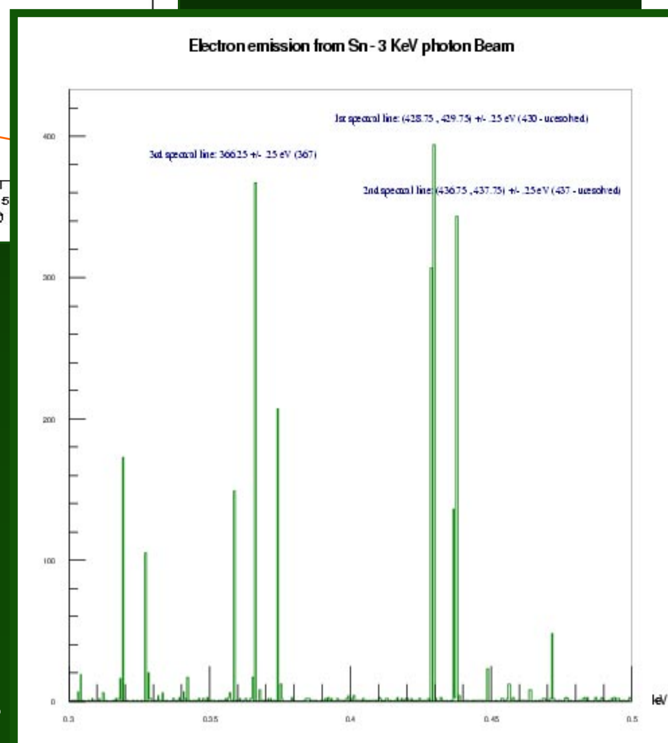
Fluorescence and Auger electrons results

Microscopic validation: against reference data



Experimental validation: test beam data, in collaboration with ESA Science Payload Division





