

Modellistica Medica

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Genova

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Lezione 32

Low Energy Electromagnetic Physics

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*) 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
 - will learn more on domains of application in the second lecture

Overview of physics

- Compton scattering

- Rayleigh scattering

- Photoelectric effect

- Pair production

- Bremsstrahlung

- Ionisation

- Polarised Compton

- + atomic relaxation

- fluorescence

- Auger effect

following photoelectric effect and ionisation

- In progress

- Polarised γ conversion, photoelectric

- More precise angular distributions (Rayleigh, photoelectric, Bremsstrahlung etc.)

- New models, based on different physics approaches

- Processes for positrons

- Development plan

- *Driven by user requirements*

- *Schedule compatible with available resources*

Software Process

A rigorous approach to software engineering

- in support of a better quality of the software
- especially relevant in the physics domain of Geant4-LowE EM
- several mission-critical applications (space, medical...)

Spiral approach

A life-cycle model that is both iterative and incremental

Collaboration-wide Geant4 software process, tailored to the WG projects

Huge effort invested into SPI

current
status →

- *Public URD*
- *Full traceability through UR/OOD/implementation/test*
- *Testing suite and testing process*
- *Public documentation of procedures*
- *Defect analysis and prevention*
- *etc....*

User requirements

Various methodologies adopted to capture URs

- Elicitation through interviews and surveys
 - *useful to ensure that UR are complete and there is wide agreement*
- Joint workshops with user groups
- Use cases
- Analysis of existing Monte Carlo codes
- Study of past and current experiments
- Direct requests from users to WG coordinators

User Requirements

GEANT4 LOW ENERGY

ELECTROMAGNETIC PHYSICS

**Posted on the WG
web site**

User Requirements Document

Status: in CVS repository

Version: 2.4

Project: Geant4-LowE

Reference: LowE-URD-V2.4

Created: 22 June 1999

Last modified: 26 March 2001

Prepared by: Petteri Nieminen (ESA) and Maria Grazia Pia (INFN)

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*)

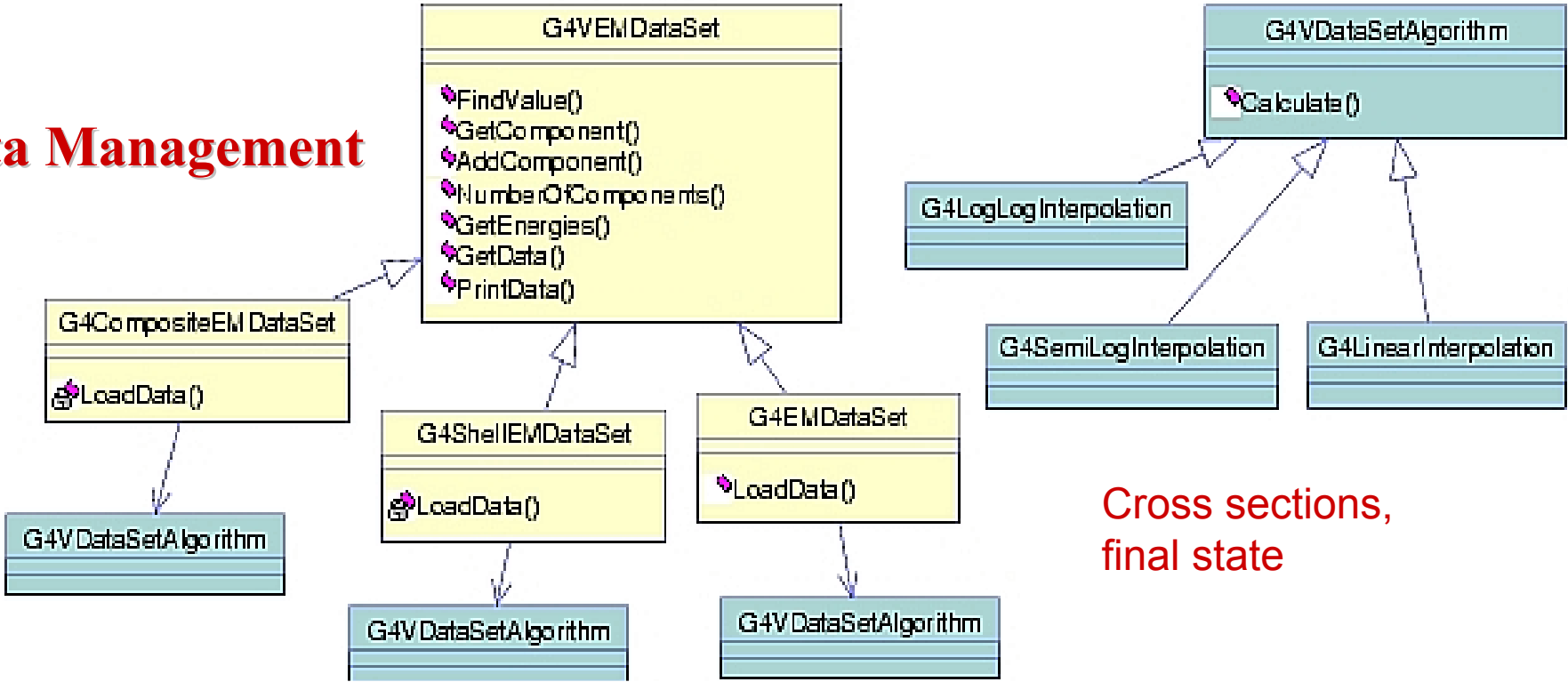
- Validity range: 250 eV - 100 GeV

- 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*)

Data Management



Cross sections,
final state

Intelligent data: know how to handle themselves through algorithm objects
 e.g.: interpolation algorithms encapsulated in objects
(to let them vary and be interchangeable)

Composite pattern to treat different physical entities (e.g. whole atom and atom with shell structure) transparently

Calculation of cross sections

Interpolation from the data libraries:

