

# Geant 4

*IEEE Nuclear Science Symposium and Medical Imaging Conference  
Short Course*

## **Simulation Techniques Using Geant4**

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<http://www.ge.infn.it/geant4/events/nss2008/geant4course.html>

This course exploits training material developed by several Geant4  
Collaboration members: thanks to all of them!

# Electromagnetic Physics

## Overview

# Electromagnetic packages in Geant4

- Standard
  - Low Energy
  - Optical
  - Muons
- 
- Different modeling approach
  - Specialized according to particle type, energy scope

# Electromagnetic physics

- electrons and positrons
- $\gamma$ , X-ray and optical photons
- muons
- charged hadrons
- ions

- **High energy extensions**

- needed for LHC experiments, cosmic ray experiments...

- **Low energy extensions**

- fundamental for space and medical applications, dark matter and  $\nu$  experiments, antimatter spectroscopy etc.

- **Alternative models for the same process**

- Multiple scattering
- energy loss { • Bremsstrahlung
- Ionisation
- Annihilation
- Photoelectric effect
- Compton scattering
- Rayleigh effect
- g conversion
- e+e- pair production
- Synchrotron radiation
- Transition radiation
- Cherenkov
- Refraction
- Reflection
- Absorption
- Scintillation
- Fluorescence
- Auger

*All obeying to the same abstract Process interface: transparent to tracking*

# Standard Electromagnetic Physics

## Overview

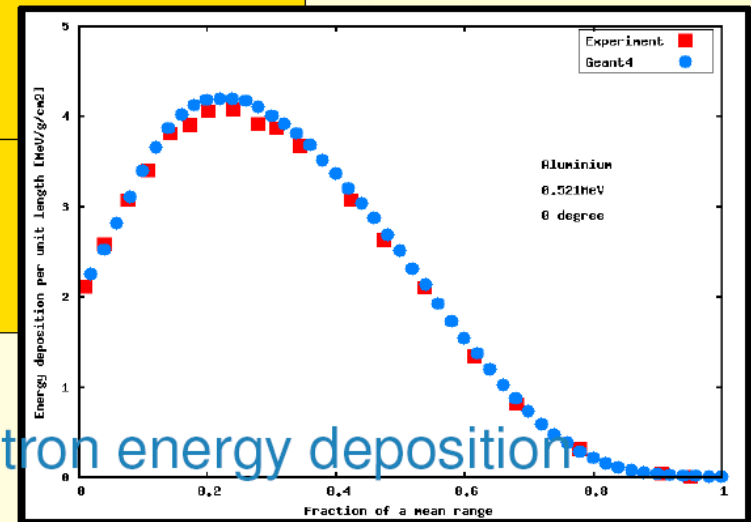
# Packages

Package	Description
Standard	Gamma, Electrons up to 100 TeV, Hadrons, Ions up to 100 TeV
Muons	Muons up to 1PeV, Energy loss propagator
X-rays	X-ray and optical photon production processes
Optical	Optical photon interactions
High-energy	Processes at high energy ( $E > 10$ GeV), Physics for exotic particles
Polarization	Simulation of polarized beams

# Processes: electrons and photons

Particle	Processes
Photons	Gamma conversion into $e^+e^-$ pair Compton scattering Photoelectric effect
Electrons, Positrons	Ionization Coulomb scattering Bremsstrahlung
Positrons	Annihilation

Example: Electron energy deposition

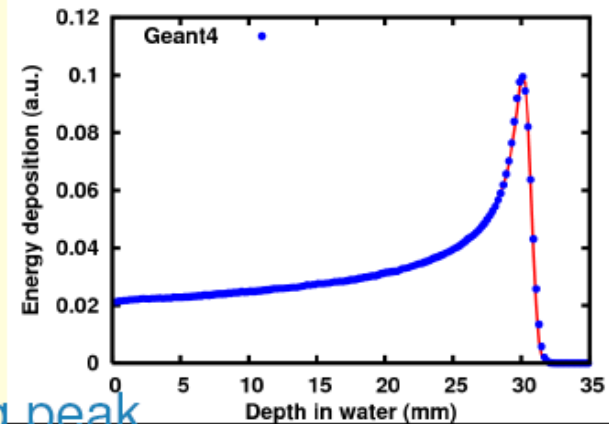


# Processes: hadrons

Particle	Processes
Hadrons, ions	Coulomb Scattering, ionization

$$\frac{dE}{dx} = 2\pi r_e^2 m c^2 n_{el} \frac{z^2}{\beta^2} \left[ \ln \left( \frac{2mc^2 \beta^2 \gamma^2 T_{up}}{I^2} \right) - \beta^2 \left( 1 + \frac{T_{up}}{T_{max}} \right) - \delta - \frac{2C_e}{Z} + F \right]$$

- Ionization:
  - $E > 2$  MeV: Bethe-Bloch formula with corrections
  - $E < 2$  MeV: Parametrization (ICRU 49, NIST)



Ex: Proton Bragg peak

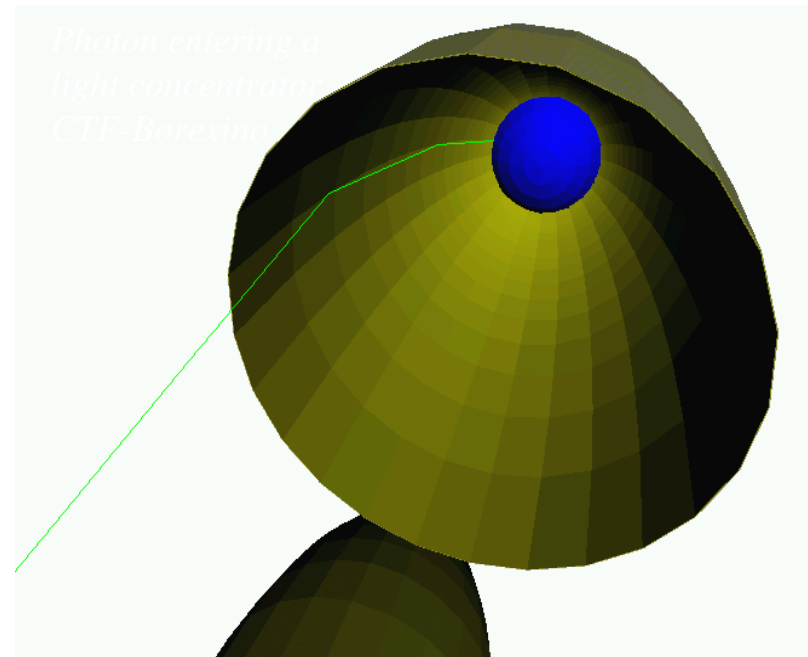


# Optical photons

*Production of optical photons in detectors is mainly due to Cherenkov effect and scintillation*

## Processes in Geant4:

- in-flight absorption
- Rayleigh scattering
- medium-boundary interactions (reflection, refraction)

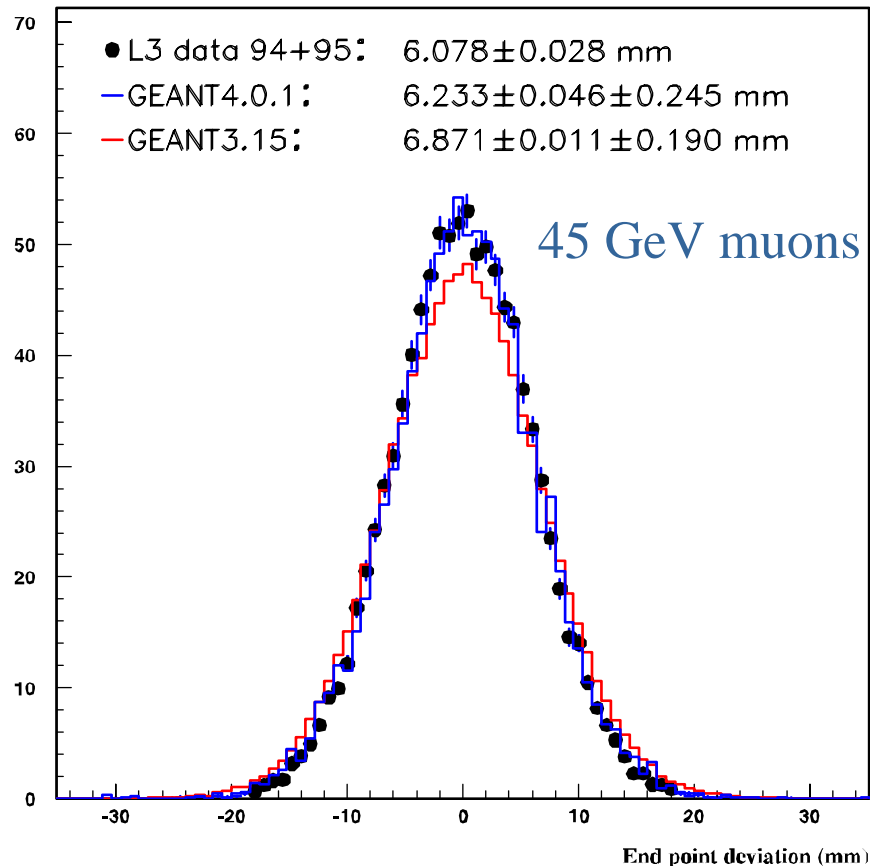


# Muons

1 keV up to 1000 PeV scale

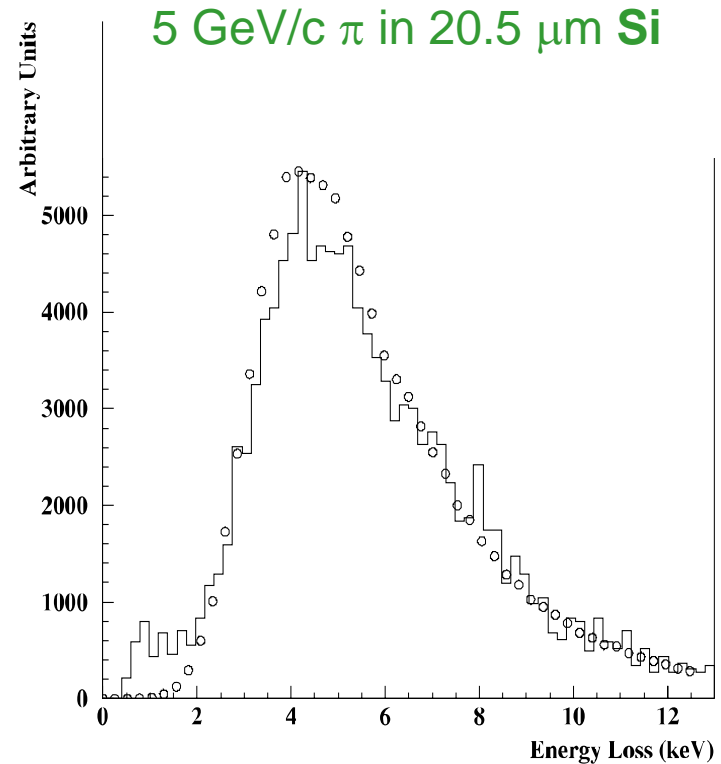
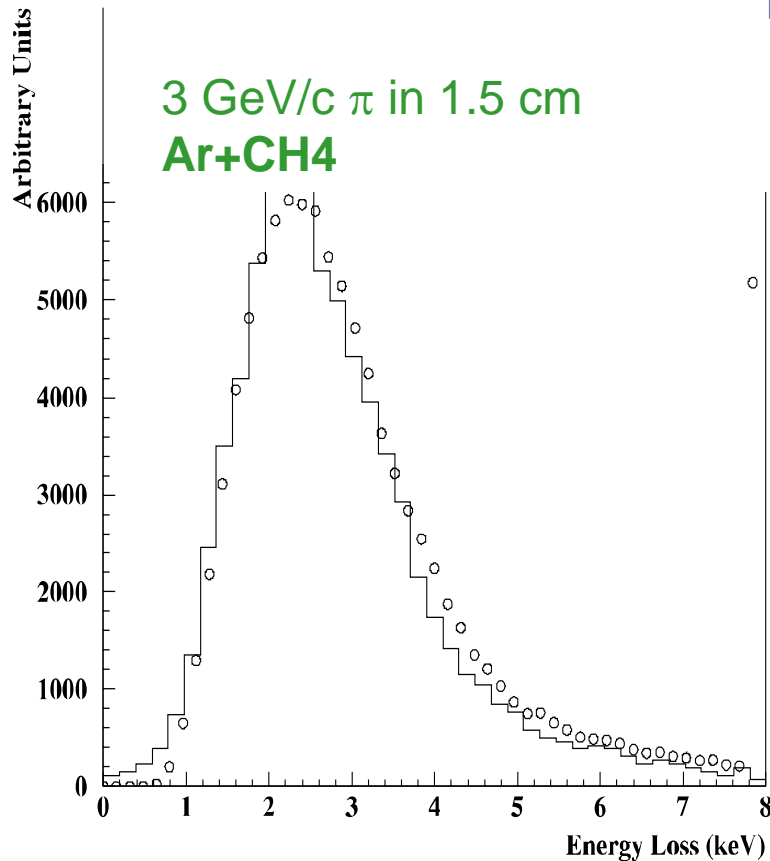
- *simulation of ultra-high energy and cosmic ray physics*
- High energy extensions based on theoretical models

Deviation of 45 GeV muons in L3



# Photo Absorption Ionisation (PAI) Model

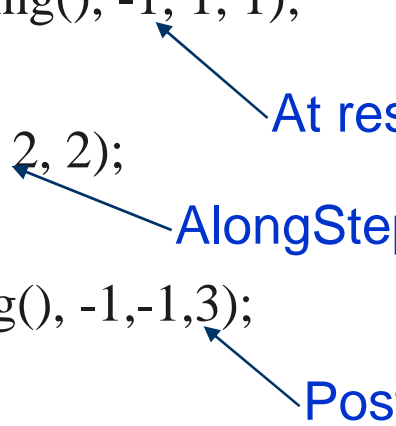
Ionisation energy loss produced by charged particles in thin layers of absorbers



Ionisation energy loss distribution produced by pions, PAI model

# Process ordering

```
void PhysicsEMElectronStandard::ConstructProcess()
{
    G4ParticleDefinition* electron = G4Electron::Definition();
    G4ProcessManager* manager = electron ->GetProcessManager();
    // Adding multiple Coloumb scattering
    manager -> AddProcess(new G4MultipleScattering(), -1, 1, 1);
    // Adding ionisation
    manager ->AddProcess(new G4eIonisation(), -1, 2, 2);
    // Adding Bremsstrahlung
    manager -> AddProcess(new G4eBremsstrahlung(), -1,-1,3);
}
```



-1 means that process is not registered for this action

# Multiple scattering

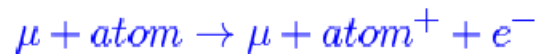
- Geant4 is a **condensed** Monte Carlo code
  - Global effects due to collisions along a macroscopic step are simulated, using approximations
- Is in contrast to detailed simulations at a microscopic level, which are exact, but require an enormous amount of time for higher energies
- **Cumulative effects**
  - Charged particles, that travel through a finite material layer are subject to a large number of Coloumb interactions, where the particles are elastically scattered
  - Summing up individual effects gives a net deflection of the particles from their initial direction
- For sufficient collisions (>20) multiple scattering angular distribution is
  - a **Gaussian** distribution for small angles
  - like **Rutherford scattering** at large angles

# Multiple scattering

- The Geant4 Multiple Scattering (MSC) model by L. Urban is applicable to all charged particles
- It is based on the Lewis theory
- Relies on transport equation of charged particles
- Uses phenomenological functions to sample angular and spatial distributions after the simulation step
  - The function parameters are chosen, in order that the moments of the distribution are the same as given by the Lewis theory
- See the *Physics Reference Manual* for details

# Ionisation

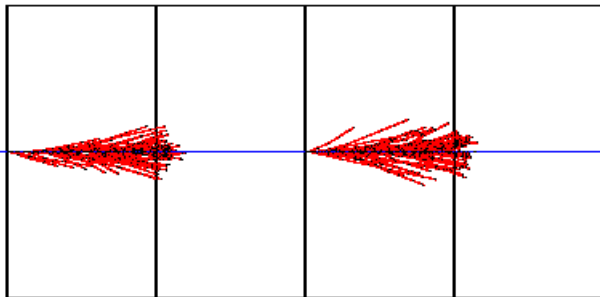
The basic mechanism is an inelastic collision of the moving charged particle with the atomic electrons of the material, ejecting off an electron from the atom :



Mean energy loss and energetic  $\delta$ -rays

$$\frac{d\sigma(Z, E, T)}{dT}$$

is the differential cross-section per atom for the ejection of an electron with kinetic energy  $T$  by an incident charged particle of total energy  $E$  moving in a material of density  $\rho$ .



One may wish to take into account separately the high-energy knock-on electrons produced above a given threshold  $T_{cut}$  (miss detection, explicit simulation ...).

$T_{cut} \gg I$  (mean excitation energy in the material).

$T_{cut} > 1$  keV in GEANT4

**Below** this threshold, the soft knock-on electrons are counted only as continuous energy lost by the incident particle.

**Above** it, they are explicitly generated. Those electrons must be **excluded** from the mean continuous energy loss count.