Sn, 3 keV photon beam, electron lines w.r.t. published experimental results

Polarised Compton scattering

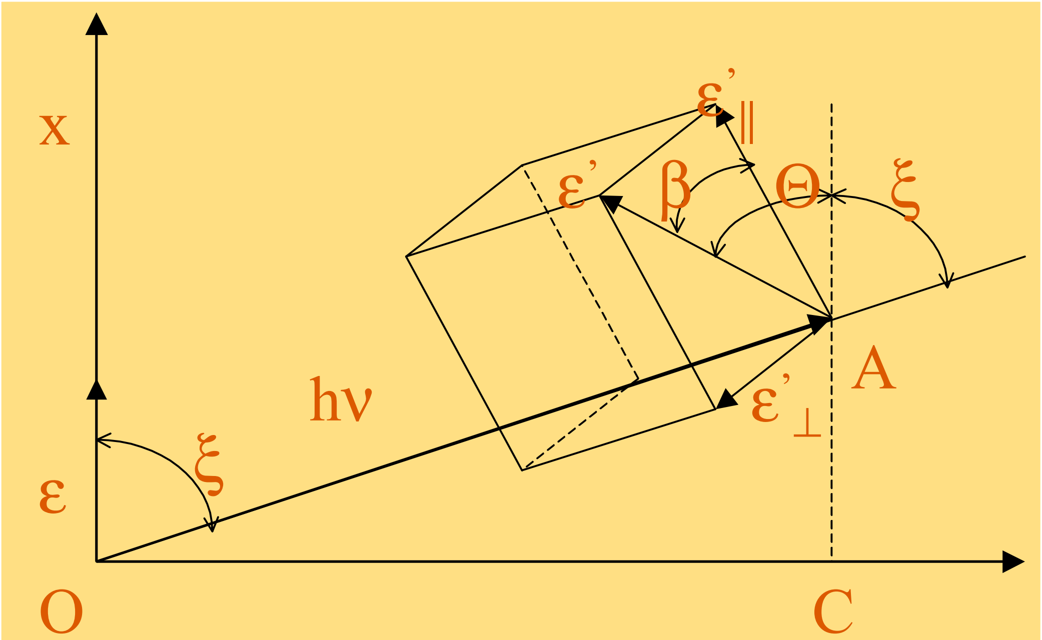
Geant 4

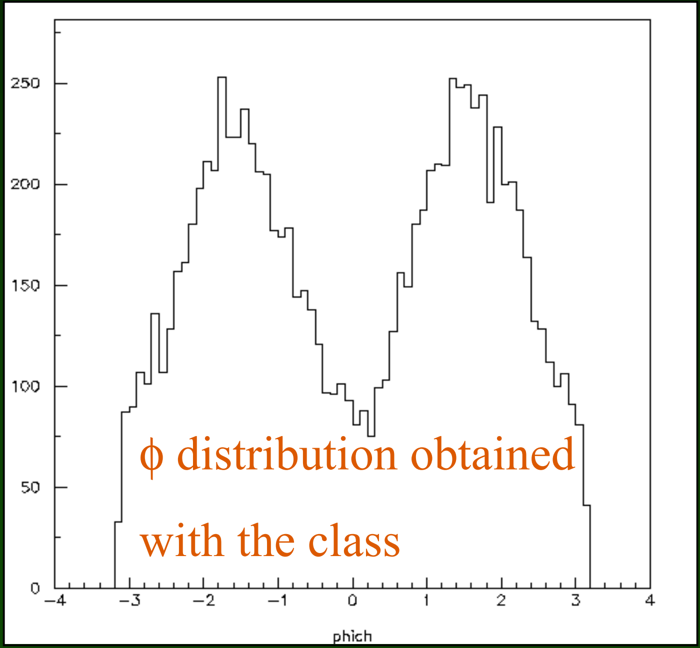
- The Klein-Nishina cross section

$$\frac{d\sigma}{d\Omega} = \frac{1}{4} r_0^2 \frac{h\nu^2}{h\nu_0^2} \left[\frac{h\nu_0}{h\nu} + \frac{h\nu}{h\nu_0} - 2 + 4\cos^2\Theta \right]$$

$h\nu_0$: energy of incident photon
$h\nu$: energy of the scattered photon
Θ : angle between the two polarization vectors

- Angular distribution of scattered radiation composed of two components: $\varepsilon'_{\parallel}$ and $\varepsilon'_{\perp}$ with respect to AOC plane





See talk by G.Depaola

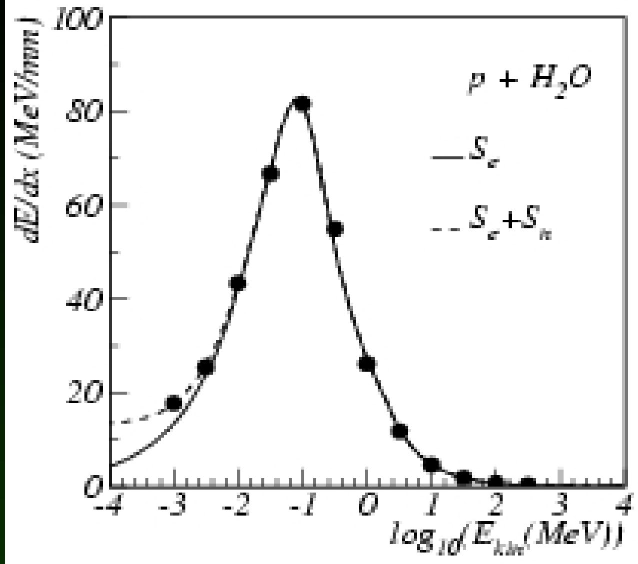
Hadron and ion EM processes

Geant 4

- Variety of models, depending on energy range, particle type and charge
- Positive charged hadrons
  - Bethe-Bloch model of energy loss, E > 2 MeV
  - 5 parameterisation models, E < 2 MeV
    - *based on Ziegler and ICRU reviews*
  - 3 models of energy loss fluctuations
- Positive charged ions
  - Scaling: $S_{ion}(T) = Z_{ion}^2 S_p(T_p), \; T_p = T \frac{m_p}{m_{ion}}$
  - 0.01 < β < 0.05 parameterisations, Bragg peak
    - *based on Ziegler and ICRU reviews*
  - β < 0.01: Free Electron Gas Model
- Models for antiprotons
  - β > 0.5 — Bethe-Bloch formula
  - 0.01 < β < 0.5 — Quantum harmonic oscillator model
  - β < 0.01 — Free electron gas mode