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

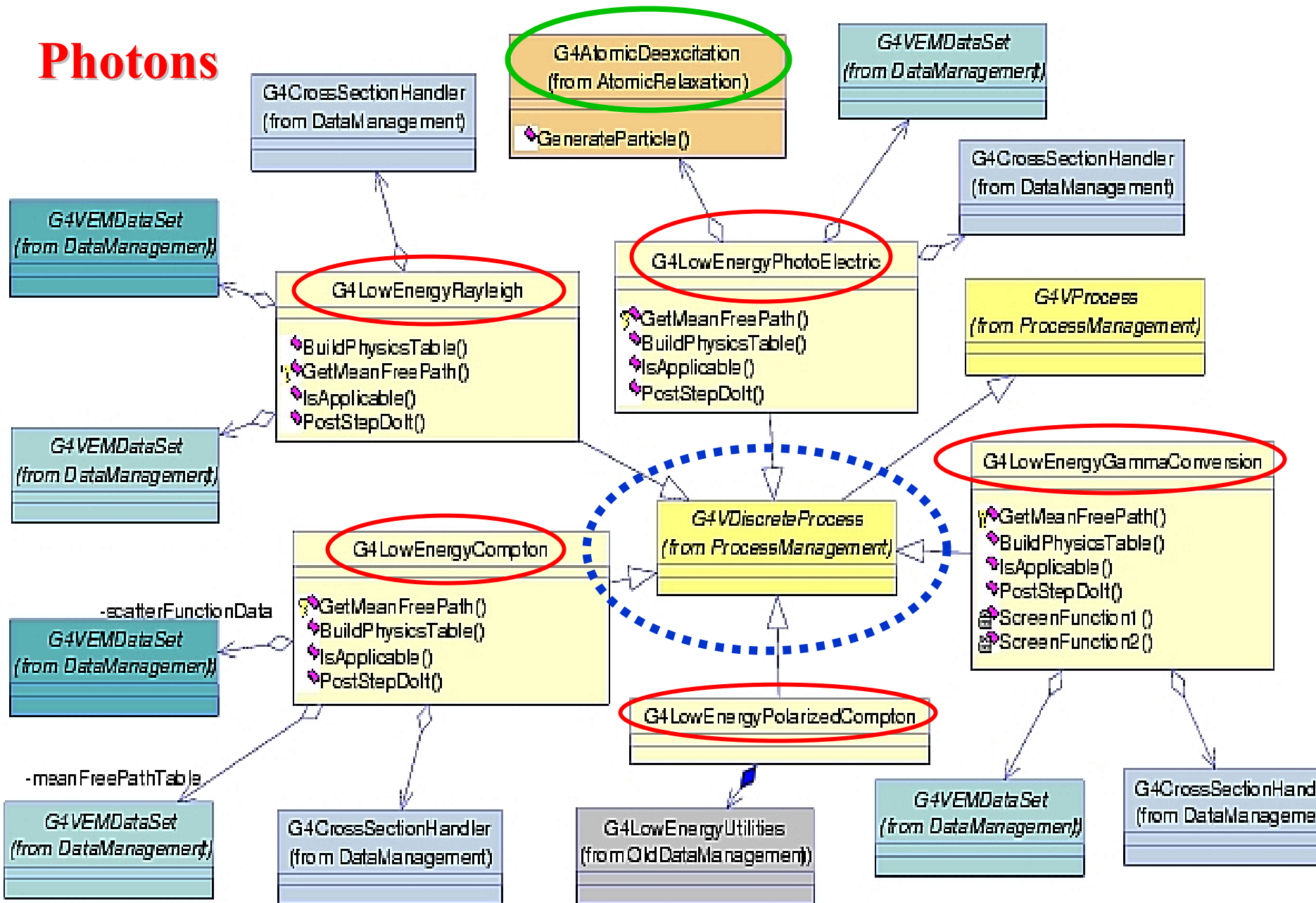
E_1 and E_2 are the lower and higher energy for which data (σ_1 and σ_2) are available

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

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 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

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
- Further improvements foreseen