# High energy knock-on electrons

- Above a given threshold  $T_{\text{cut}}$  high energy knock-on electrons are explicitly taken into account
  - i.e.  $\delta$ -rays are explicitly generated (particles excluded from continuous energy loss)
- Below  $T_{\text{cut}}$  the soft electrons are only considered as continuous energy loss of the incident particle



# Energy loss fluctuations

- Urban model of fluctuations,
  - based on a simple modelling approach of particle-atom interactions:
- Atoms are assumed to have only two energy levels: E1 and E2
- The particle-atom interaction can be:
  - excitation of the atom with energy loss  $E = E1 - E2$
  - 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 electrons and photons
  - Slow model, should only be applied for sensitive region

# Low Energy Electromagnetic Physics

## Overview

# What is

- 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*)/100 eV for electrons and photons
  - down to the approximately the ionisation 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

# Overview of physics

- Compton scattering
- Rayleigh scattering
- Photoelectric effect
- Pair production
  
- Bremsstrahlung
- Ionisation
  
- Polarised Compton
  
- + atomic relaxation
  - fluorescence
  - Auger effect

*following processes leaving a vacancy in an atom*

in two “flavours” of models:

- based on the **Livermore Library**
- à la **Penelope**

+ models for hadrons/ions

# LowE processes based on Livermore Library

# Photons and electrons

different approach w.r.t.  
Geant4 standard e.m.  
package

- Based on evaluated data libraries from LLNL:
  - EADL (*Evaluated Atomic Data Library*)
  - EEDL (*Evaluated Electrons Data Library*)
  - EPDL97 (*Evaluated Photons Data Library*)especially formatted for Geant4 distribution (*courtesy of D. Cullen, LLNL*)
- Validity range: 250 eV - 100 GeV
  - The processes can be used down to 100 eV, with degraded accuracy
  - In principle the validity range of the data libraries extends down to ~10 eV
- Elements  $Z=1$  to  $Z=100$ 
  - Atomic relaxation:  $Z > 5$  (*transition data available in EADL*)

# Calculation of cross sections

Interpolation from the data libraries:

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

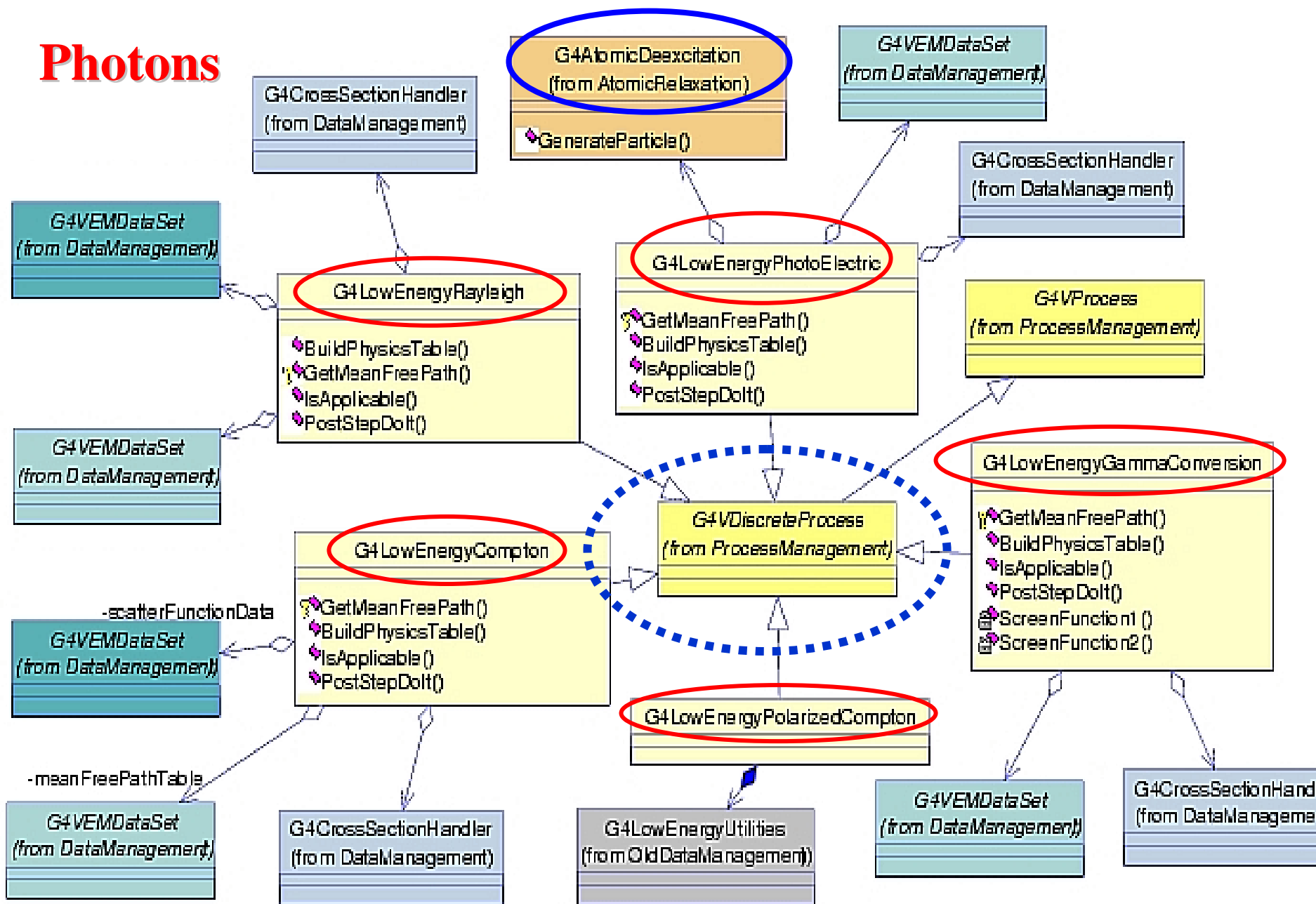
*E<sub>1</sub> and E<sub>2</sub> are the lower and higher energy for which data ( $\sigma_1$  and  $\sigma_2$ ) are available*

Mean free path for a process, at energy E:

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

*n<sub>i</sub> = atomic density of the i<sup>th</sup> element contributing to the material composition*

# Photons





# Compton scattering

Klein-Nishina  
cross section:

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

- Energy distribution of the scattered photon according to the *Klein-Nishina formula*, multiplied by **scattering function**  $F(q)$  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

# 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
- This process is only available in the *lowenergy* package
  - Not available in the *standard* package

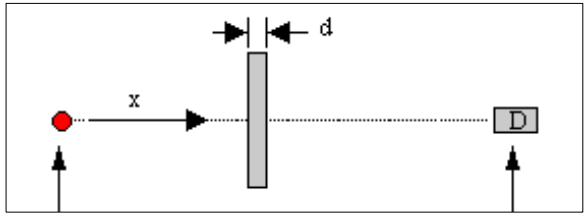
# Photoelectric effect

- 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
  - Various angular distribution generators (“naïve”, Sauter-Gavrila, Gavrila)
- Deexcitation via the atomic relaxation sub-process
  - Initial vacancy + following chain of vacancies created
- *Improved angular distribution in preparation*

# $\gamma$ conversion

- The secondary  $e^-$  and  $e^+$  energies are sampled using Bethe-Heitler cross sections with Coulomb correction
- $e^-$  and  $e^+$  assumed to have symmetric angular distribution
- Energy and polar angle sampled w.r.t. the incoming photon using Tsai differential cross section
- Azimuthal angle generated isotropically
- Choice of which particle in the pair is  $e^-$  or  $e^+$  is made randomly

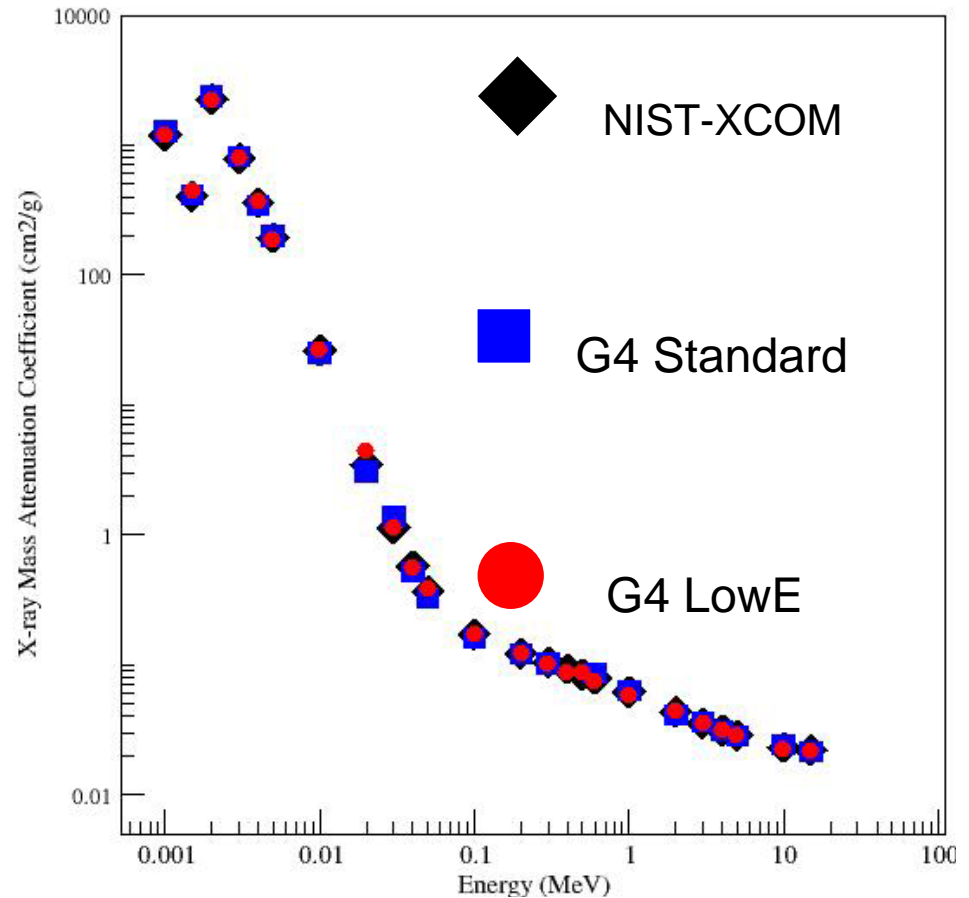
# Photons: mass attenuation coefficient



$$\chi^2_{N-L} = 13.1 - \nu = 20 - p = 0.87$$

$$\chi^2_{N-S} = 23.2 - \nu = 15 - p = 0.08$$

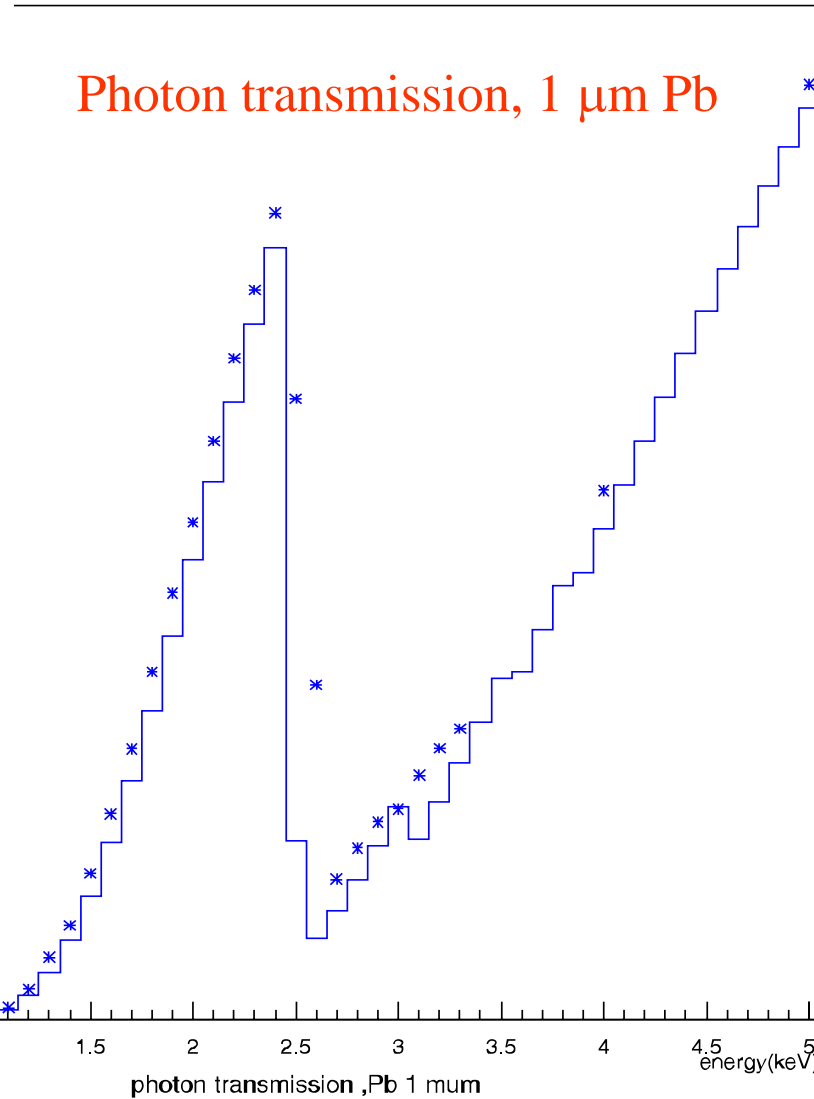
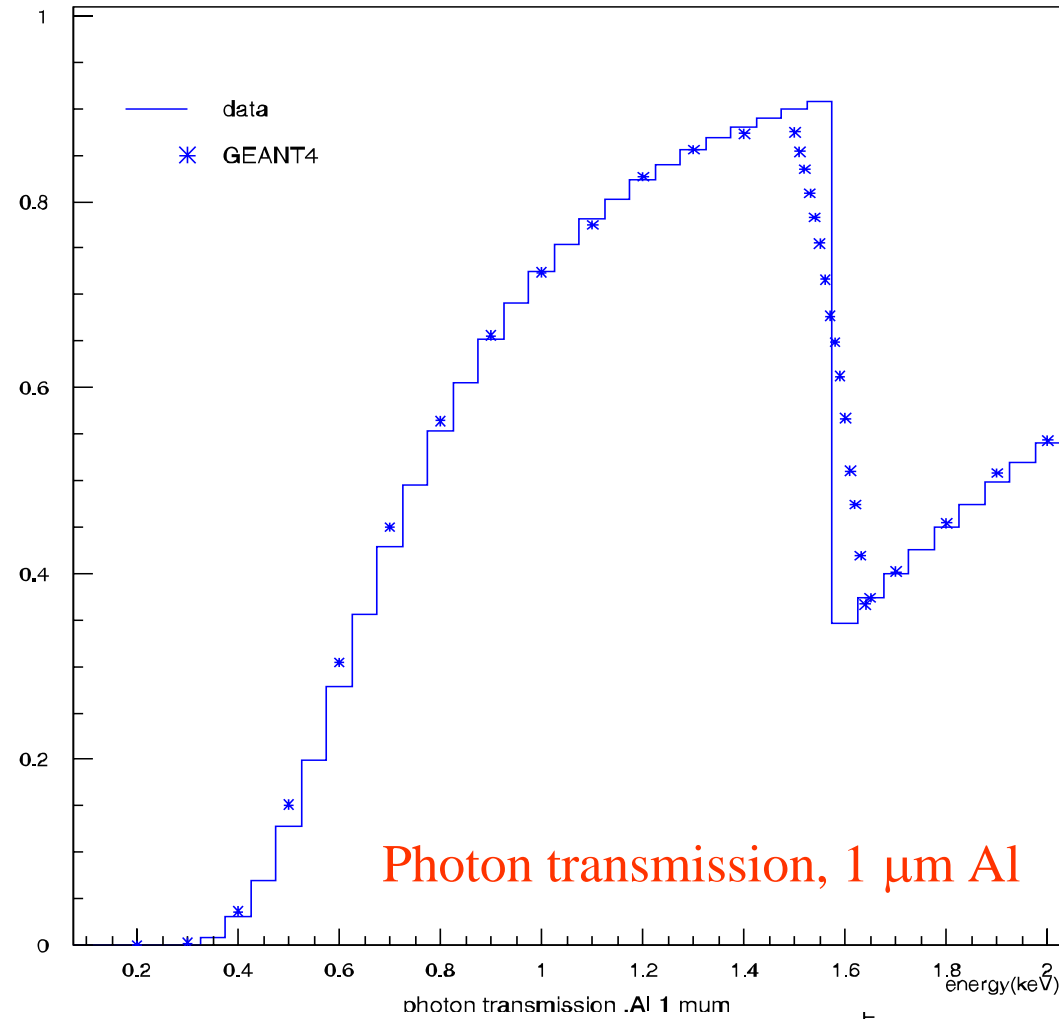
Comparison against NIST data



# Photons, evidence of shell effects

photon transmission , Al 1 micrometer

photon transmission , Pb 1 micrometer



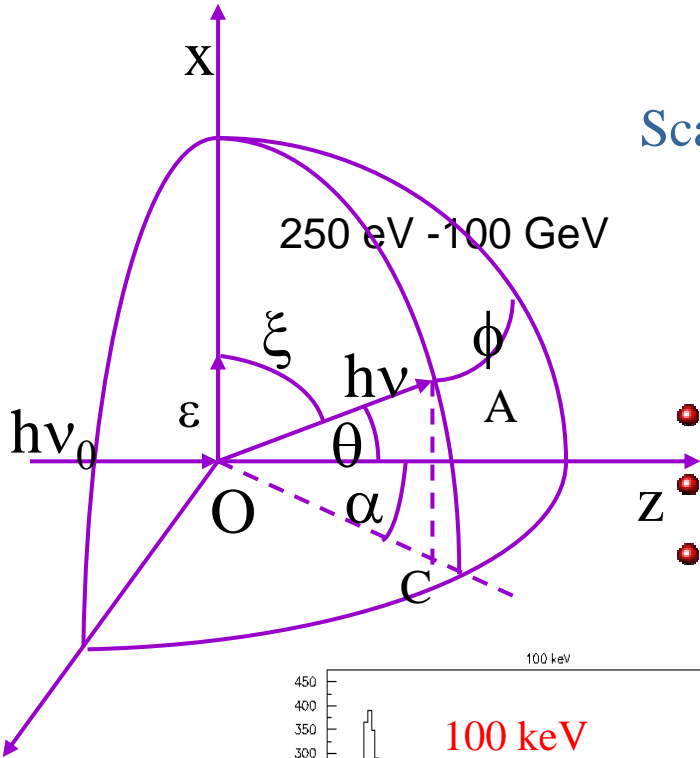
# Polarisation

Cross section: 
$$\frac{d\sigma}{d\Omega} = \frac{1}{2} r_0^2 \frac{h\nu^2}{h\nu_0^2} \left[ \frac{h\nu_0}{h\nu} + \frac{h\nu}{h\nu_0} - 2 \sin^2 \theta \cos^2 \phi \right]$$

$$\cos \xi = \sin \theta \cos \phi \Rightarrow \sin \xi = \sqrt{1 - \sin^2 \theta \cos^2 \phi} = N$$