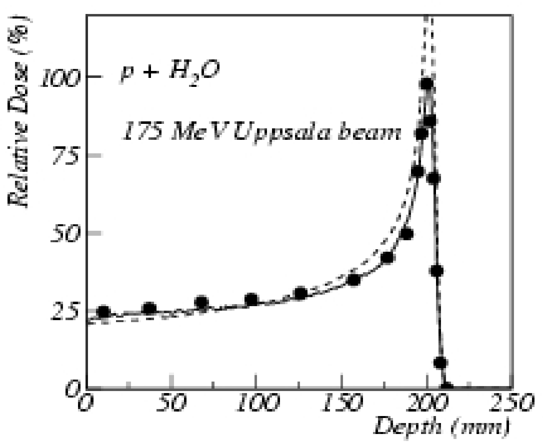
Positive charged hadrons

- Density correction for high energy
- Shell correction term for intermediate energy
- Spin dependent term
- Barkas and Bloch terms
- Chemical effect for compound materials
- Nuclear stopping power
- PIXE included (preliminary)

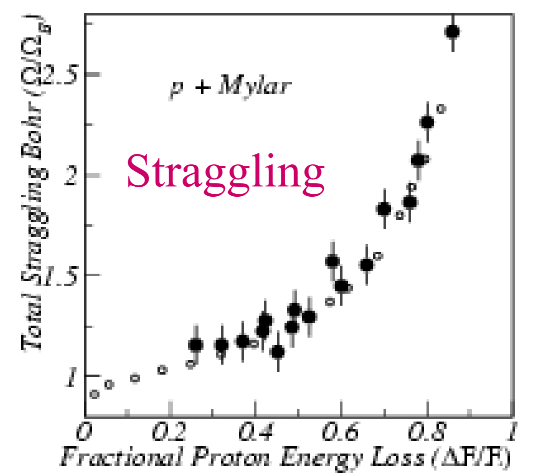


Nuclear stopping power

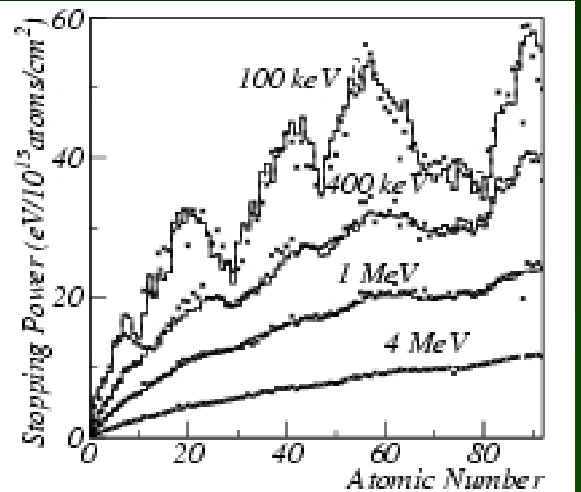
- The precision of the stopping power simulation for protons in the energy from 1 keV to 10 GeV is of the order of a few per cent