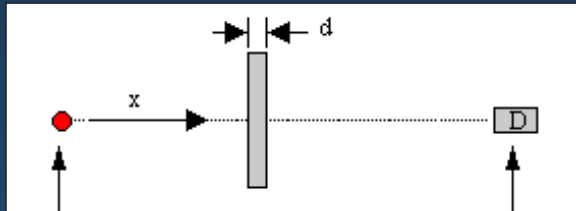
Photoelectric effect

- **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

γ 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

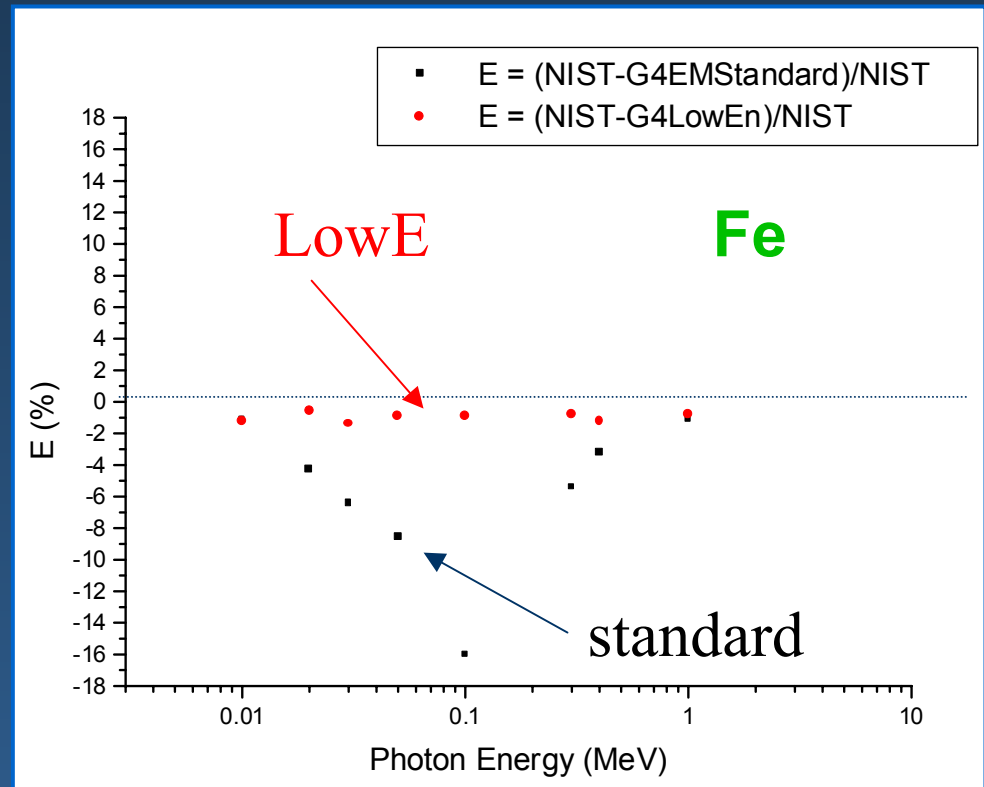
Photons: mass attenuation coefficient



Comparison against NIST data

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

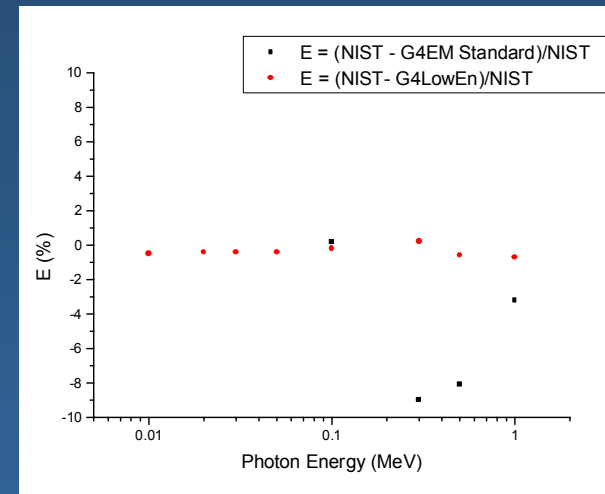
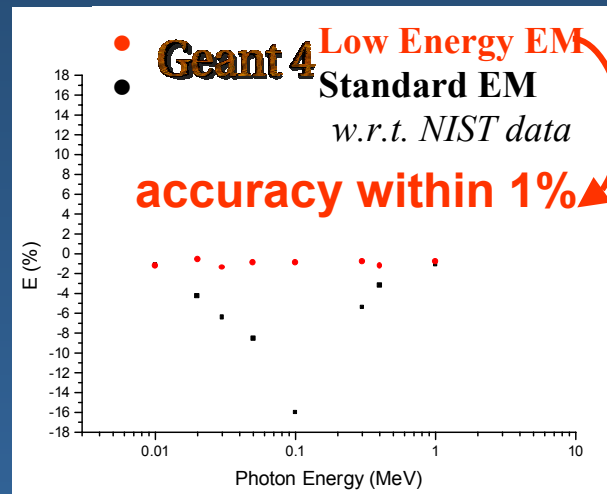
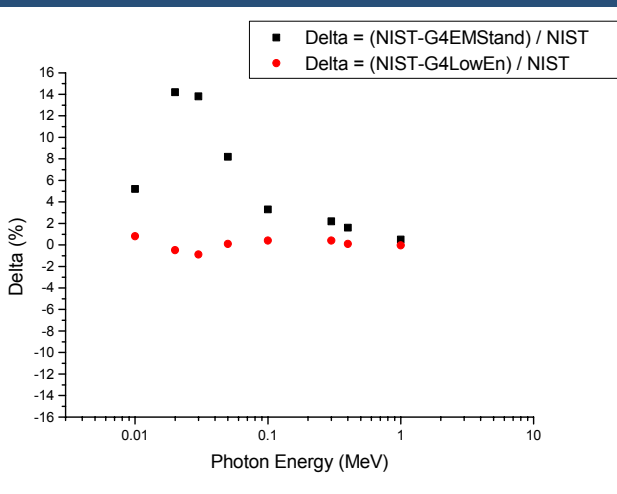
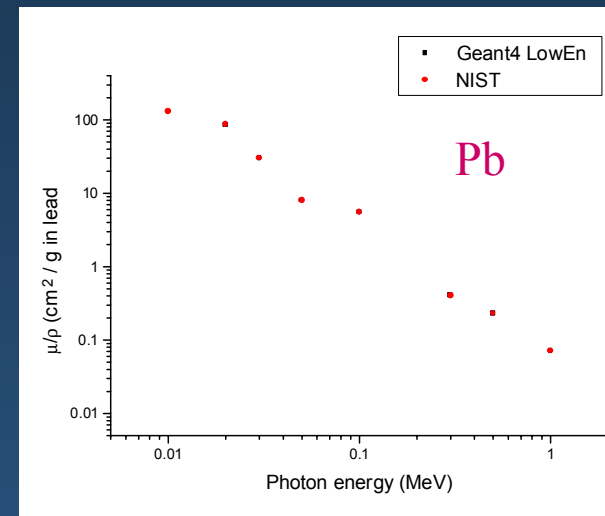
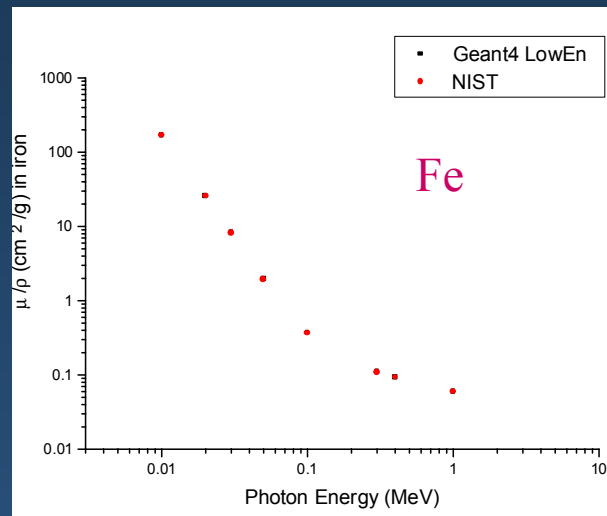
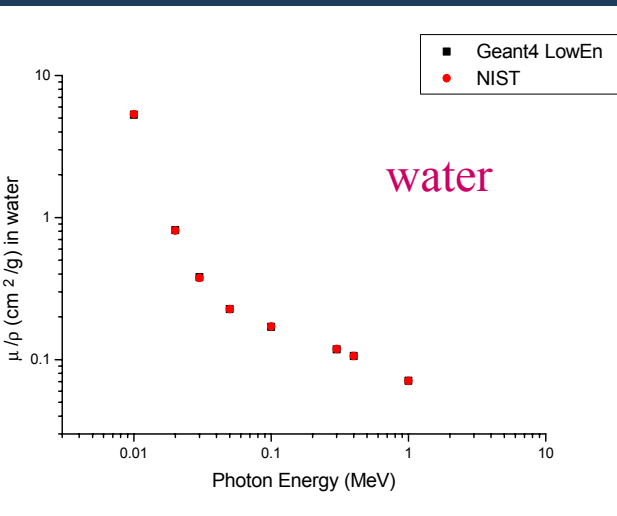
LowE accuracy $\sim 1\%$