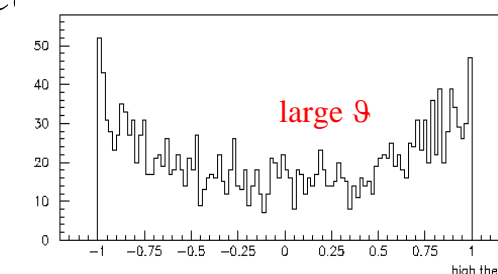
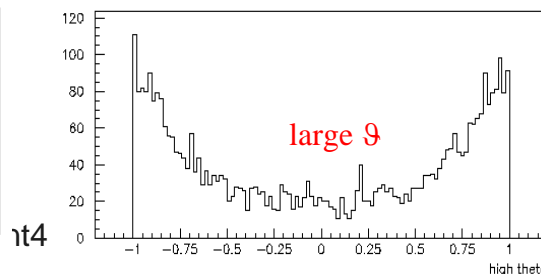
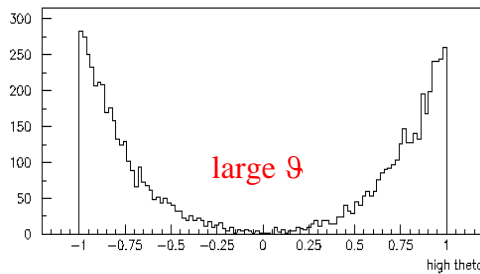
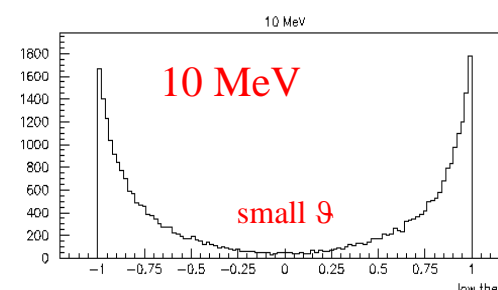
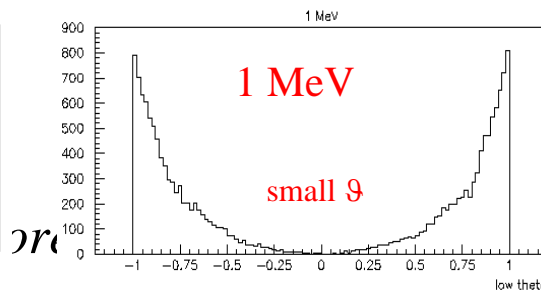
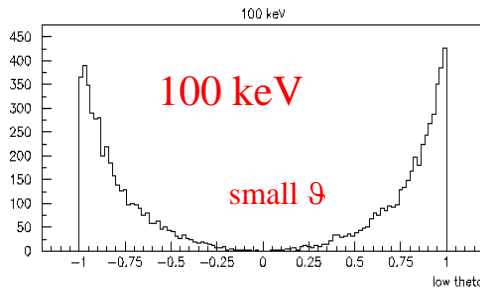
Scattered Photon Polarization 
$$\bar{\epsilon}_\perp = \frac{1}{N} (\cos \theta \hat{j} - \sin \theta \sin \phi \hat{k}) \sin \beta$$

$$\bar{\epsilon}_\parallel = \left( N \hat{i} - \frac{1}{N} \sin^2 \theta \sin \phi \cos \phi \hat{j} - \frac{1}{N} \sin \theta \cos \theta \cos \phi \hat{k} \right) \cos \beta$$



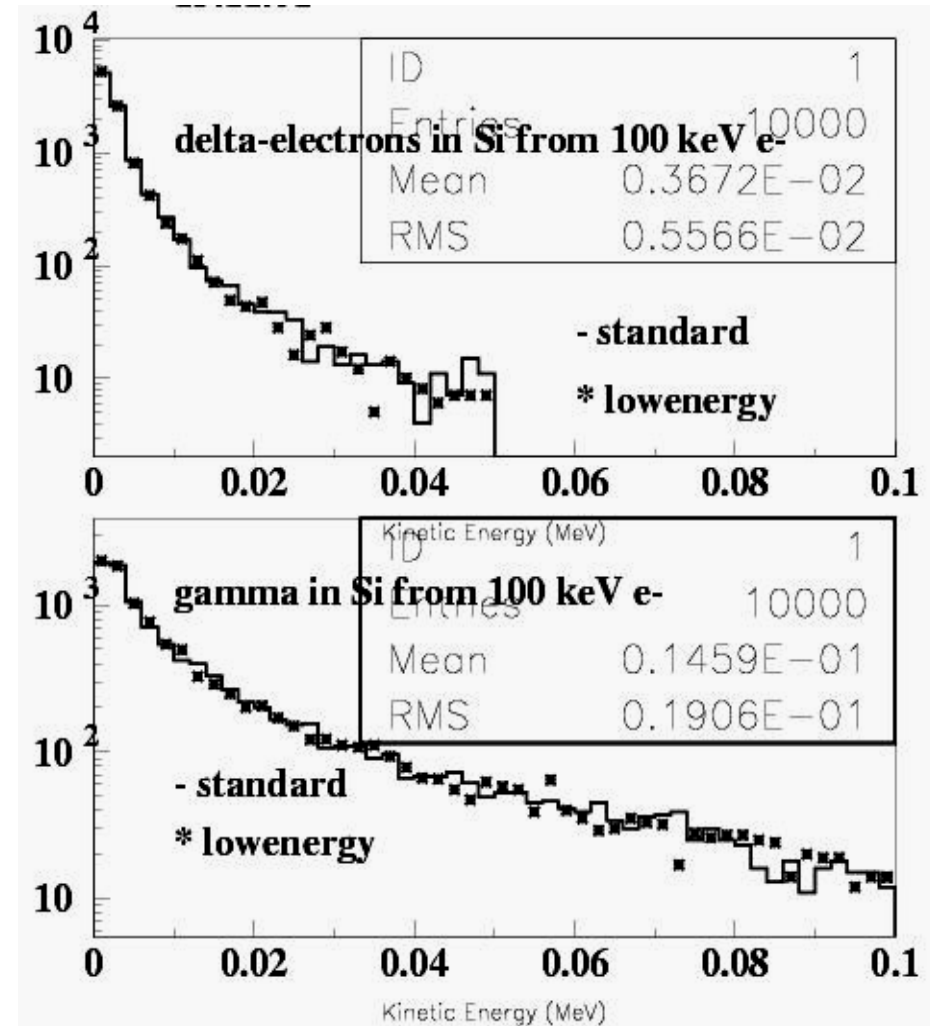
- $\theta$  Polar angle
- $\phi$  Azimuthal angle
- $\epsilon$  Polarization vector

Low Energy  
Polarised Compton



# Electron Bremsstrahlung

- Parameterisation of EEDL data
  - 16 parameters for each atom
  - At high energy the parameterisation reproduces the Bethe-Heitler formula
  - Precision is  $\sim 1.5\%$



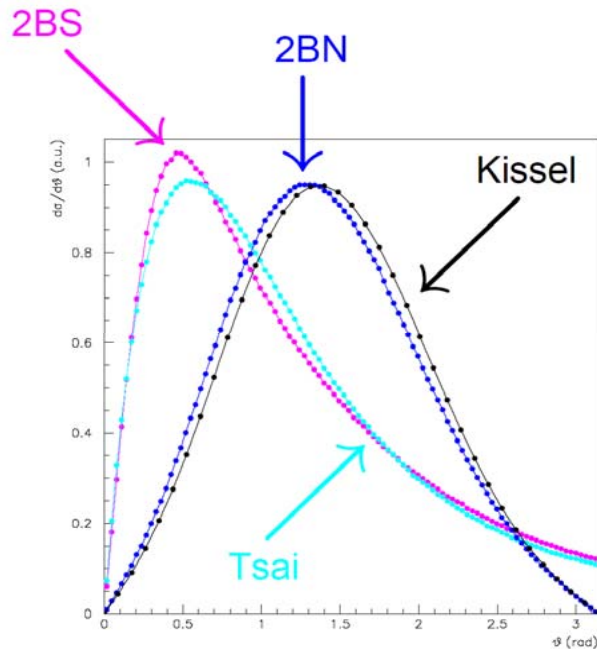


# Bremsstrahlung Angular Distributions

Three LowE generators available in GEANT4 6.0 release:

G4ModifiedTsai, G4Generator2BS and G4Generator2BN

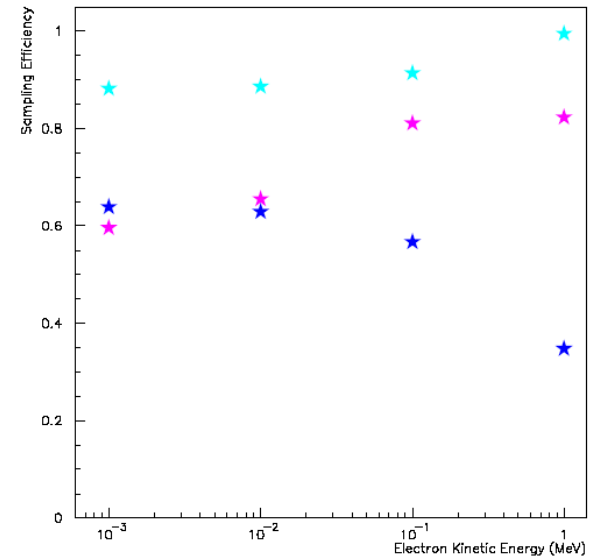
G4Generator2BN allows a correct treatment at low energies (< 500 keV)



T=10 keV (k/T=0.5)

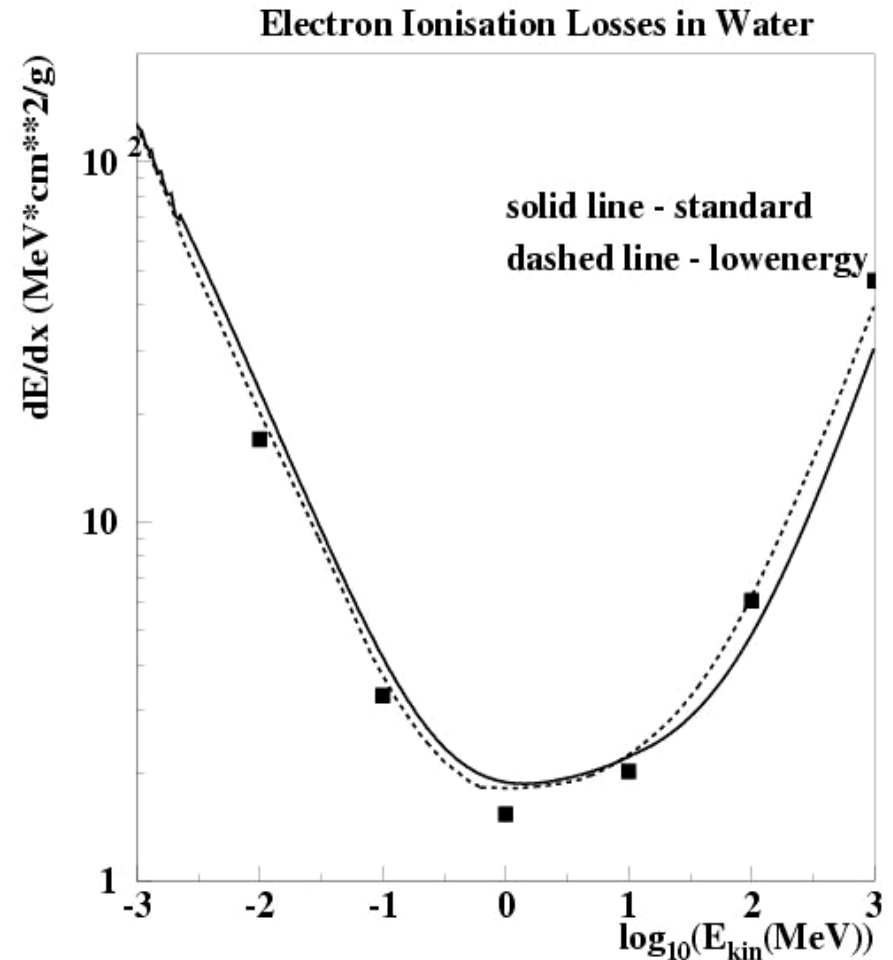
- ★ Tsai
- ★ 2BS (k/T=0.3)
- ★ 2BN (k/T=0.3)

Tungsten (W) - Z=74



# Electron ionisation

- Parameterisation based on 5 parameters for each shell
- Precision of parametrisation is better than 5% for 50 % of shells, less accurate for the remaining shells



# Electrons: range

Range in various simple and composite materials

Compared to NIST database

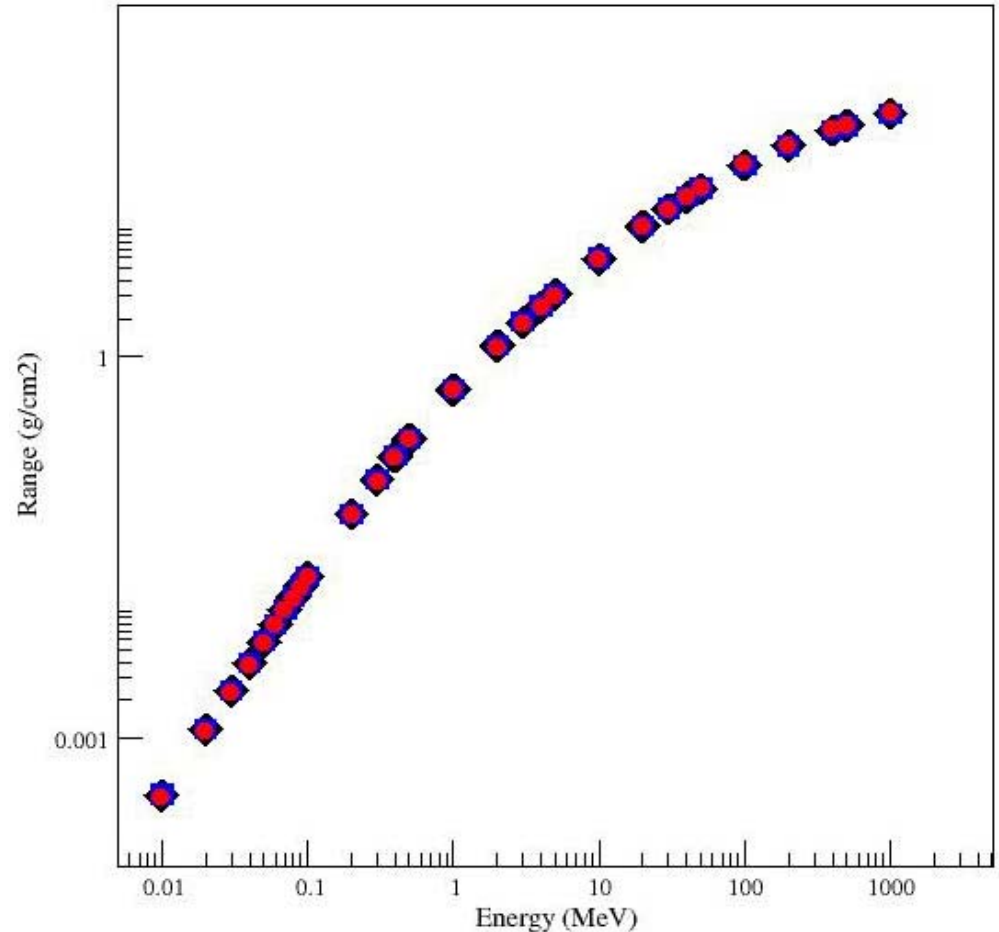
◆ NIST-ESTAR

■ G4 Standard

● G4 LowE

Electrons - CSDA Range - Aluminium

(Geant4-05-02)