Bragg peak *(with hadronic interactions)*



Straggling



Stopping power

Z dependence for various energies

Ziegler and ICRU models

Positive ion and antiproton results

- Positive ions
  - Effective charge model
  - Nuclear stopping power

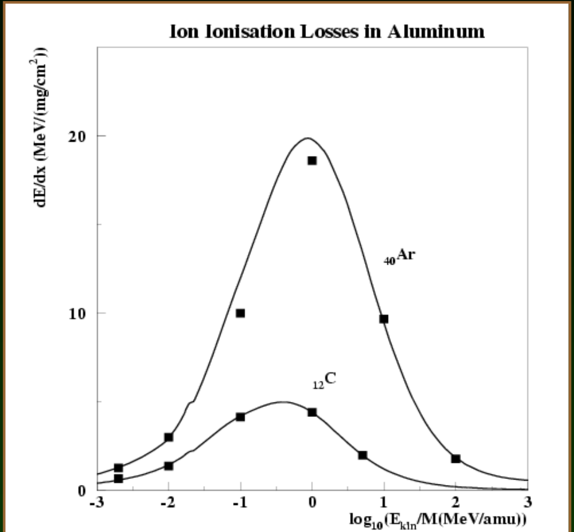
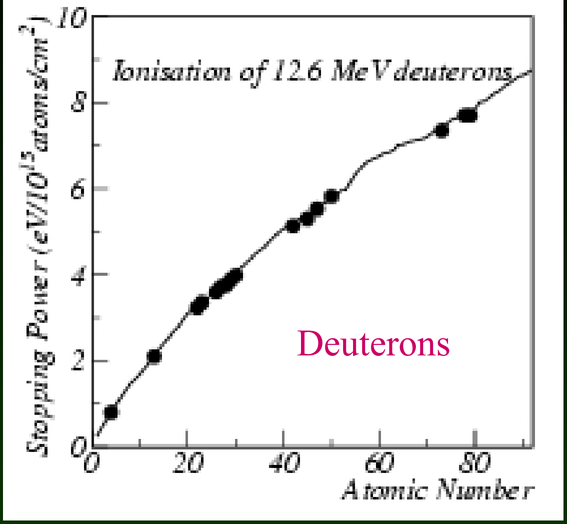
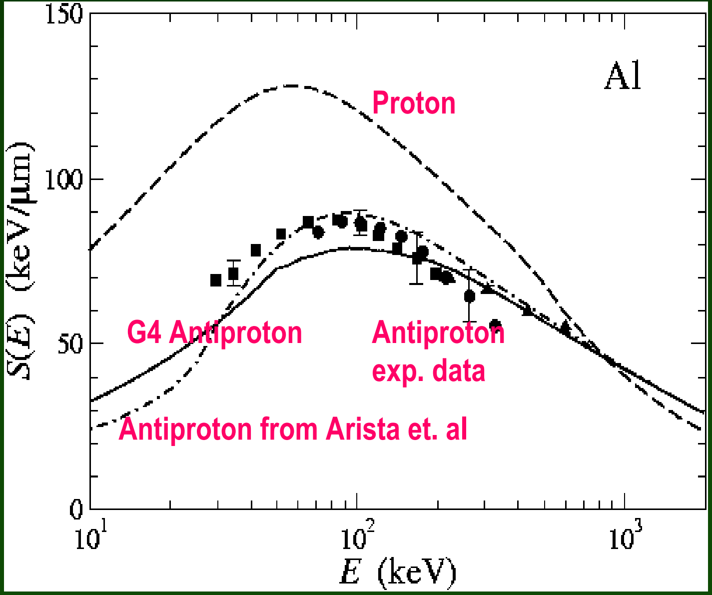
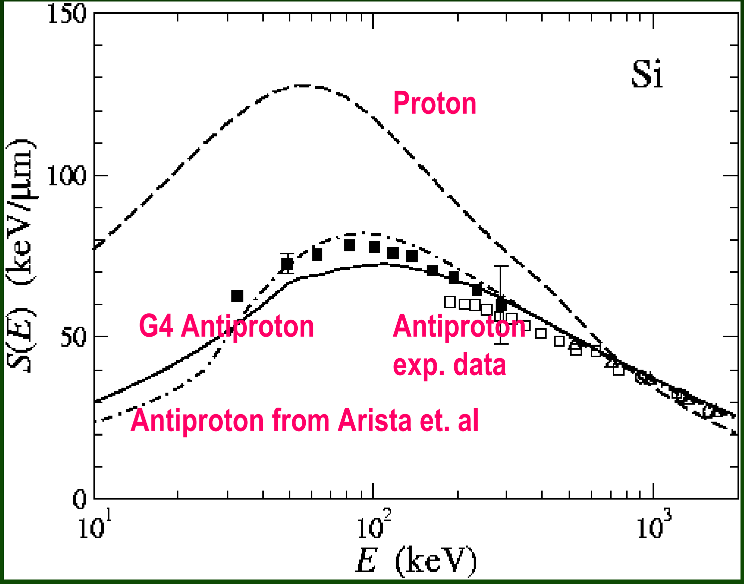


Figure 9: Ion electronic stopping power in aluminum. Points - the best fit on the data from Ref.[12], solid line - GEANT4 parameterisation. The accuracy of the data is about 5 %.