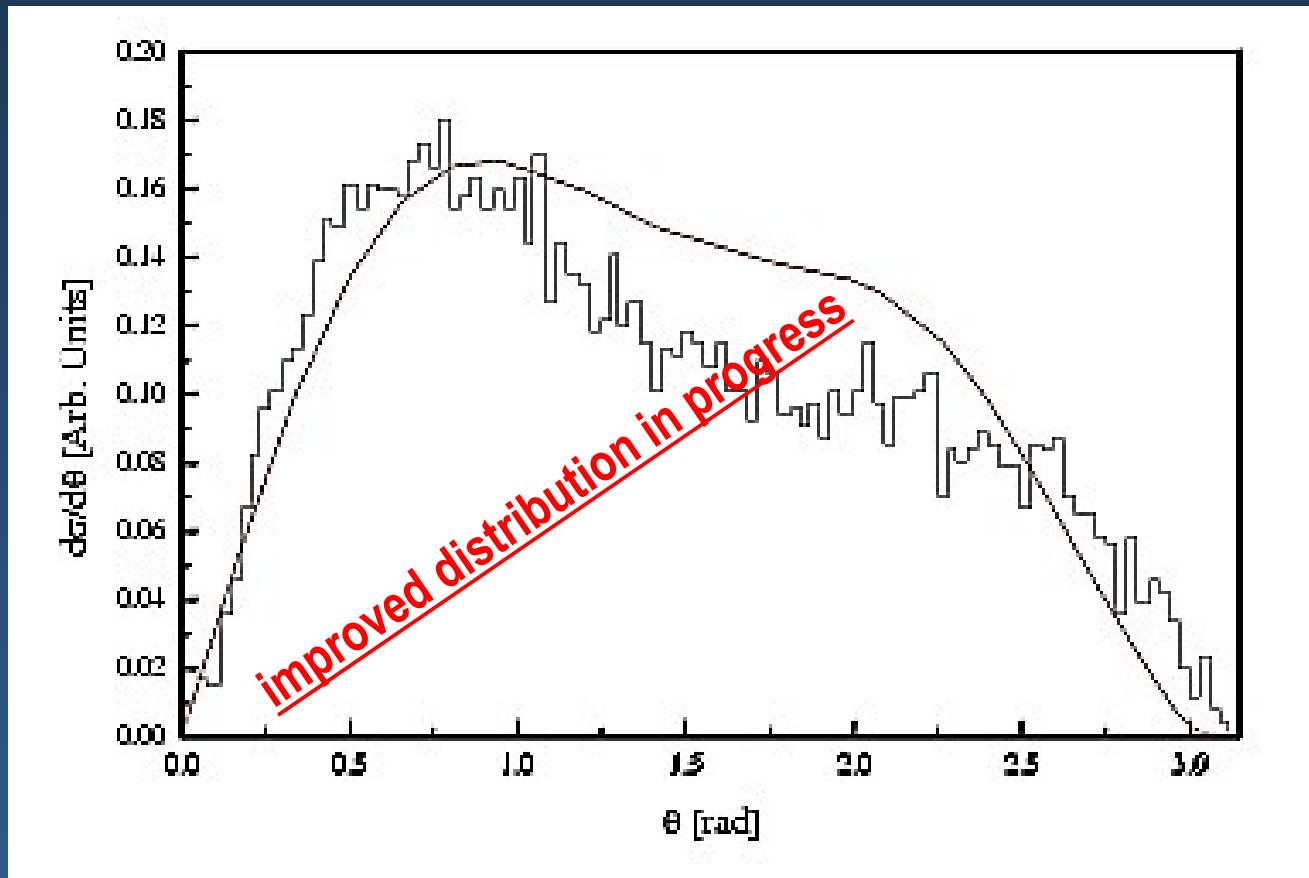
This test will be introduced into the Test & Analysis project for a systematic verification