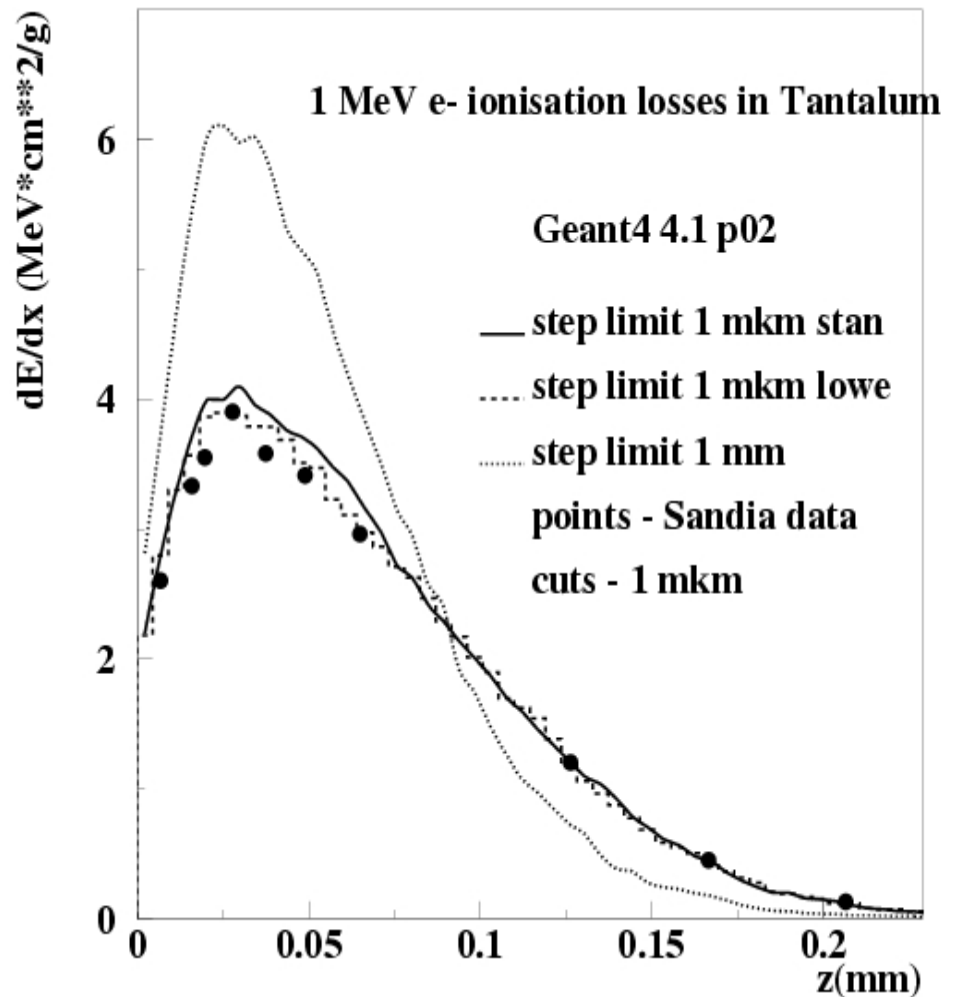


# Electrons: dE/dx

Ionisation energy loss in various materials

Compared to Sandia database

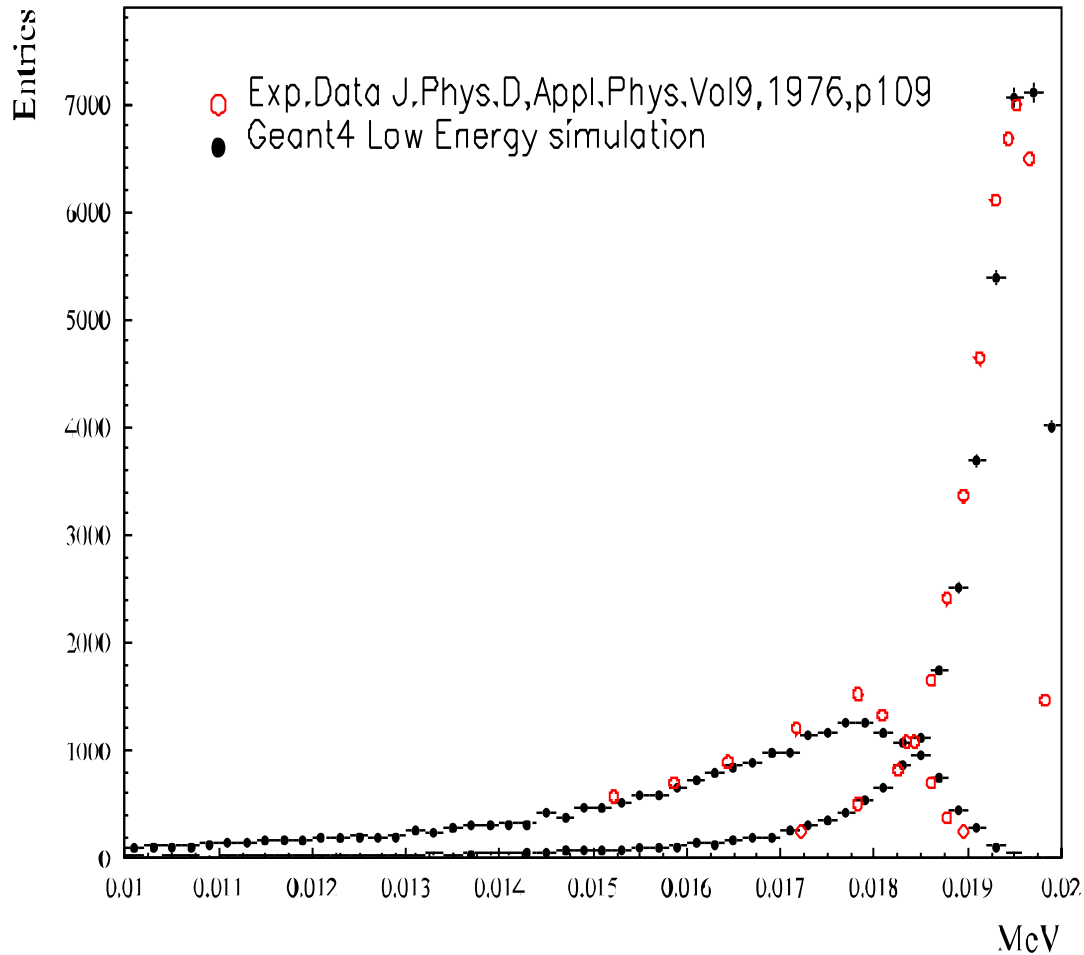
More systematic verification planned



Also Fe, Ur

# Electrons, transmitted

20 keV electrons, 0.32 and 1.04  $\mu\text{m}$  Al



# Geant4 validation vs. NIST database

- All Geant4 physics models of electrons, photons, protons and  $\alpha$  compared to NIST database
  - Photoelectric, Compton, Rayleigh, Pair Production cross-sections
  - Photon attenuation coefficients
  - Electron, proton,  $\alpha$  stopping power and range
- Quantitative comparison
  - Statistical goodness-of-fit tests
- Other validation projects in progress

# NIST Test

- Photon Mass Attenuation Coefficient
- Photon Partial Interaction Coefficient
  - related to the cross section of a specific photon interaction process
- Electron CSDA range and Stopping Power
- Proton CSDA range and Stopping Power
- $\alpha$  CSDA range and Stopping Power

## Elements

Be, Al, Si, Fe, Ge, Ag, Cs, Au, Pb, U  
(span the periodic element table)

## Energy range

photon	1 keV – 100 GeV
electron	10 keV – 1 GeV
proton	1 keV – 10 GeV
$\alpha$	1 keV – 1 GeV

Simulation configuration reproducing NIST conditions  
(ionisation potential, fluctuations, production of secondaries etc.)

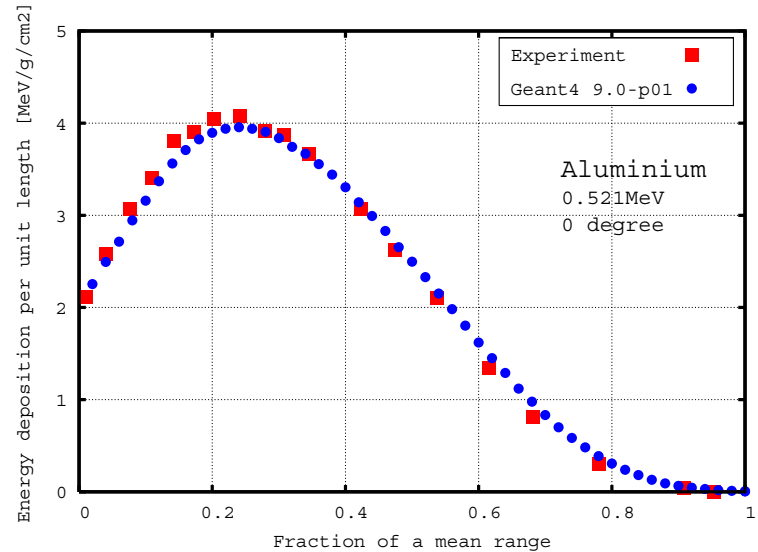
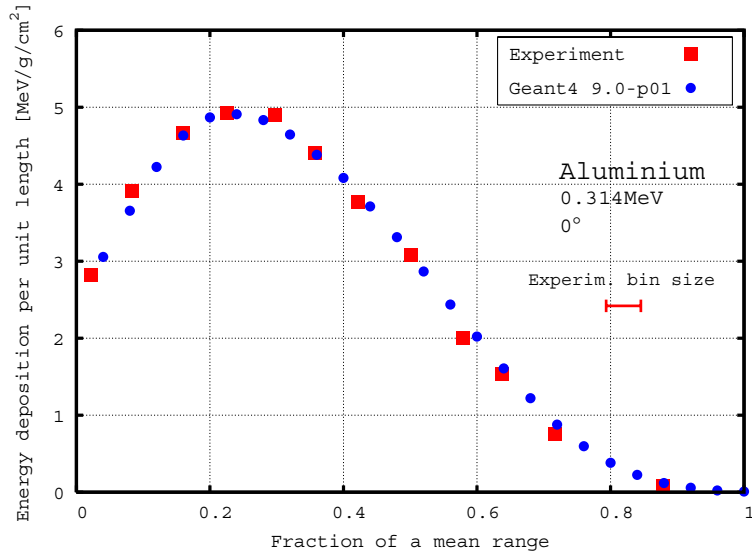
## Geant4 models: electrons and photons

Standard  
Low Energy EEDL/EPDL  
Low Energy Penelope

## Geant4 models: protons and $\alpha$

Standard  
Low Energy ICRU49  
Low Energy Ziegler 1977  
Low Energy Ziegler 1985  
Low Energy Ziegler 2000  
(Low Energy: free electron gas +  
parameterisations + Bethe-Bloch)

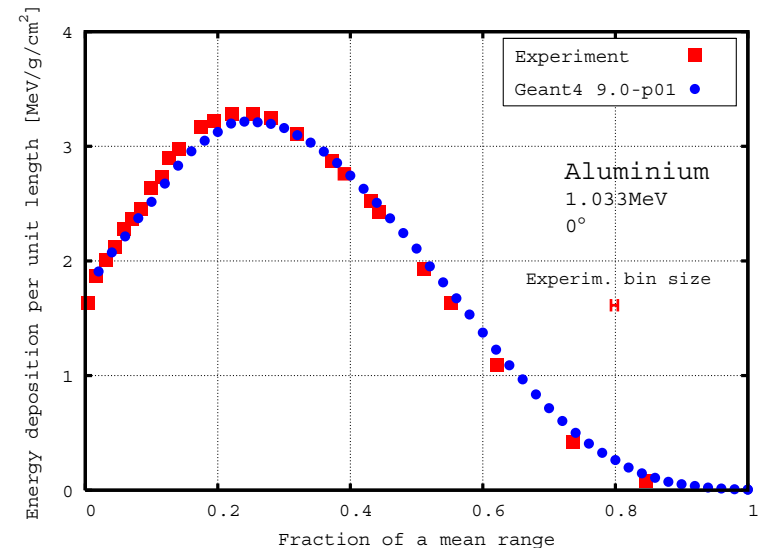
# Dosimetry with Geant4 LowE EM package



## Energy deposit in calorimeter

### Experimental data

G.J. Lockwood et al.,  
 “Calorimetric Measurement of Electron  
 Energy Deposition in Extended  
 Media - Theory vs. Experiment”,  
 SAND79-0414 UC-34a, 1987.



A. Lechner, M.G. Pia, M. Sudhakar

IEEE NSS 2007 Conf. Rec. IEEE NPSS Best Student Paper Award



# Effect of secondary production threshold

Geant4 Low Energy  
Electromagnetic

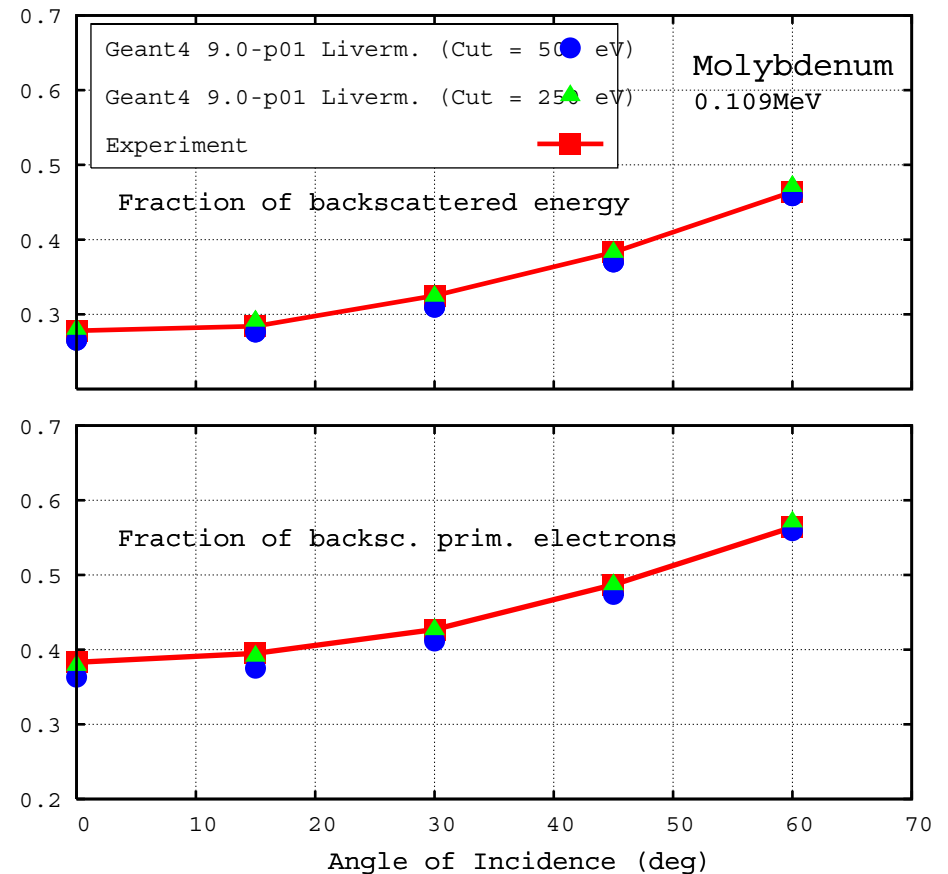
250 eV

EGS

Geant4 Standard  
Electromagnetic

MCNP

1 keV



**Example 5.2. Registration of electromagnetic low energy electron/photon processes.**

```
void LowEnPhysicsList::ConstructEM()
{
    theParticleIterator->reset();

    while( (*theParticleIterator)() ){

        G4ParticleDefinition* particle = theParticleIterator->value();
        G4ProcessManager* pmanager = particle->GetProcessManager();
        G4String particleName = particle->GetParticleName();

        if (particleName == "gamma") {

            theLEPhotoElectric      = new G4LowEnergyPhotoElectric();
            theLECompton             = new G4LowEnergyCompton();
            theLEGammaConversion    = new G4LowEnergyGammaConversion();
            theLERayleigh           = new G4LowEnergyRayleigh();

            pmanager->AddDiscreteProcess(theLEPhotoElectric);
            pmanager->AddDiscreteProcess(theLECompton);
            pmanager->AddDiscreteProcess(theLERayleigh);
            pmanager->AddDiscreteProcess(theLEGammaConversion);

        }
        else if (particleName == "e-") {

            theLEIonisation = new G4LowEnergyIonisation();
            theLEBremsstrahlung = new G4LowEnergyBremsstrahlung();
            theeminusMultipleScattering = new G4MultipleScattering();

            pmanager->AddProcess(theeminusMultipleScattering,-1,1,1);
            pmanager->AddProcess(theLEIonisation,-1,2,2);
            pmanager->AddProcess(theLEBremsstrahlung,-1,-1,3);

        }
    }
}
```

# Processes à la Penelope

- The whole physics content of the Penelope Monte Carlo code has been re-engineered into Geant4 (*except for multiple scattering*)
  - processes for photons: release 5.2, for electrons: release 6.0
- Physics models by F. Salvat et al.
- Power of the OO technology:
  - extending the software system is easy
  - all processes obey to the same abstract interfaces
  - using new implementations in application code is simple
- Profit of Geant4 advanced geometry modeling, interactive facilities *etc.*
  - same physics as original Penelope

# Hadrons and ions

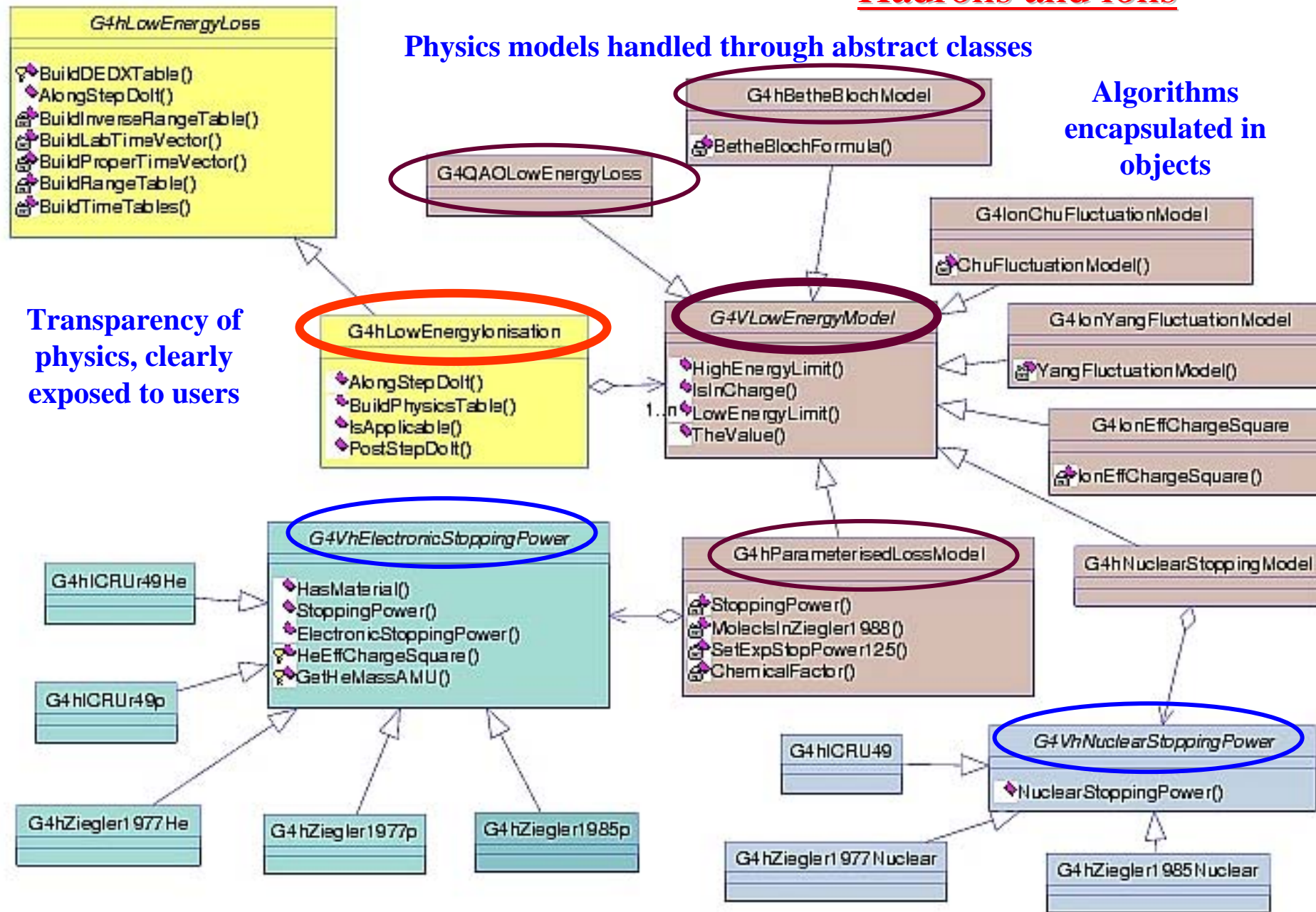
- Variety of models, depending on
  - energy range
  - particle type
  - charge
- Composition of models across the energy range, with different approaches
  - analytical
  - based on data reviews + parameterisations
- Specialised models for fluctuations
- Open to extension and evolution