- Antiprotons





How to use the Low Energy EM processes: differences in the Physics list

Geant 4

- Code (here and later) taken from the Geant4 "Underground Physics" advanced example

```
// gamma
#include "G4LowEnergyRayleigh.hh"
#include "G4LowEnergyPhotoElectric.hh"
#include "G4LowEnergyCompton.hh"
#include "G4LowEnergyGammaConversion.hh"

// e-
#include "G4LowEnergyIonisation.hh"
#include "G4LowEnergyBremsstrahlung.hh"

// e+
#include "G4eIonisation.hh"
#include "G4eBremsstrahlung.hh"
#include "G4eplusAnnihilation.hh"


// alpha and GenericIon and deuterons, triton, He3:
#include "G4hLowEnergyIonisation.hh"
```

Geant 4

…Low Energy implementation…

- Process creation

```
G4LowEnergyPhotoElectric*   lowePhot = new G4LowEnergyPhotoElectric();
G4LowEnergyIonisation*      loweIon  = new G4LowEnergyIonisation();
G4LowEnergyBremsstrahlung*  loweBrem = new G4LowEnergyBremsstrahlung();
```

- And special cut for the secondary Fluorescence photons

```
// fluorescence: specific cuts for flourescence
// from photons, electrons and bremsstrahlung photons

G4double fluorcut = 250*eV;
lowePhot->SetCutForLowEnSecPhotons(fluorcut);
loweIon ->SetCutForLowEnSecPhotons(fluorcut);
loweBrem->SetCutForLowEnSecPhotons(fluorcut);
```

…Low Energy implementation…

- Attach the processes…

```
G4String particleName = particle->GetParticleName();

// gamma
if (particleName == "gamma") {
  pmanager->AddDiscreteProcess(new G4LowEnergyRayleigh());
  pmanager->AddDiscreteProcess(lowePhot);
  pmanager->AddDiscreteProcess(new G4LowEnergyCompton());
  pmanager->AddDiscreteProcess(new G4LowEnergyGammaConversion());
}
```

```
// electron
else if (particleName == "e-") {
  pmanager->AddProcess(aMultipleScattering,      -1, 1, 1);
  pmanager->AddProcess(loweIon,                  -1, 2, 2);
  pmanager->AddProcess(loweBrem,                 -1,-1, 3);
}
```

- Special setting for the Low Energy physics

```
//special for low energy physics
  G4double lowlimit=250*eV;
  G4Gamma   ::SetEnergyRange(lowlimit,100*GeV);
  G4Electron::SetEnergyRange(lowlimit,100*GeV);
  G4Positron::SetEnergyRange(lowlimit,100*GeV);
```

- Hadron EM processes

```
// charged hadrons
else if (particleName == "proton"     ||
         particleName == "alpha"      ||
         particleName == "deuteron"   ||
         particleName == "triton"     ||
         particleName == "He3"        ||
         particleName == "GenericIon" ||
         (particleType == "nucleus" && particleCharge != 0)) {
  pmanager->AddProcess(aMultipleScattering, -1, 1, 1);
  pmanager->AddProcess(ahadronLowEIon,      -1, 2, 2);
}
```

Conclusions

- Geant4 electromagnetic physics covers a wide energy range of interactions of photons, electrons and positrons, muons, charged hadrons and ions
  - Often with a variety of complementary and alternative physics models
- Thanks to the modular design and the OO technology:
  - Open to extensions and implementation of new models
- A set of models has been developed to extend the Geant4 coverage of electromagnetic interactions of photons and electrons down to 250 eV, and of hadrons down to < 1 keV
  - Based on the exploitation of evaluated data
- Wide user community in astrophysics, space applications, medical field, HEP, in the U.S., Europe, and elsewhere
- Further electromagnetic physics developments and refinements are underway

To learn more

- Geant4 Physics Reference Manual
- Application Developer Guide

- Useful links
  - http://cern.ch/geant4
  - http://www.ge.infn.it/geant4/lowE/
  - http://www.llnl.gov/cullen1/
  - http://www.icru.org/pubs.htm