Photon attenuation: Geant4 vs. NIST data

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



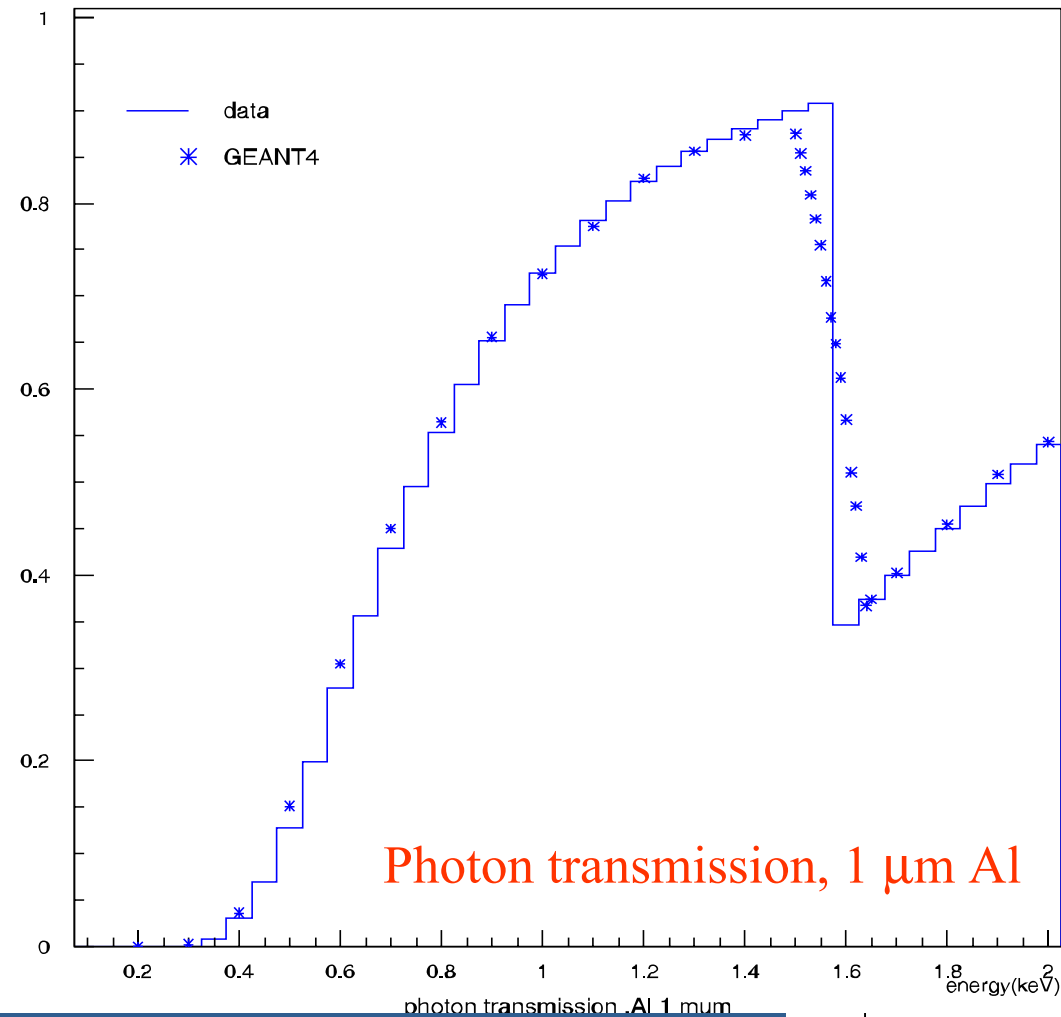
Photons: angular distributions



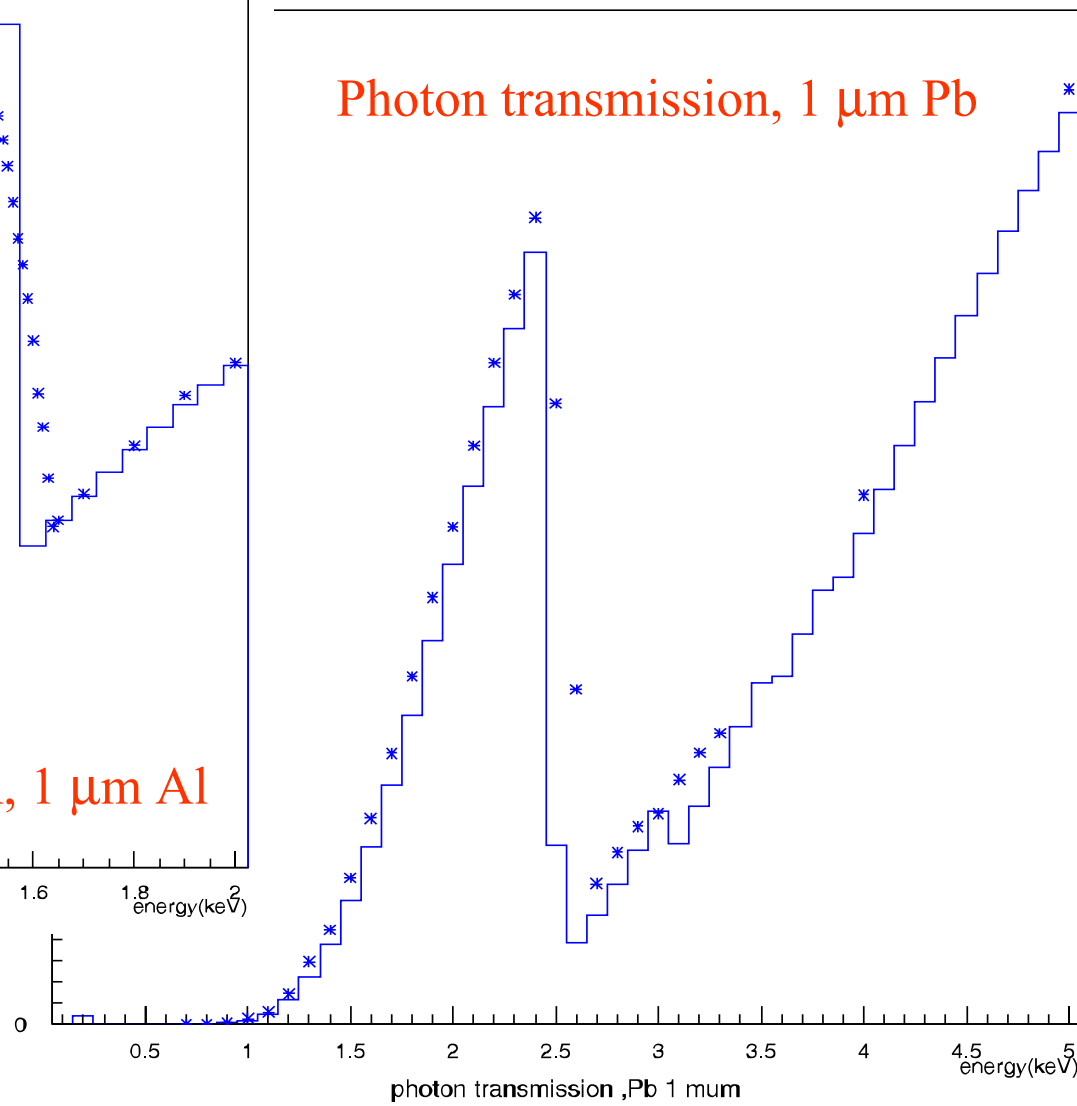
Rayleigh scattering: Geant4-LowE and expected distribution

Photons, evidence of shell effects

photon transmission , Al 1 micrometer



photon transmission , Pb 1 micrometer



Polarisation

Cross section:

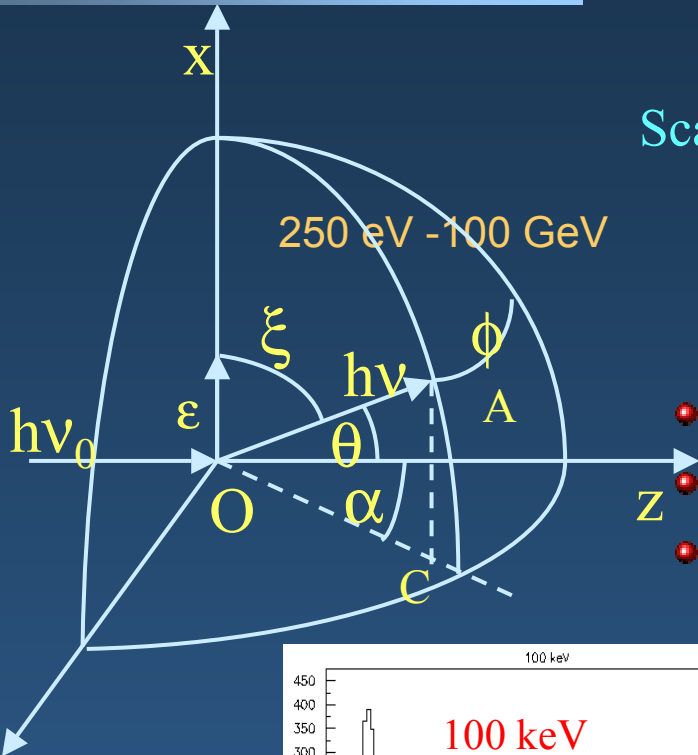
$$\frac{d\sigma}{d\Omega} = \frac{1}{2} r_0^2 \frac{h\nu^2}{h\nu_0^2} \left[\frac{h\nu_0}{h\nu} + \frac{h\nu}{h\nu_0} - 2 \sin^2 \theta \cos^2 \phi \right]$$

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

Scattered Photon Polarization

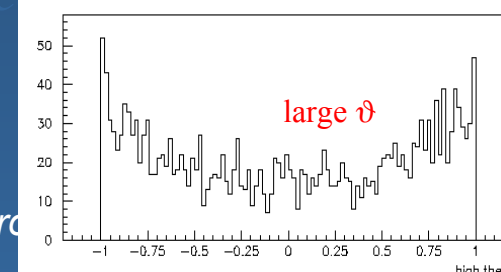
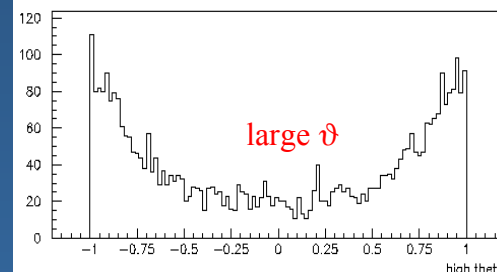
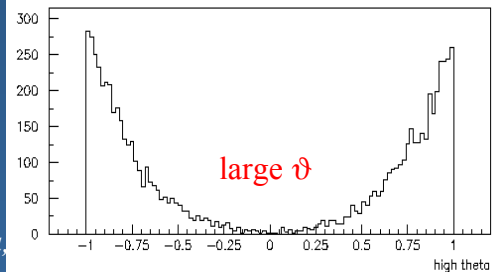
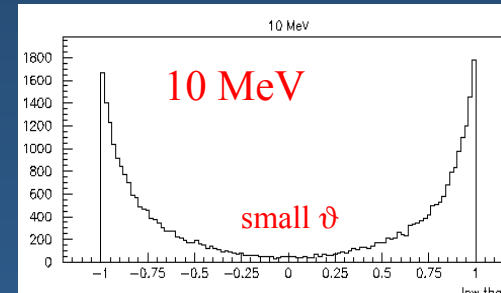
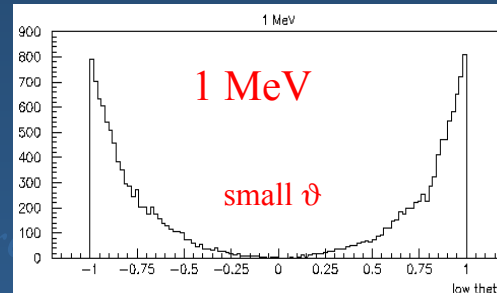
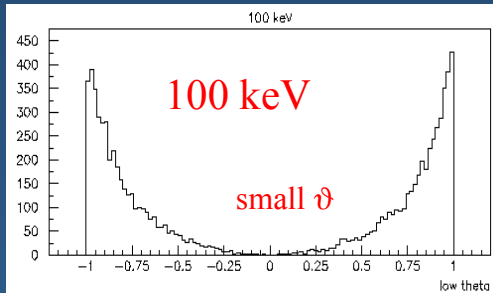
$$\overline{\epsilon}'_{\perp} = \frac{1}{N} (\cos \theta \hat{j} - \sin \theta \sin \phi \hat{k}) \sin \beta$$