# Hadrons and ions

Physics models handled through abstract classes

Algorithms encapsulated in objects

Transparency of physics, clearly exposed to users

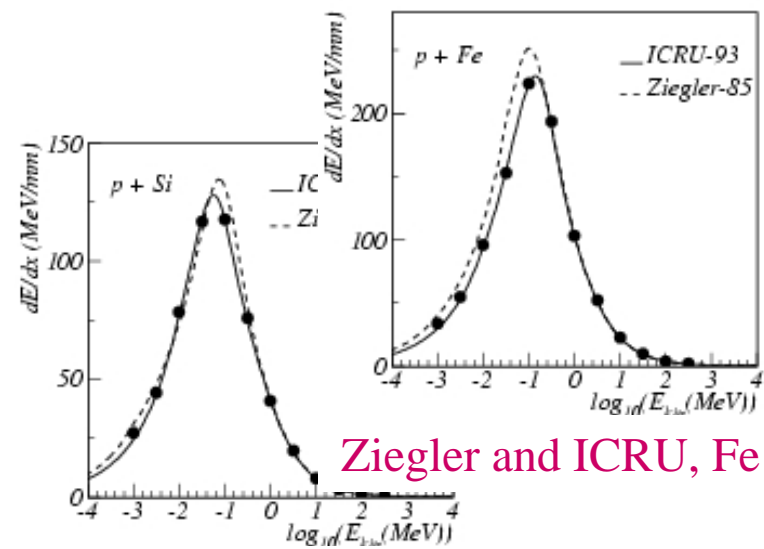


Interchangeable and transparent access to data sets

# 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

- Density correction for high energy
- Shell correction term for intermediate energy

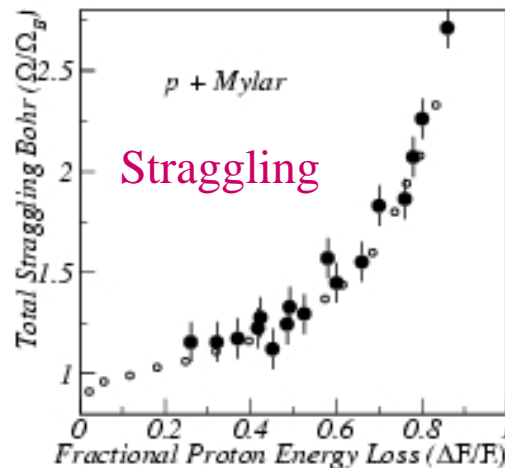


Ziegler and ICRU, Fe

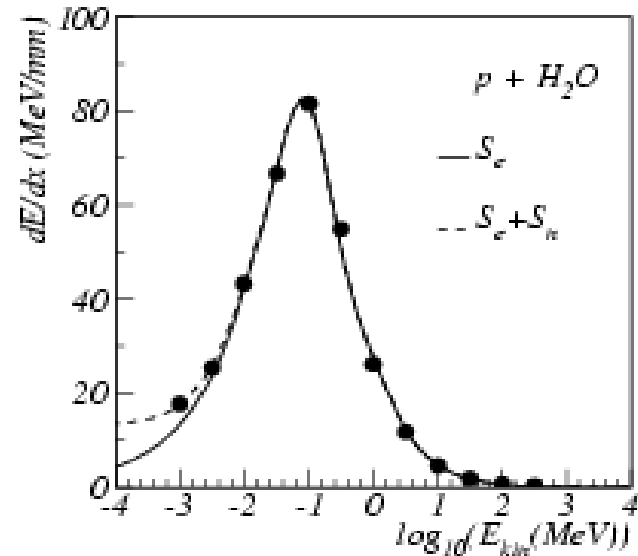
Ziegler and ICRU, Si

- Spin dependent term
- Barkas and Bloch terms

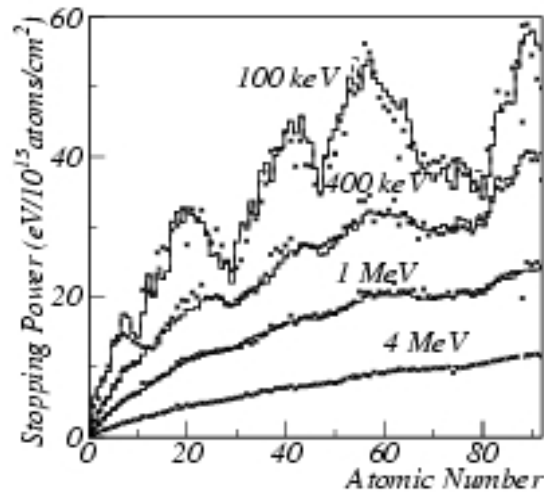
- Chemical effect for compounds
- Nuclear stopping power
- PIXE included



Straggling



Nuclear stopping power

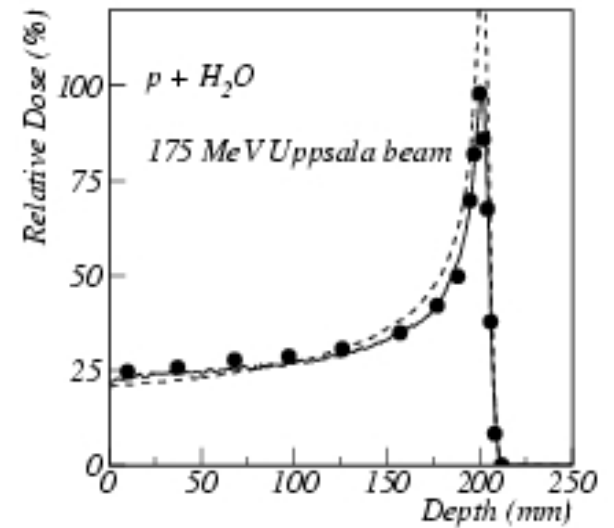
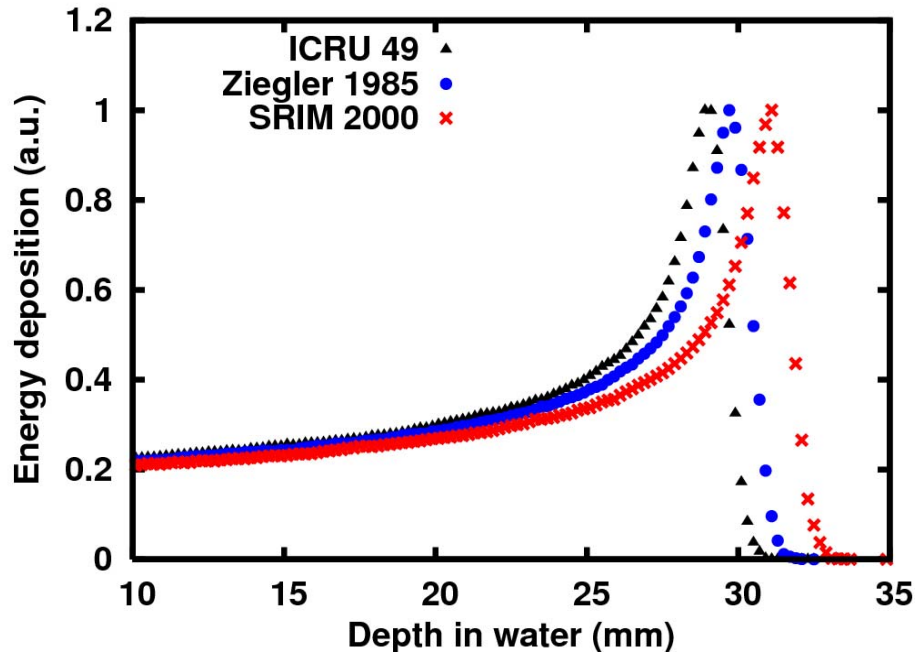


Stopping power

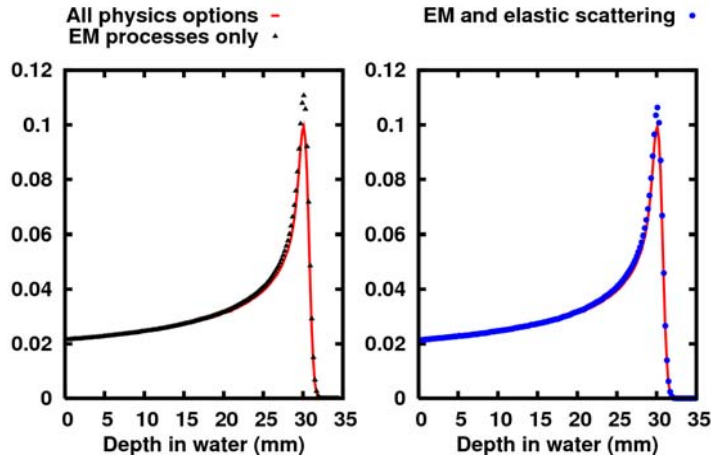
Z dependence for various energies

Ziegler and ICRU models

Further activity in progress



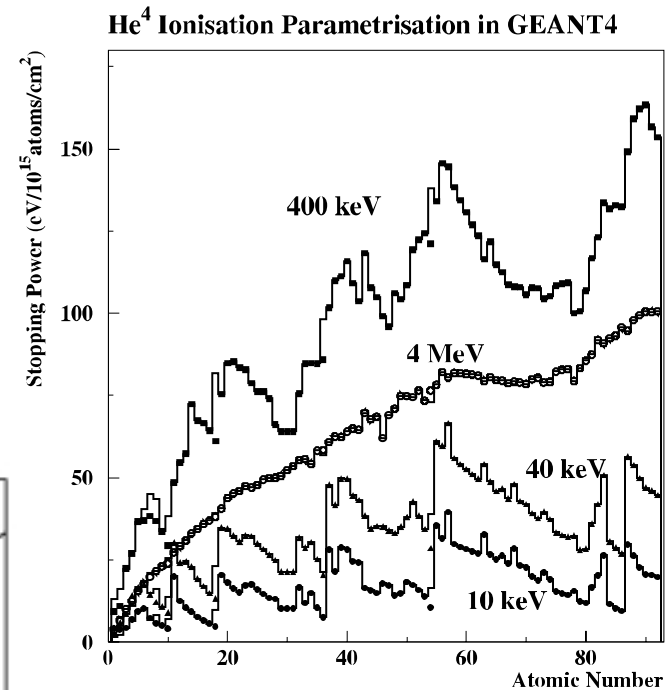
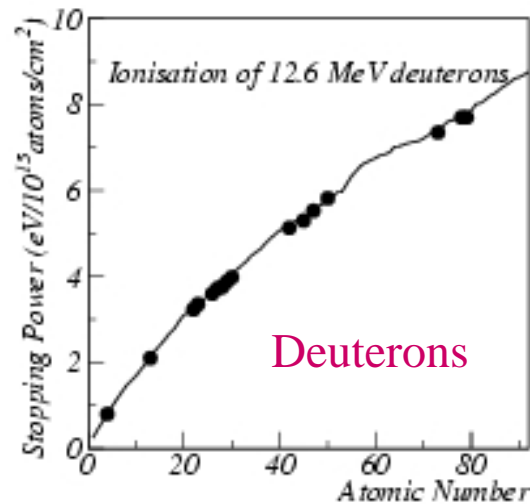
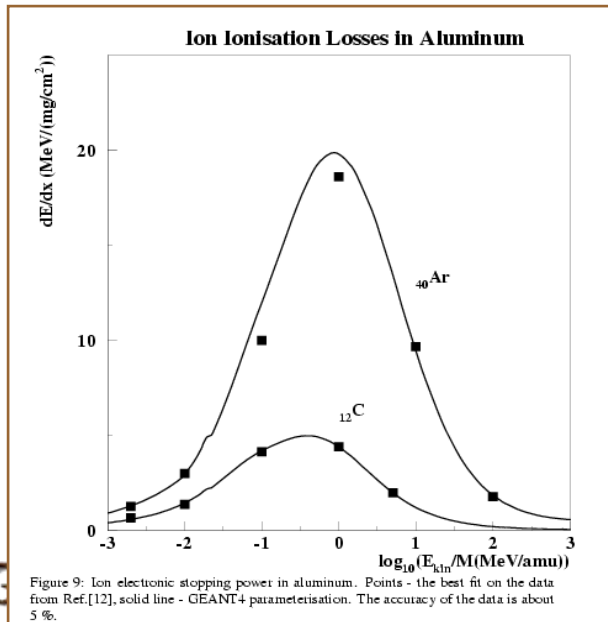
Bragg peak  
(with hadronic interactions)



# Positive charged ions

- Scaling:  $S_{ion}(T) = Z_{ion}^2 S_p(T_p), T_p = T \frac{m_p}{m_{ion}}$
- $0.01 < \beta < 0.05$  parameterisations, Bragg peak  
- based on Ziegler and ICRU reviews
- $\beta < 0.01$ : Free Electron Gas Model

- Effective charge model  
- Nuclear stopping power





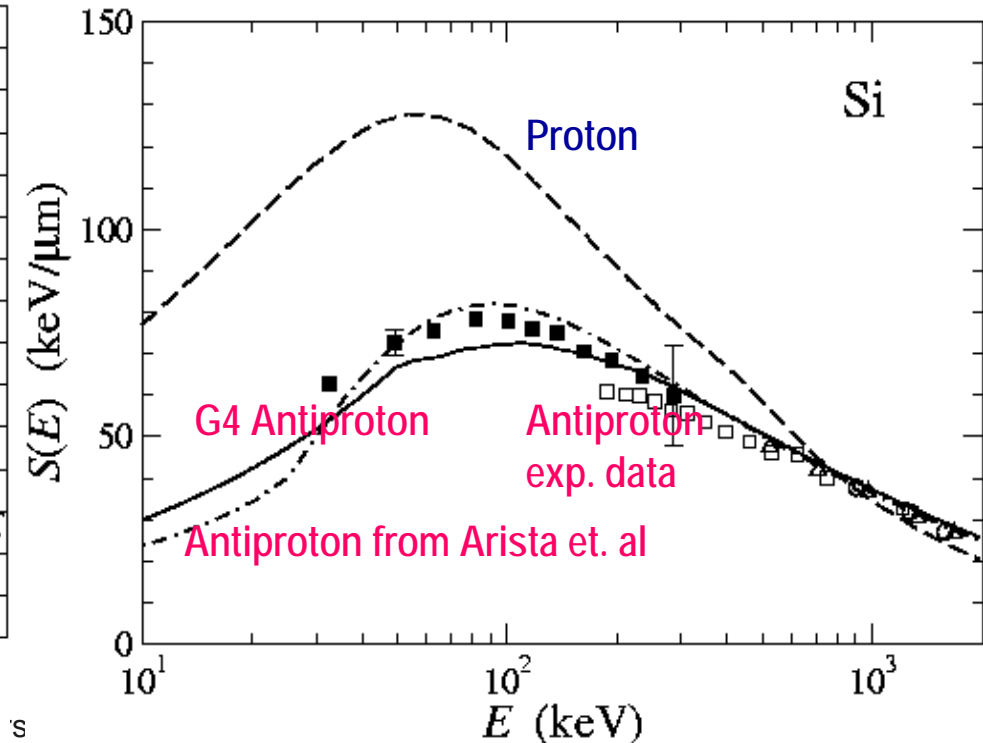
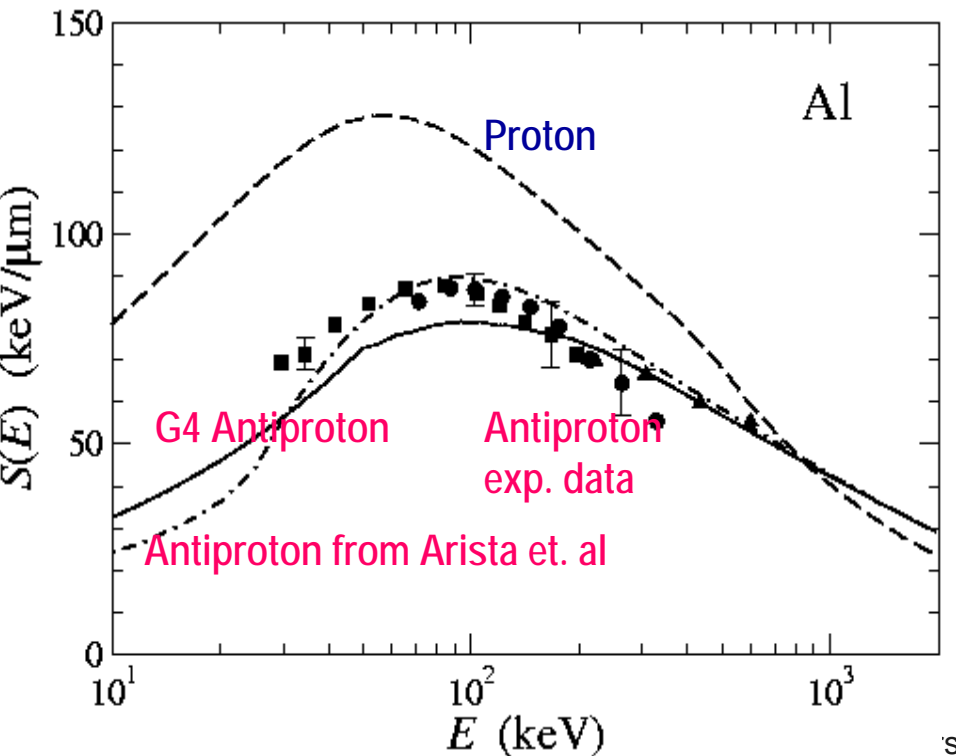
# Models for antiprotons

- $\beta > 0.5$
- $0.01 < \beta < 0.5$
- $\beta < 0.01$

Bethe-Bloch formula

Quantum harmonic oscillator model

Free electron gas model

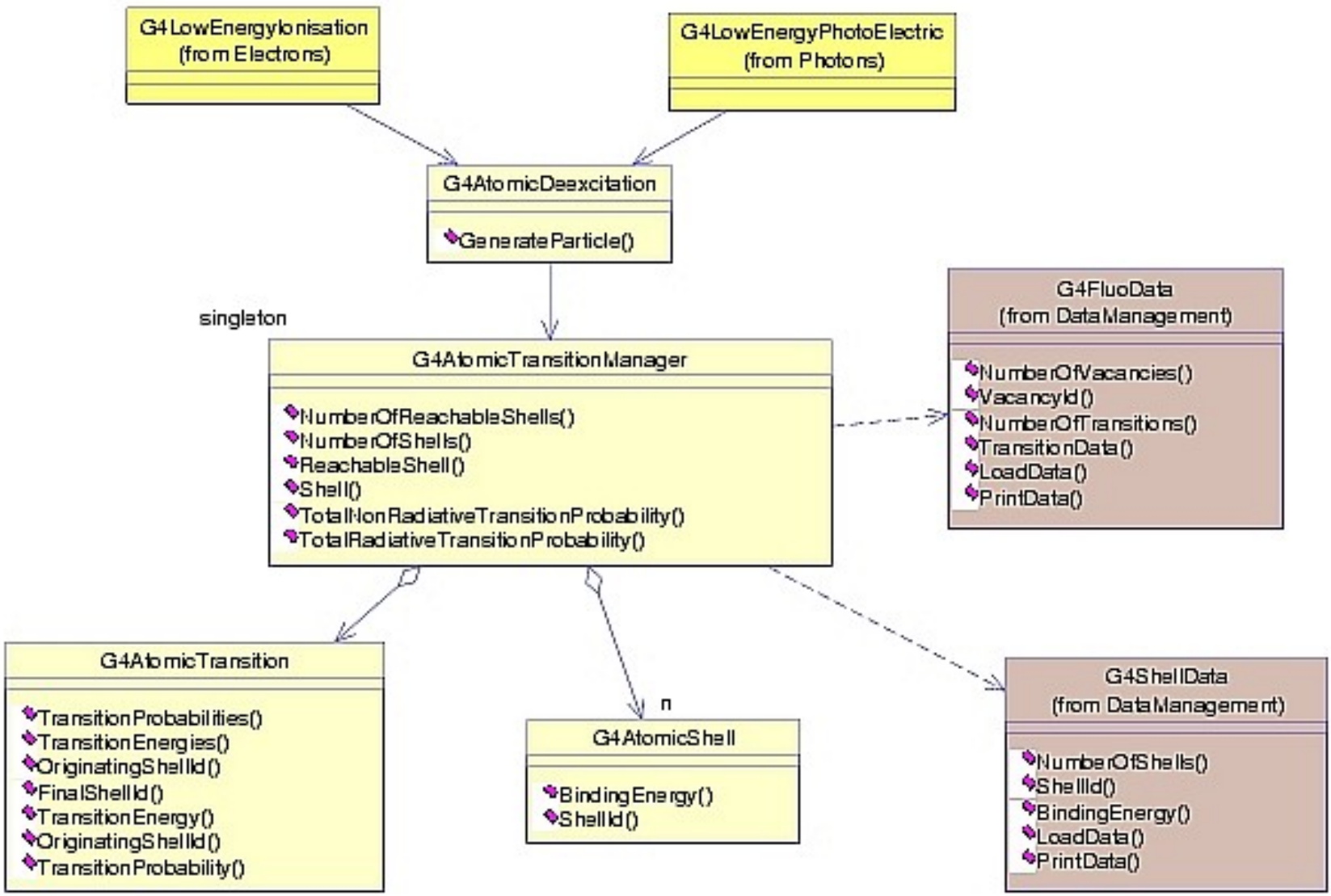


# Options for G4hLowEnergyIonisation

*G4hLowEnergyIonisation\* hIonisation = new G4hLowEnergyIonisation;  
hIonisation->Set...();*

- SetHighEnergyForProtonParametrisation(G4double)
- SetLowEnergyForProtonParametrisation(G4double)
- SetHighEnergyForAntiProtonParametrisation(G4double)
- SetLowEnergyForAntiProtonParametrisation(G4double)
- **SetElectronicStoppingPowerModel**(const G4ParticleDefinition\*,const G4String& )
- **SetNuclearStoppingPowerModel**(const G4String&)
- **SetNuclearStoppingOn**()
- **SetNuclearStoppingOff**()
- SetBarkasOn()
- SetBarkasOff()
- SetFluorescence(const G4bool)
- ActivateAugerElectronProduction(G4bool)
- SetCutForSecondaryPhotons(G4double)
- SetCutForSecondaryElectrons(G4double)

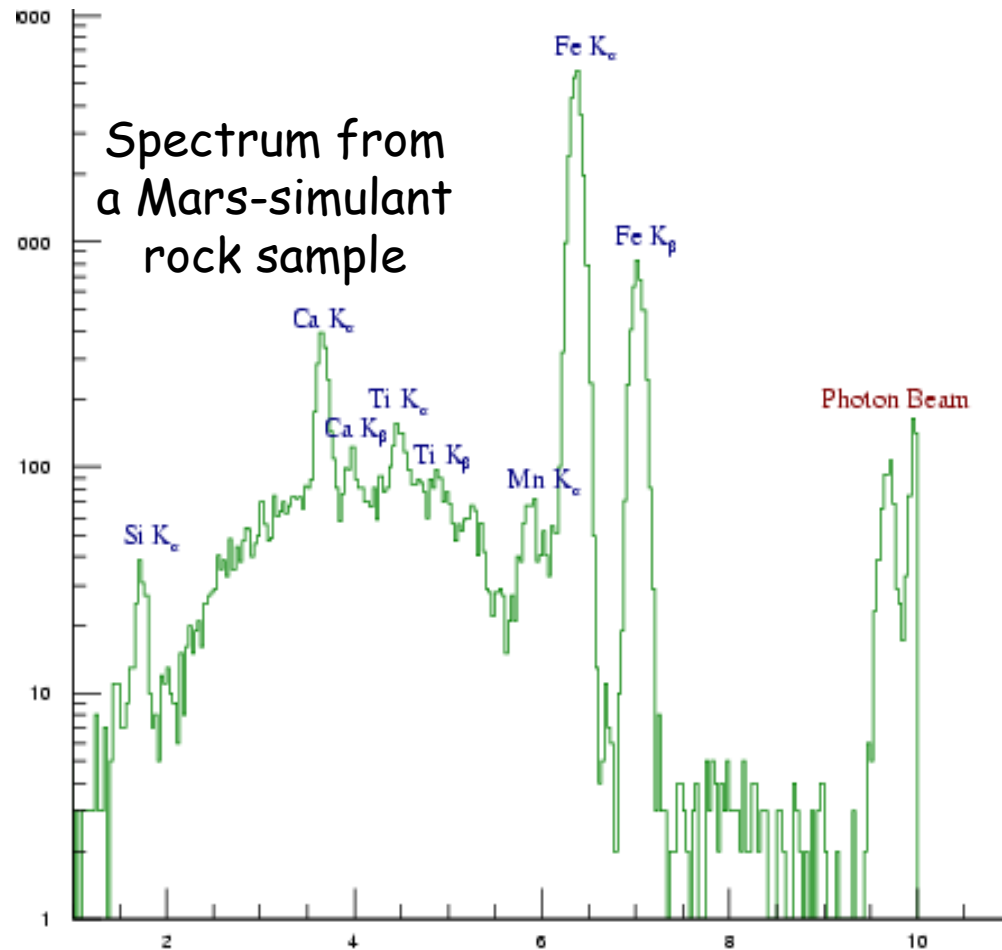
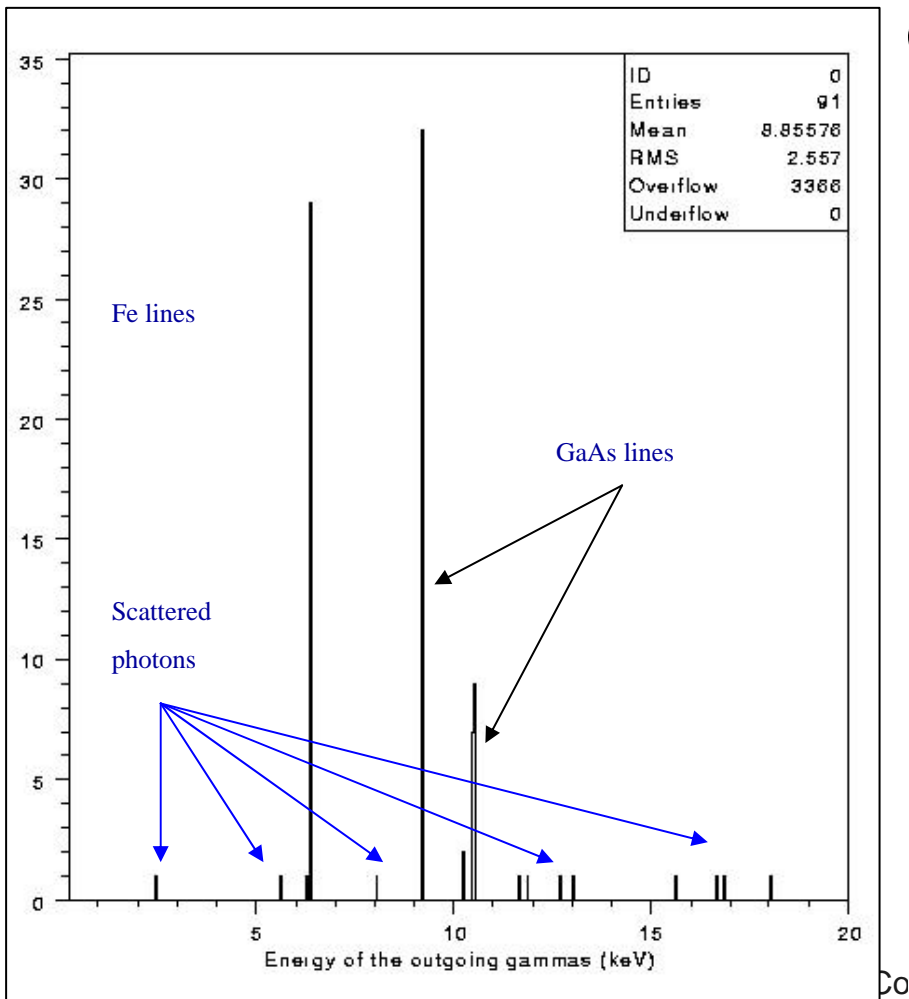
# Atomic relaxation



# Fluorescence

Microscopic validation:  
against reference data

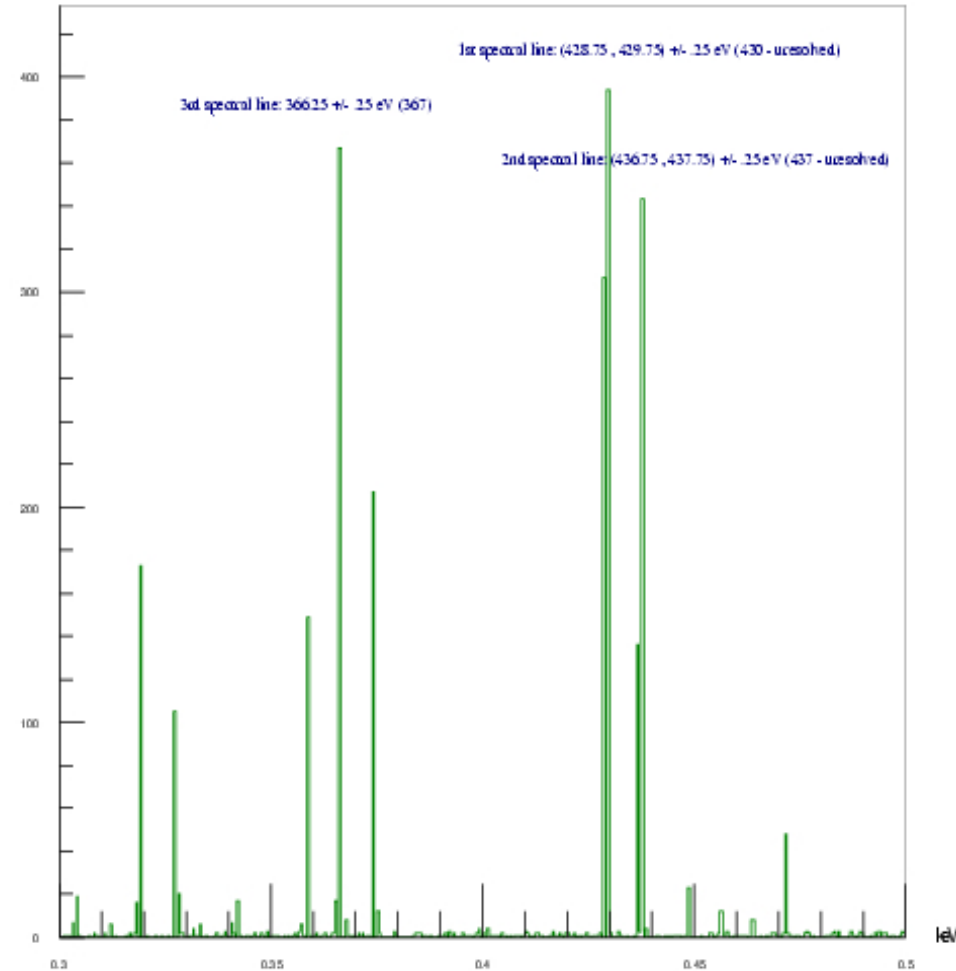
Experimental validation:  
test beam data, in collaboration with  
ESA Advanced Concepts & Science  
Payload Division



# Auger effect

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

Electron emission from Sn - 3 KeV photon Beam



# PIXE

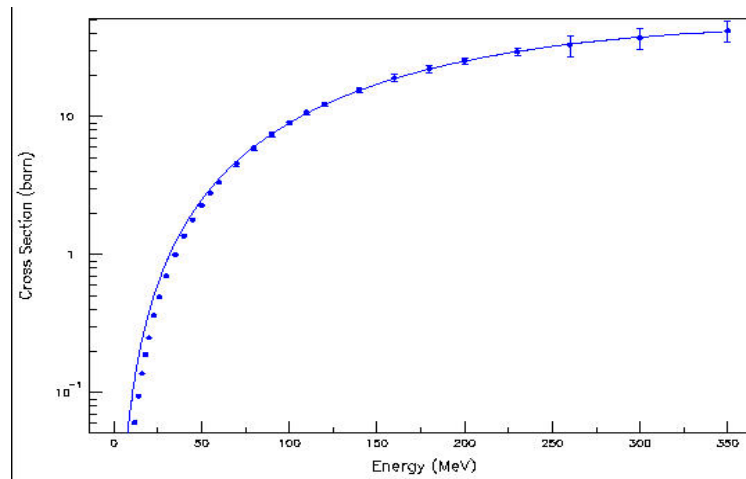
- Model based on experimental data
  - Parameterisation of Paul & Sacher data library for ionisation cross sections
  - Uses the EADL-based package of atomic deexcitation for the generation of fluorescence and Auger secondary products
- Geant4 9.1 implementation: protons, K-shell
- Further developments (and problems)

Talk by G. Weidenspointner  
NSS session N41-4 on  
Thursday morning

Example of p ionisation cross section,  
K shell

parameterisation (solid line)

Experimental data



# Further documentation on Geant4 Atomic Relaxation

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 54, NO. 3, JUNE 2007

585

## Geant4 Atomic Relaxation

**2007**

Susanna Guatelli, Alfonso Mantero, Barbara Mascialino, Petteri Nieminen, and Maria Grazia Pia

594

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 54, NO. 3, JUNE 2007

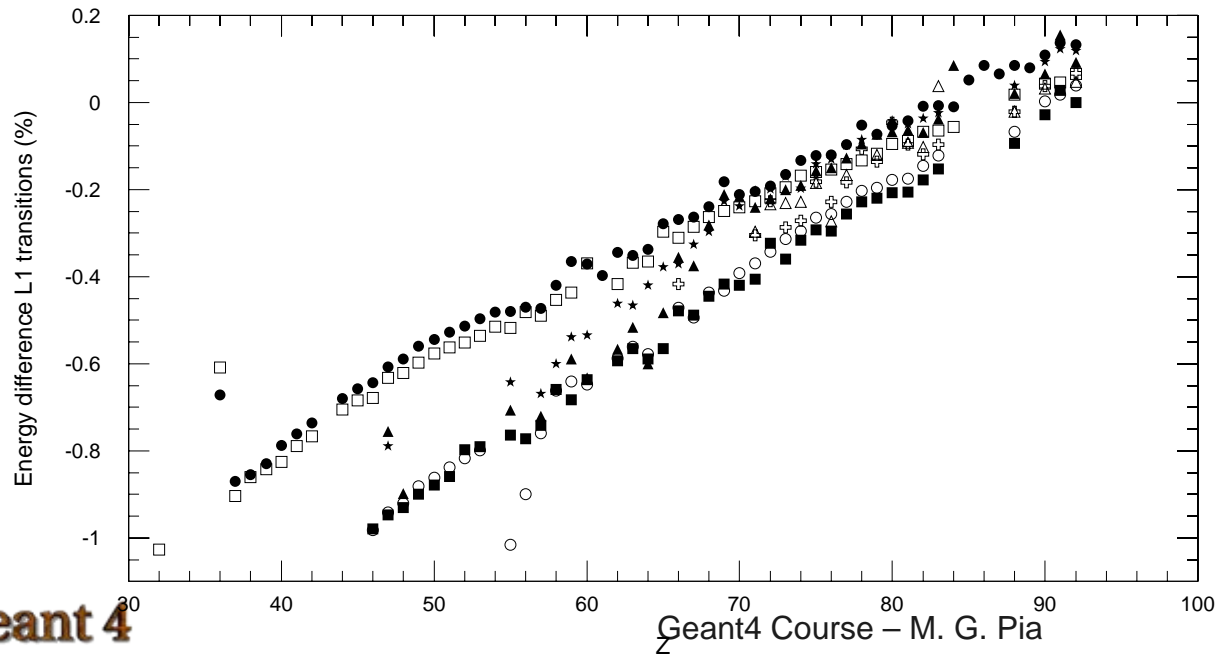
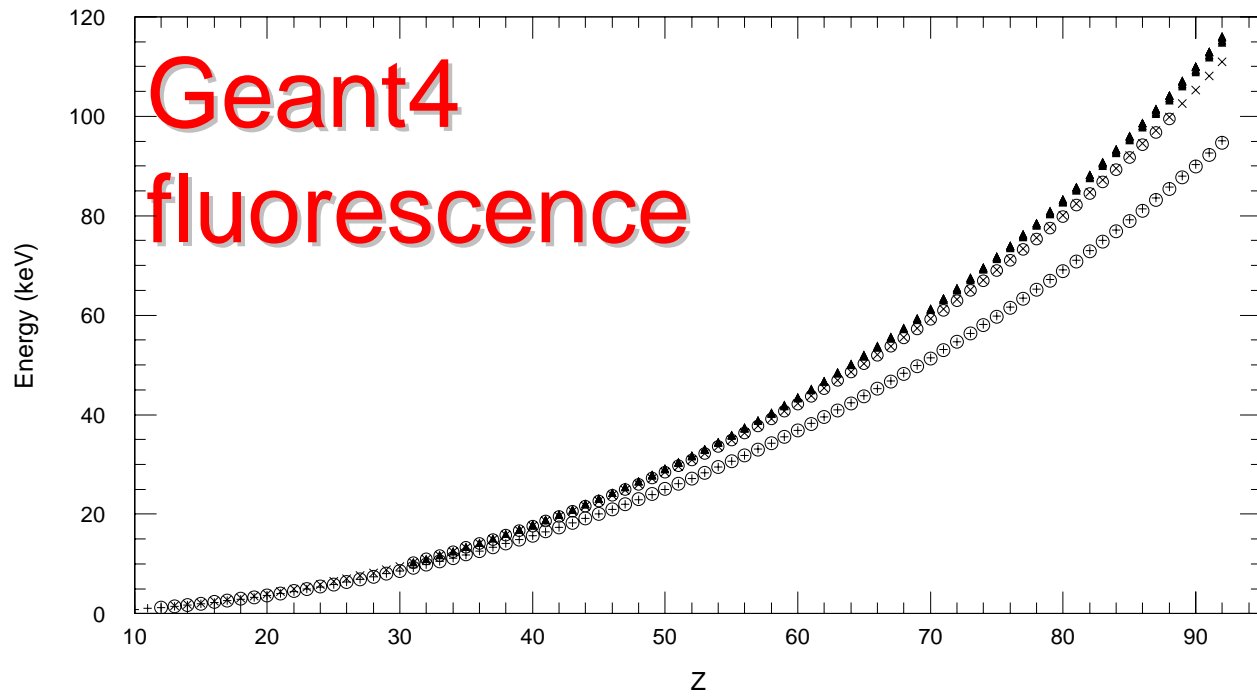
## Validation of Geant4 Atomic Relaxation Against the NIST Physical Reference Data

**2007**

S. Guatelli, A. Mantero, B. Mascialino, M. G. Pia, and V. Zampichelli

More in preparation (M.G. Pia et al.)