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

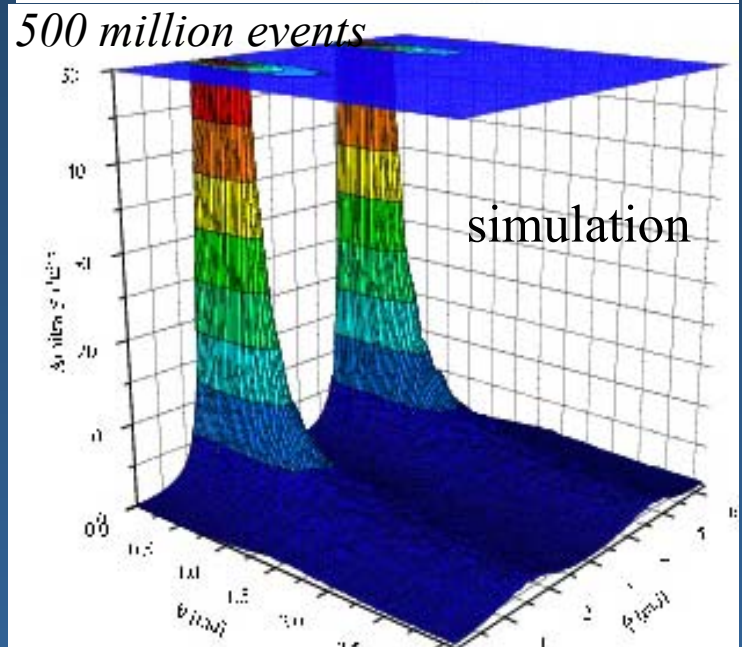
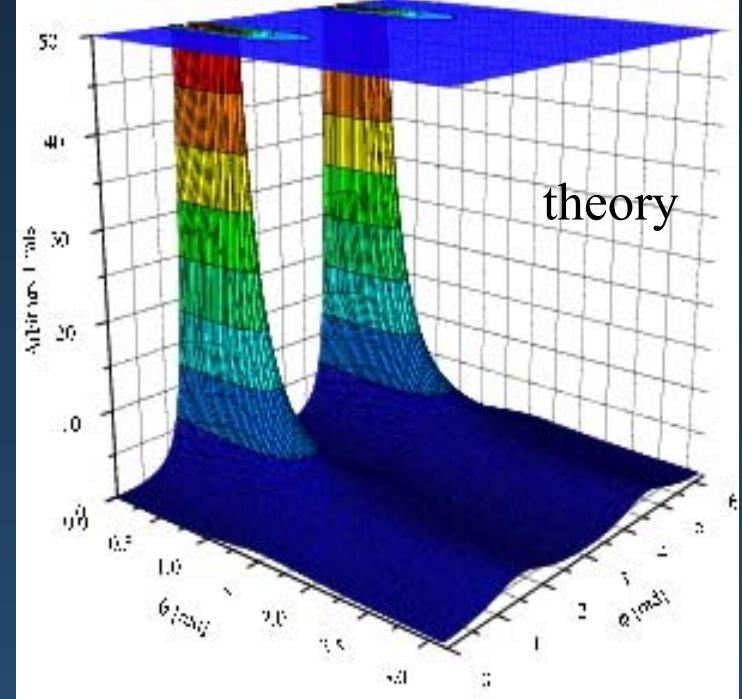
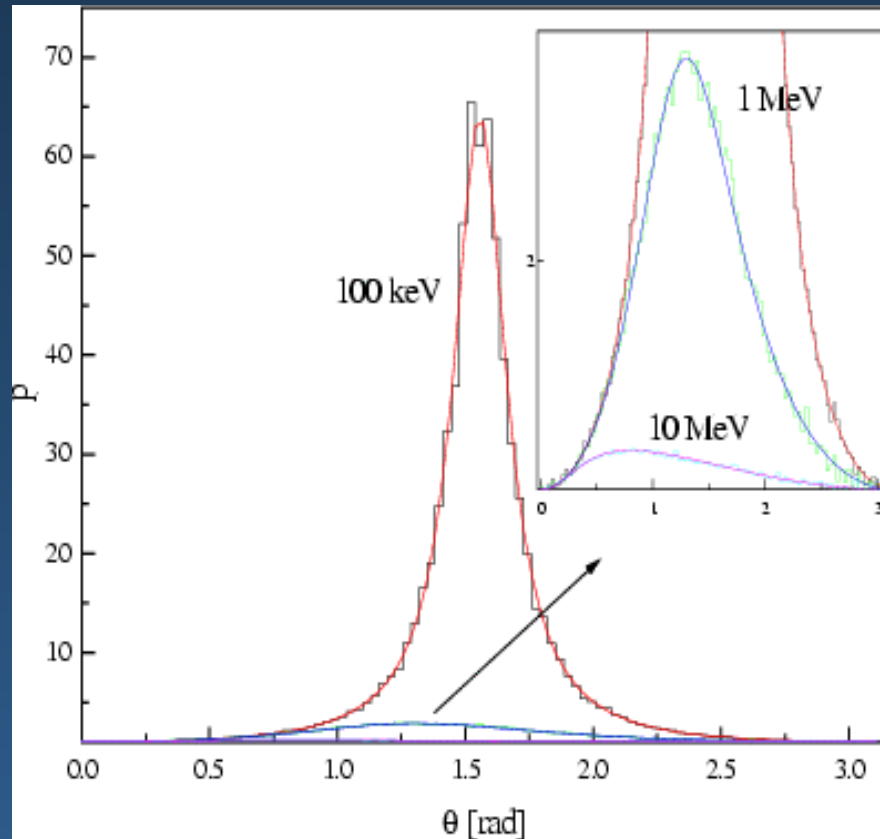