**2008**



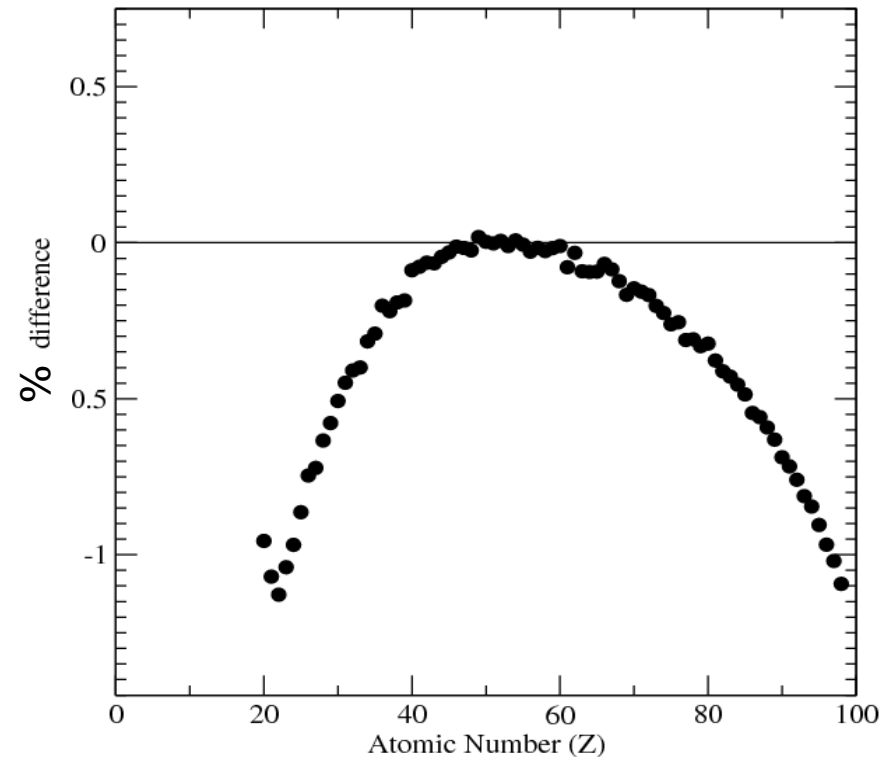
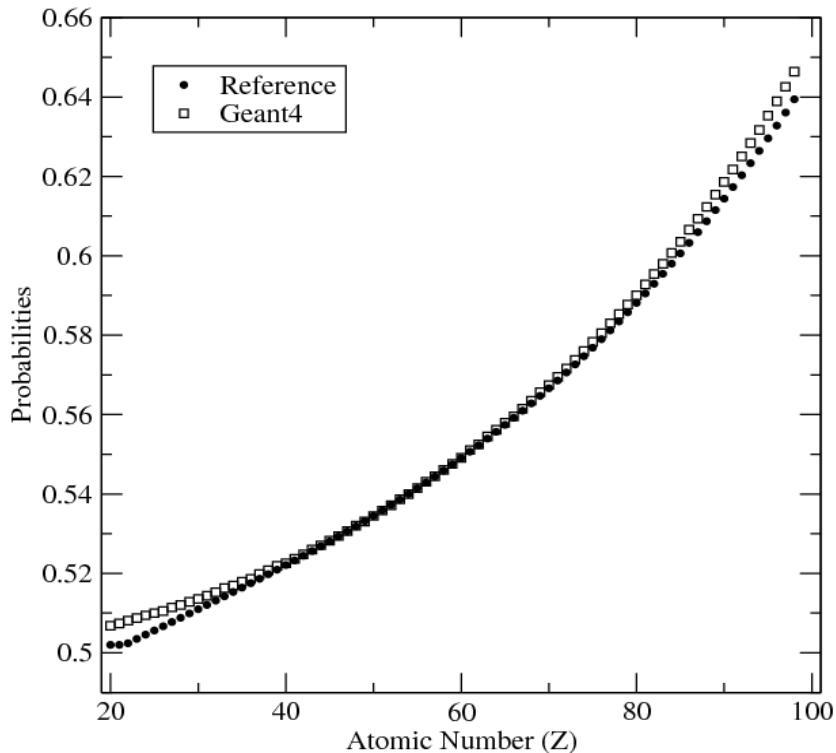


# Goodness of fit test

Transition	p-value
KL <sub>2</sub>	1
KL <sub>3</sub>	1
KM <sub>2</sub>	1
KM <sub>4</sub>	1
KM <sub>5</sub>	1
KN <sub>2</sub>	1
KN <sub>3</sub>	1
L <sub>1</sub> M <sub>2</sub>	1
L <sub>1</sub> M <sub>3</sub>	1
L <sub>1</sub> M <sub>4</sub>	1
L <sub>1</sub> M <sub>5</sub>	1
L <sub>1</sub> N <sub>2</sub>	1
L <sub>1</sub> N <sub>3</sub>	1
L <sub>1</sub> N <sub>4</sub>	0.997
L <sub>1</sub> N <sub>5</sub>	1
L <sub>2</sub> M <sub>1</sub>	1
L <sub>2</sub> M <sub>3</sub>	1
L <sub>2</sub> M <sub>4</sub>	1
L <sub>2</sub> N <sub>2</sub> or L <sub>2</sub> N <sub>3</sub>	1
L <sub>2</sub> N <sub>3</sub>	1
L <sub>2</sub> N <sub>4</sub>	1
L <sub>2</sub> N <sub>6</sub>	1
L <sub>3</sub> M <sub>1</sub>	1
L <sub>3</sub> M <sub>2</sub>	1
L <sub>3</sub> M <sub>3</sub>	1
L <sub>3</sub> M <sub>4</sub>	1
L <sub>3</sub> M <sub>5</sub>	1
L <sub>3</sub> N <sub>2</sub> or L <sub>3</sub> N <sub>3</sub>	1
L <sub>3</sub> N <sub>2</sub>	1
L <sub>3</sub> N <sub>3</sub>	1
L <sub>3</sub> N <sub>4</sub>	1
L <sub>3</sub> N <sub>5</sub>	1

Goodness-of-fit test	p-value
Anderson-Darling	1
Cramer-von Mises	1
Kolmogorov-Smirnov	1
Kuiper	1
Watson	1

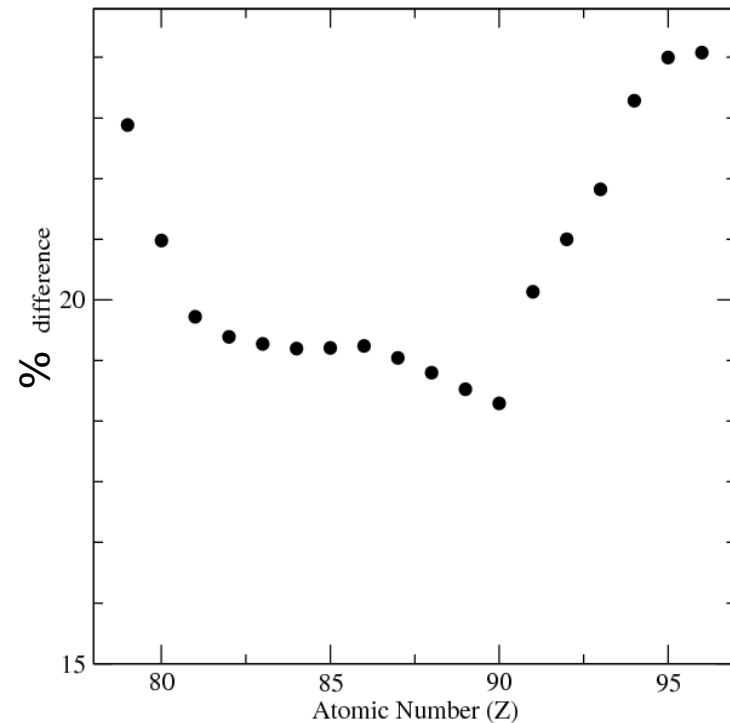
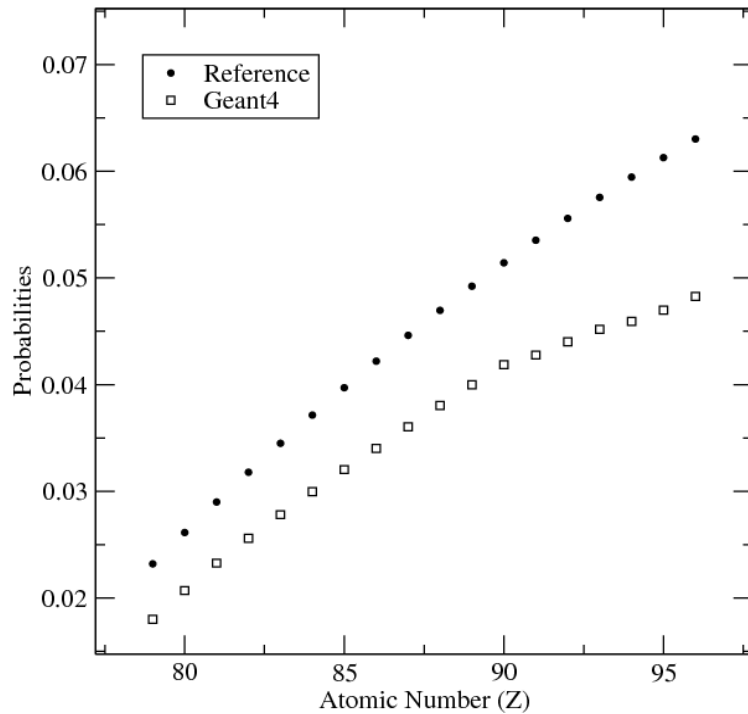
# Fluorescence transition probabilities



Experimental reference:

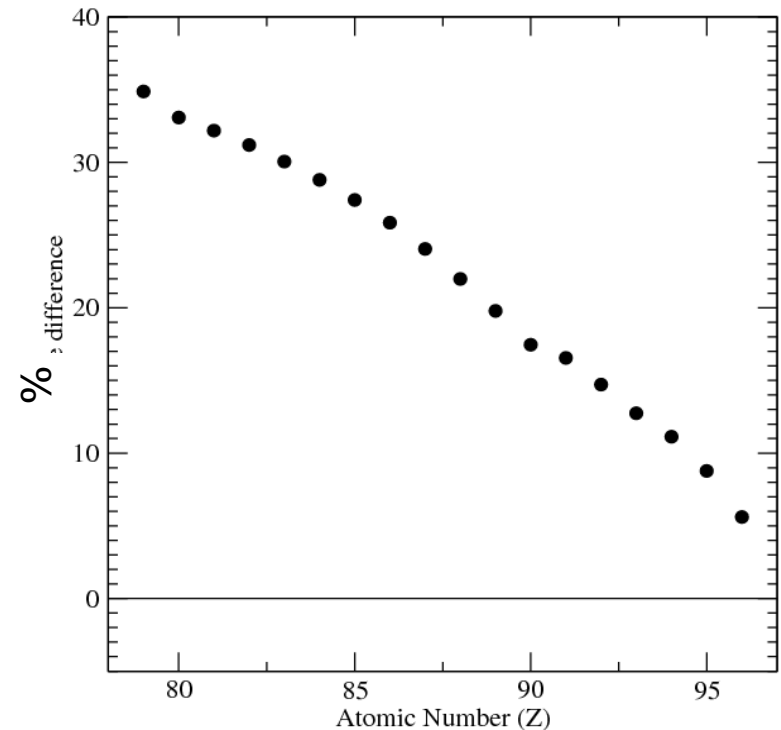
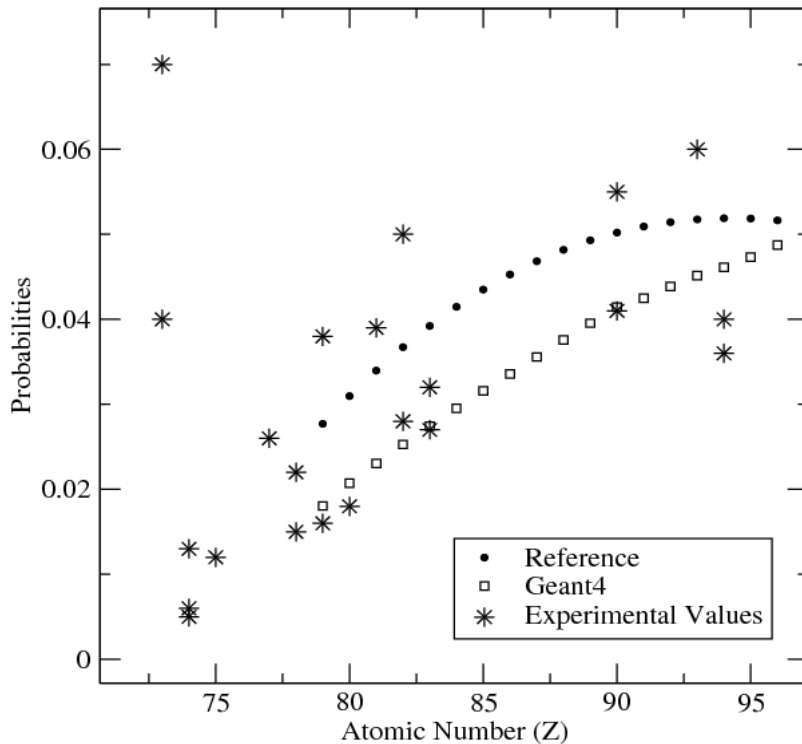
W.T. Elam, B.D. Ravel, J.R. Sieber, *A new atomic database for X-ray spectroscopic calculations*, Radiat. Phys. Chem. 63 (2002) 121–128

# Bad but harmless...



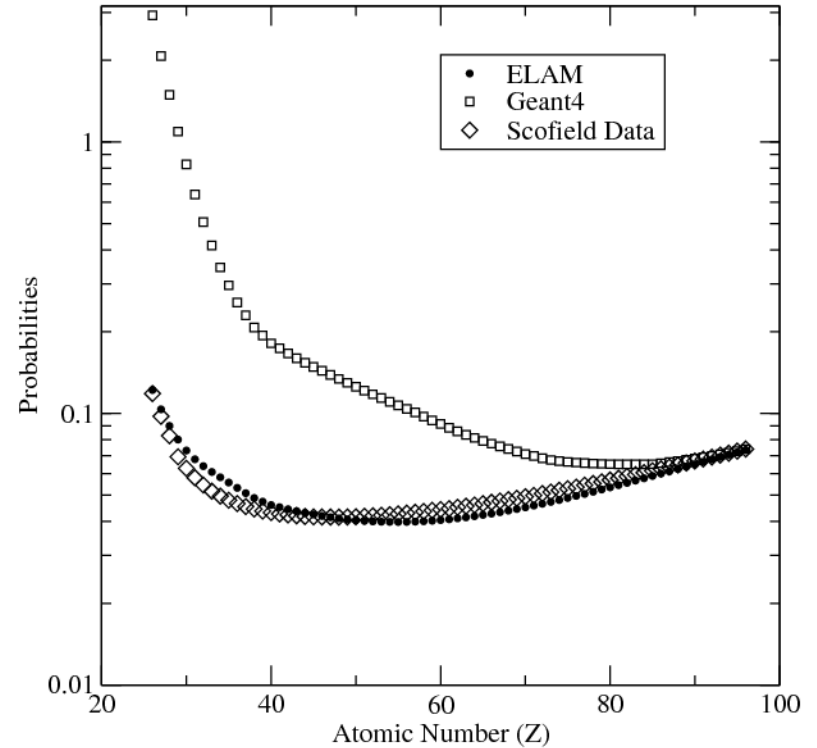
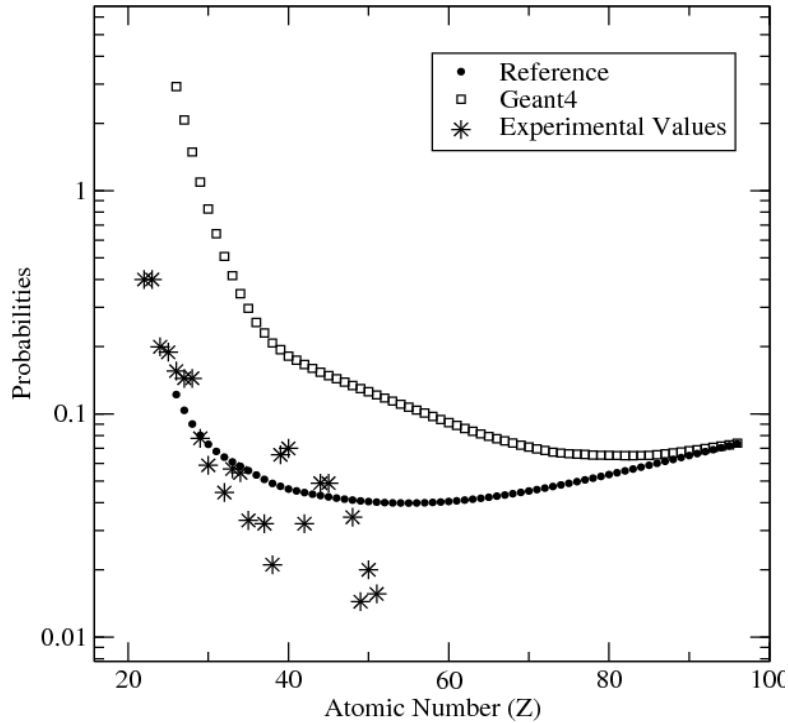
25% absolute error  $\Rightarrow$  0.04% error in an experimental use case

# Hard to say...



Controversial experimental data

# Hidden for 17 years...



**The error is in EADL!**

# In progress

- Extensions down to the eV scale
  - In water (for radiobiology studies)
  - Other materials (gas, solids)
- Difficult domain
  - Models must be specialised by material
  - Cross sections, final state generation, angular distributions

# 1<sup>st</sup> development cycle: Very-low energy extensions

Physics of interactions in water down to the eV scale

- **Complex domain**

- **Physics:** collaboration with theorists
- **Technology:** innovative design technique introduced in Geant4 (1<sup>st</sup> time in Monte Carlo)

- **Experimental complexity as well**

- Scarce experimental data
- Collaboration with experimentalists for model validation
- Geant4 physics validation at low energies is difficult!