- θ Polar angle
- ϕ Azimuthal angle
- ϵ Polarization vector

Low Energy Polarised Compton



Polarisation

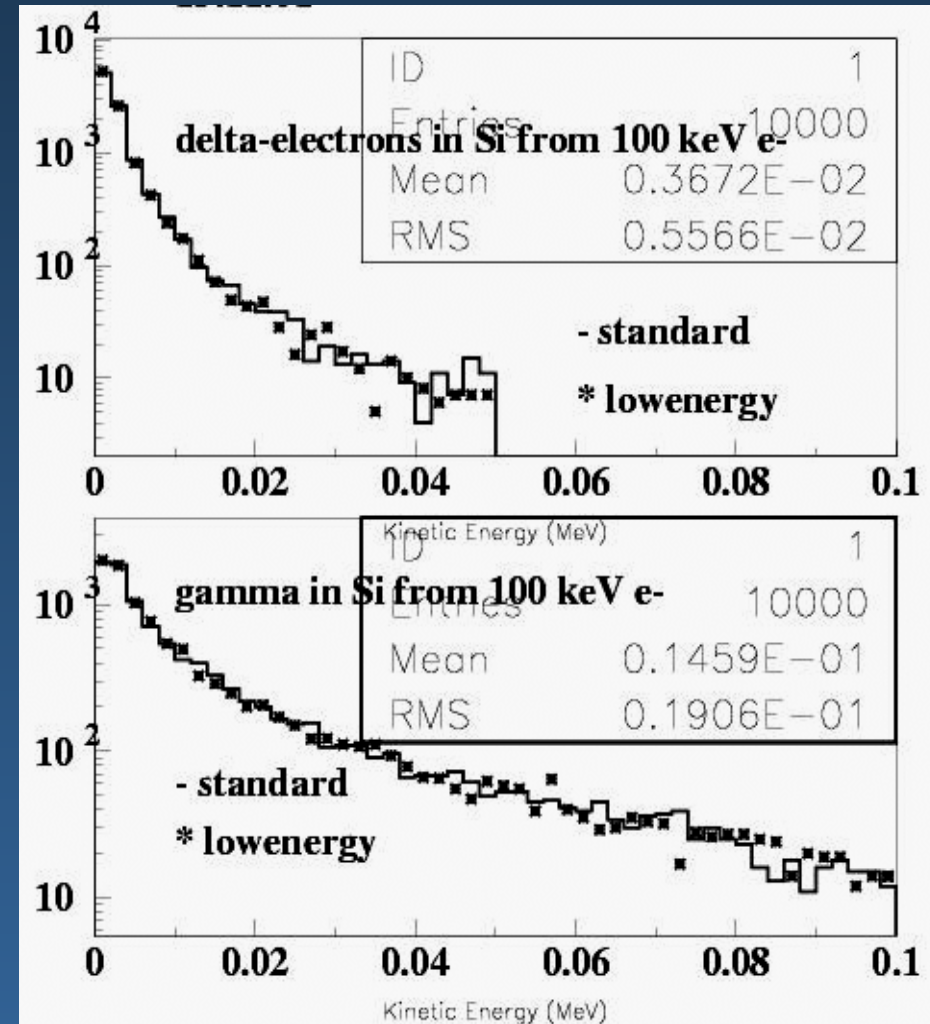


Polarisation of a non-polarised photon beam, simulation and theory

Ratio between intensity with perpendicular and parallel polarisation vector w.r.t. scattering plane, linearly polarised photons