# Geant4-DNA physics processes

Specialised processes for low energy interactions with water

- **Models in liquid water**

- More realistic than water vapour
- Theoretically more challenging
- Hardly any experimental data
- New measurements needed

- **Status**

- 1st  $\beta$ -release Geant4 8.1 2006
- Full release December 2007
- Further extensions in progress

- **Current focus**

- Experimental comparisons

**Toolkit:** offer a wide choice among available alternative models for each process

Particle	Processes
$e^-$	Elastic scattering Excitation Ionisation
p	Charge decrease Excitation Ionisation
H	Charge increase Ionisation
He $^{++}$	Charge decrease Excitation Ionisation
He $^+$	Charge decrease Charge increase Excitation Ionisation
He	Charge increase Excitation Ionisation



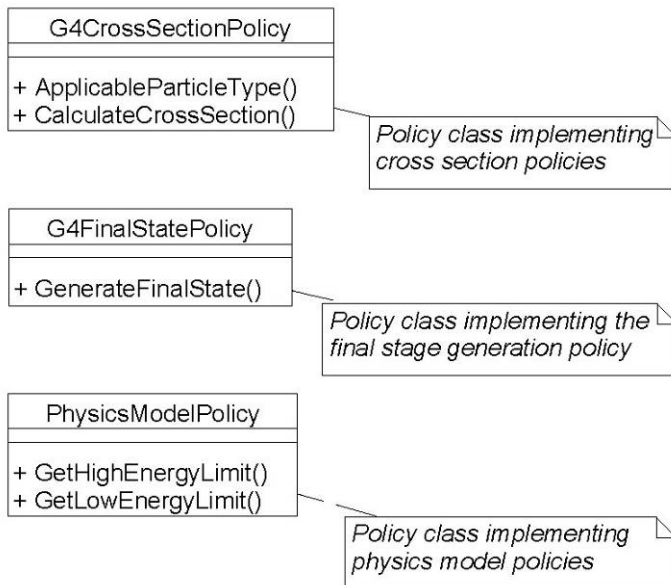
# What is behind...

## Policy-based class design

- A policy defines a class or class template interface
- Policy host classes are parameterised classes
  - classes that use other classes as a parameter
- Advantage w.r.t. a conventional strategy pattern
  - Policies are not required to inherit from a base class
  - The code is bound at compilation time
    - No need of virtual methods, resulting in faster execution

New  
technique

1<sup>st</sup> time  
introduced  
in Monte  
Carlo

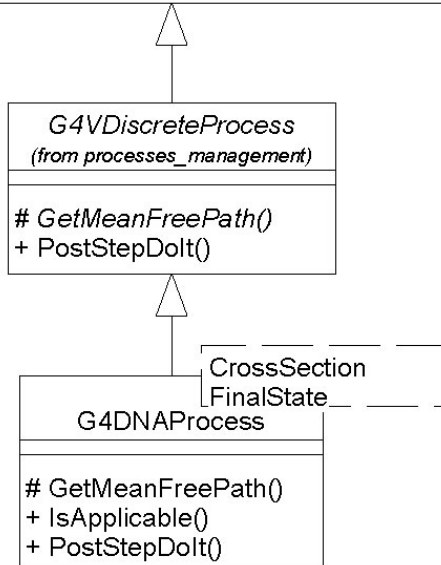
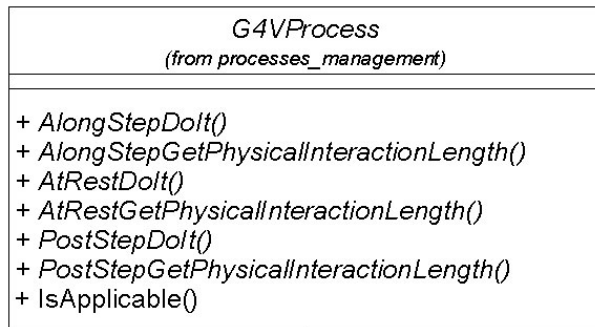


**Weak dependency** of the policy and the policy based class on the policy interface

**Highly customizable** design  
Open to extension

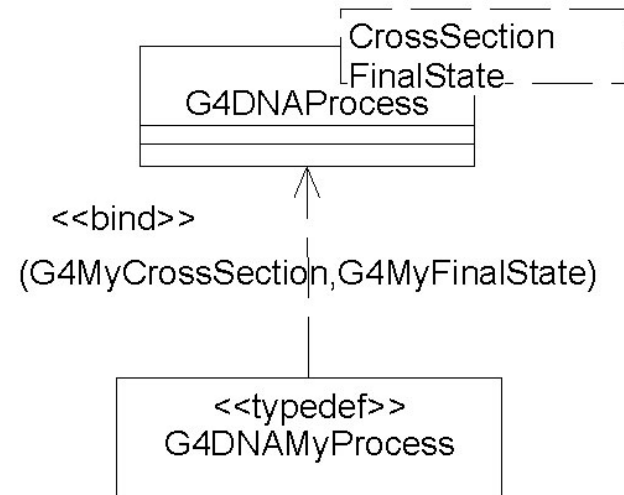
# Geant4-DNA physics process

Handled transparently  
by Geant4 kernel



Deprived of any intrinsic  
physics functionality

Configured by  
**template specialization**  
to acquire physics properties



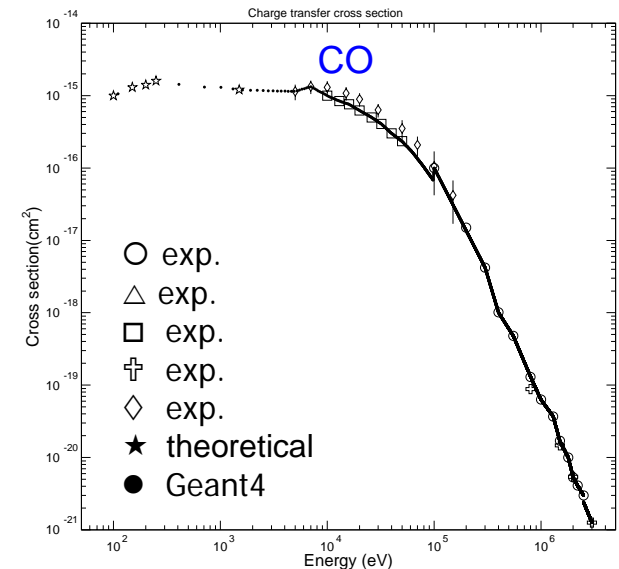
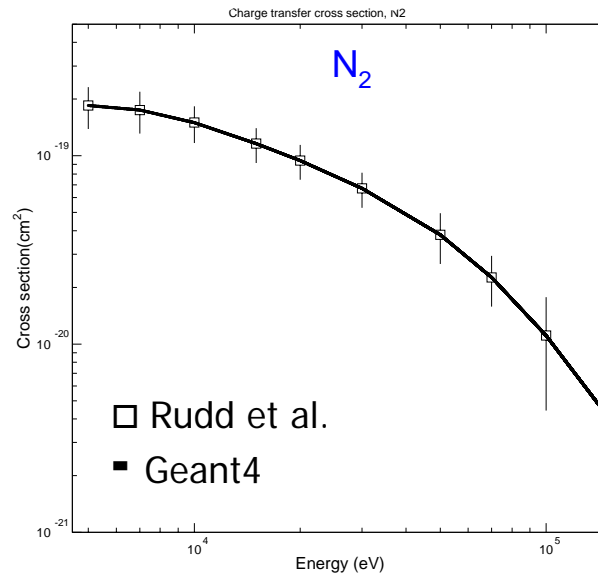
# From cells to plasma...

## Proton charge transfer processes for 12 materials

(He, water vapour, N<sub>2</sub>, CO, CO<sub>2</sub>, hydrocarbons)

Relevant to astrophysics and fusion reactor design

Development  
metrics  
in Easter egg



Design investment  
pays back!

M.E. Rudd et al., *Phys. Rev. A* 28, 3244-3257, 1983  
L.H. Toburen et al., *Phys. Rev.* 171, 114 - 122, 1968  
S.L. Varghese et al., *Phys. Rev. A* 31, 2202-2209, 1985  
M.B. Shah and H.B. Gilbody, *J. Phys. B* 23, 1491-1499, 1990  
R.S. Gao et al., *Phys. Rev. A* 41, 5929-5933, 1990  
M. Kimura et al., *Phys. Rev. A* 61, 032708, 2000

# How to use policy-based processes

## // Definition

```
typedef G4DNAProcess<G4CrossSectionElasticScreenedRutherford,G4FinalStateElasticScreenedRutherford> ElasticScreenedRutherford;  
typedef G4DNAProcess<G4CrossSectionElasticScreenedRutherford,G4FinalStateElasticBrennerZaider> ElasticBrennerZaider;  
typedef G4DNAProcess<G4CrossSectionExcitationEmfietzoglou,G4FinalStateExcitationEmfietzoglou> ExcitationEmfietzoglou;  
typedef G4DNAProcess<G4CrossSectionExcitationBorn,G4FinalStateExcitationBorn> ExcitationBorn;  
typedef G4DNAProcess<G4CrossSectionIonisationBorn,G4FinalStateIonisationBorn> IonisationBorn;  
typedef G4DNAProcess<G4CrossSectionIonisationRudd,G4FinalStateIonisationRudd> IonisationRudd;  
typedef G4DNAProcess<G4CrossSectionExcitationMillerGreen,G4FinalStateExcitationMillerGreen> ExcitationMillerGreen;  
typedef G4DNAProcess<G4CrossSectionChargeDecrease,G4FinalStateChargeDecrease> ChargeDecrease;  
typedef G4DNAProcess<G4CrossSectionChargeIncrease,G4FinalStateChargeIncrease> ChargeIncrease;
```

## // Registration

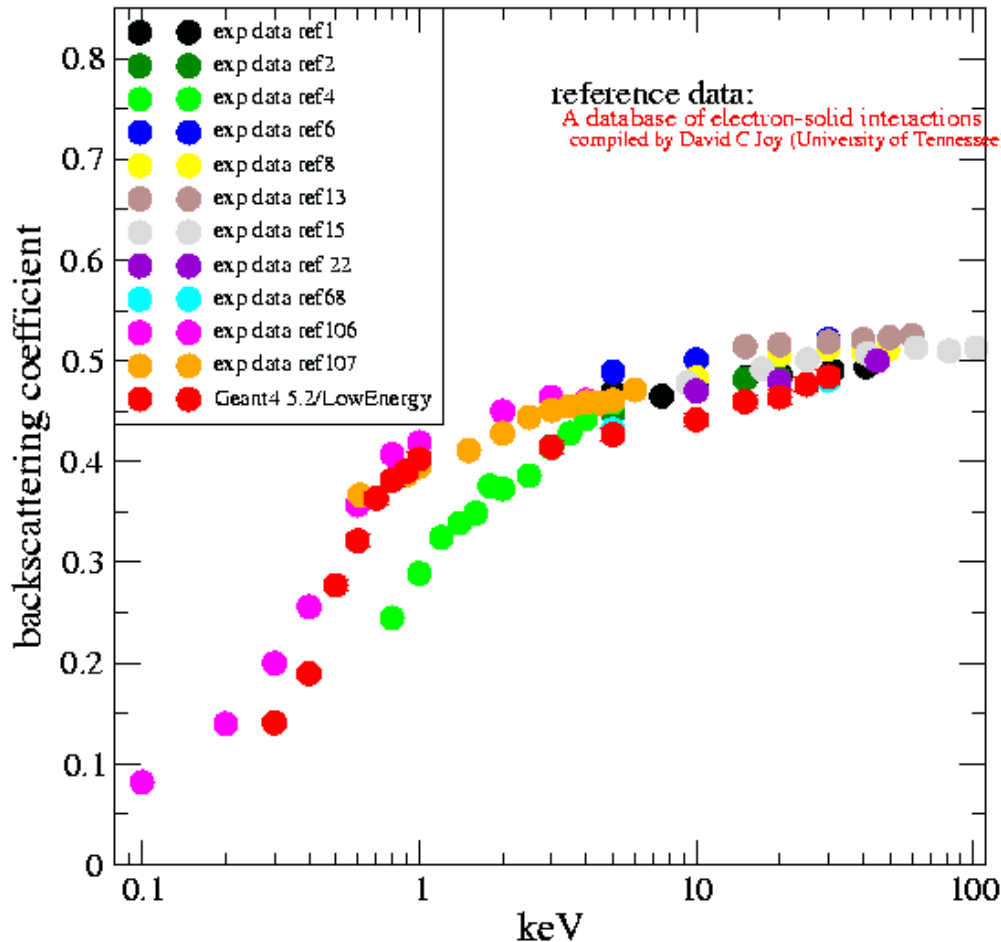
```
...  
if (particleName == "e-")  
{  
    processManager->AddDiscreteProcess(new ExcitationEmfietzoglou);  
    processManager->AddDiscreteProcess(new ElasticScreenedRutherford);  
    processManager->AddDiscreteProcess(new ElasticBrennerZaider);  
    processManager->AddDiscreteProcess(new IonisationBorn);  
}
```

# Physics models and their validation

- S. Chauvie et al.,  
**Geant4 physics processes for microdosimetry simulation: design foundation and implementation of the first set of models**  
*IEEE Trans. Nucl. Sci.*, vol. 54, no. 6, Dec. 2007
- S. Chauvie, P. Nieminen, M. G. Pia  
**Geant4 model for the stopping power of low energy negatively charged hadrons**  
*IEEE Trans. Nucl. Sci.*, vol. 54, no. 3, pp. 578-584, Jun. 2007
- S. Guatelli, A. Mantero, B. Mascialino, P. Nieminen, M. G. Pia  
**Geant4 Atomic Relaxation**  
*IEEE Trans. Nucl. Sci.*, vol. 54, no. 3, pp. 585-593, Jun. 2007
- S. Guatelli, A. Mantero, B. Mascialino, P. Nieminen, M. G. Pia, V. Zampichelli  
**Validation of Geant4 Atomic Relaxation against the NIST Physical Reference Data**  
*IEEE Trans. Nucl. Sci.*, vol. 54, no. 3, Jun. 2007, pp. 594-603
- K. Amako et al.,  
**Comparison of Geant4 electromagnetic physics models against the NIST reference data**  
*IEEE Trans. Nucl. Sci.*, vol. 52, no. 4, pp. 910-918, Aug. 2005

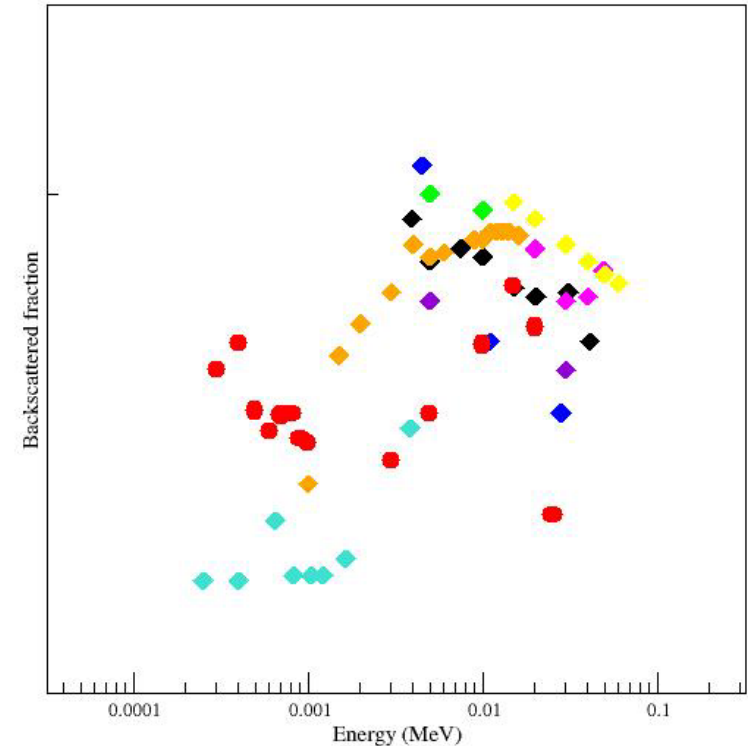
# The problem of validation: finding reliable data

backscattering for e-  
e- energy range: 0.1 keV -> 102. keV



Backscattering low energies - Au

Electrons - Backscattering - Iron  
(Geant4-05-02 LowE)



**Note: Geant4 validation is not always easy**

experimental data often exhibit large differences!

# Summary

- OO technology provides the mechanism for a rich set of electromagnetic physics models in Geant4
  - further extensions and refinements are possible, without affecting Geant4 kernel or user code
- Two main approaches in Geant4:
  - Standard package
  - Low Energy package

each one offering a variety of models for specialised applications
- Extensive validation activity and results
- More on Physics Reference Manual and web site