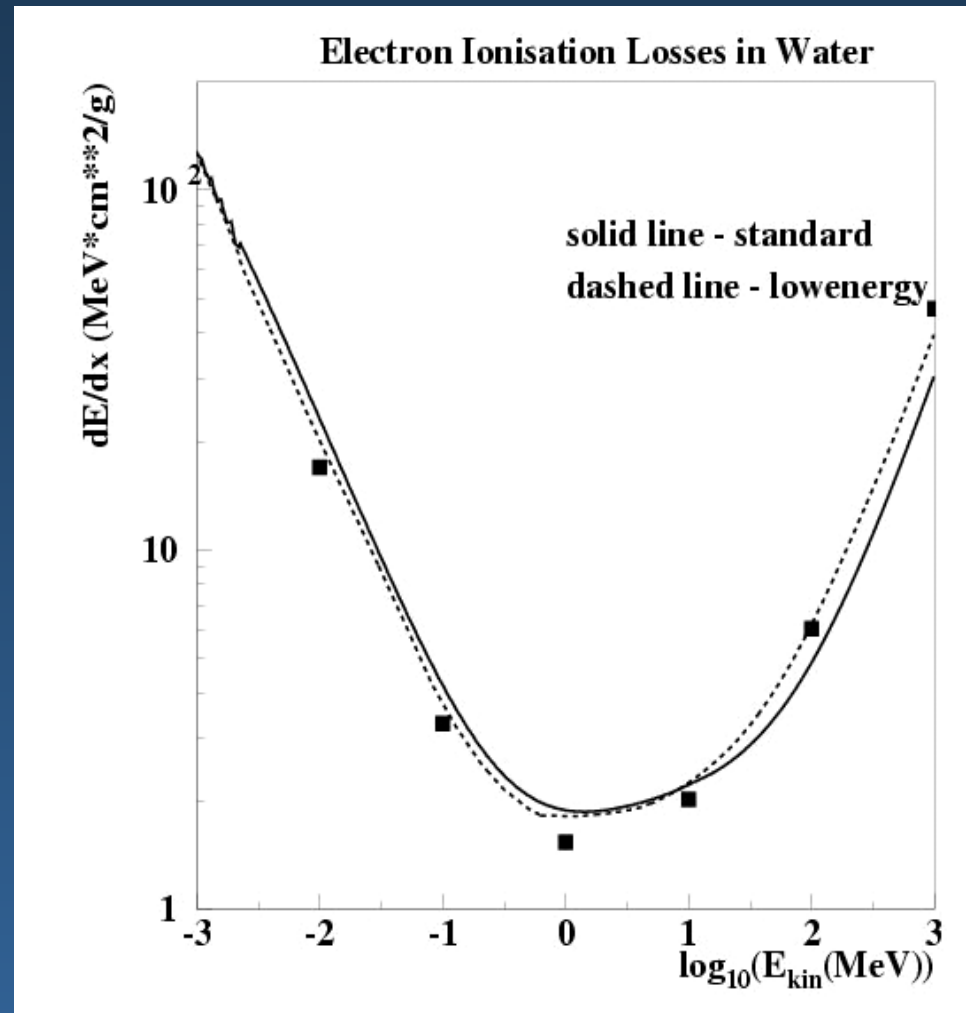
Electron Bremsstrahlung

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



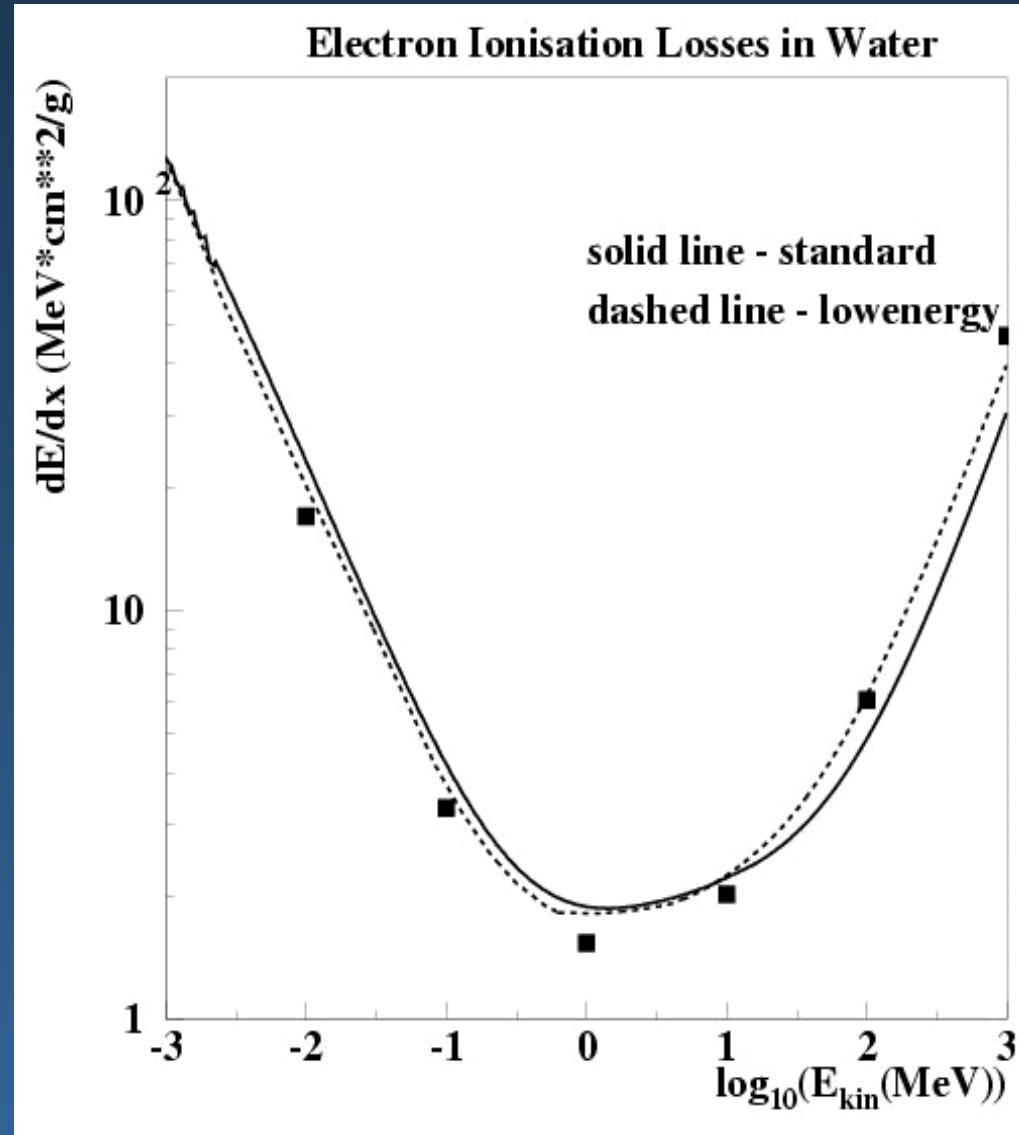
Electron ionisation

- 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
- Work in progress to improve the parameterisation and the performance



Electron ionisation

- New parameterisations of EEDL data library recently released
 - precision is now better than 5 % for ~ 50% of the shells, poorer for the 50% left
- Plans
 - Systematic verification over shell, Z and energy
 - Need Test & Analysis Project for automated verification (*all shells, 99 elements!*)

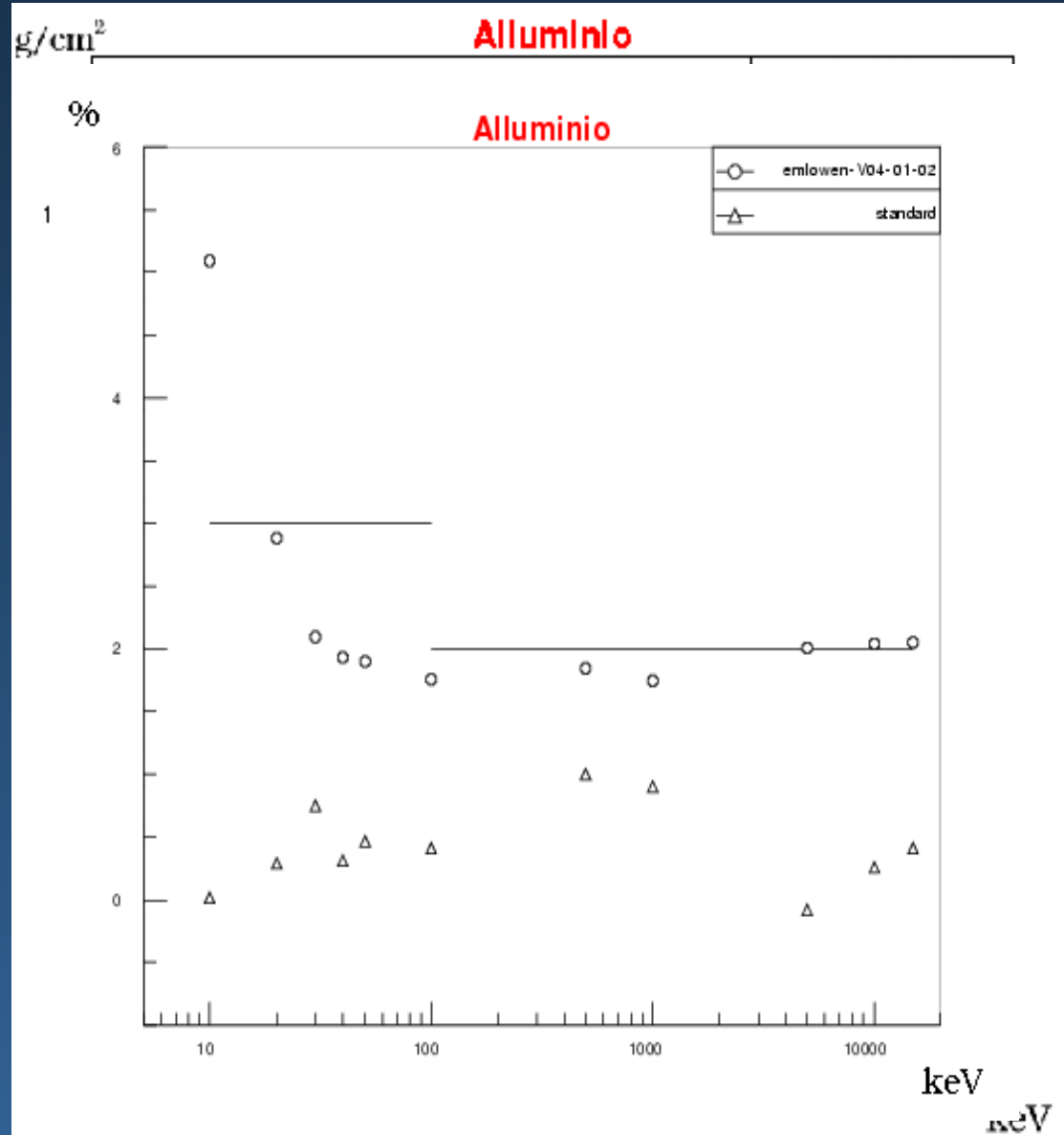


Electrons: range

Range in various simple and composite materials

Compared to NIST database

Also Be, Fe, Au, Pb, Ur, air, water, bone, muscle, soft tissue

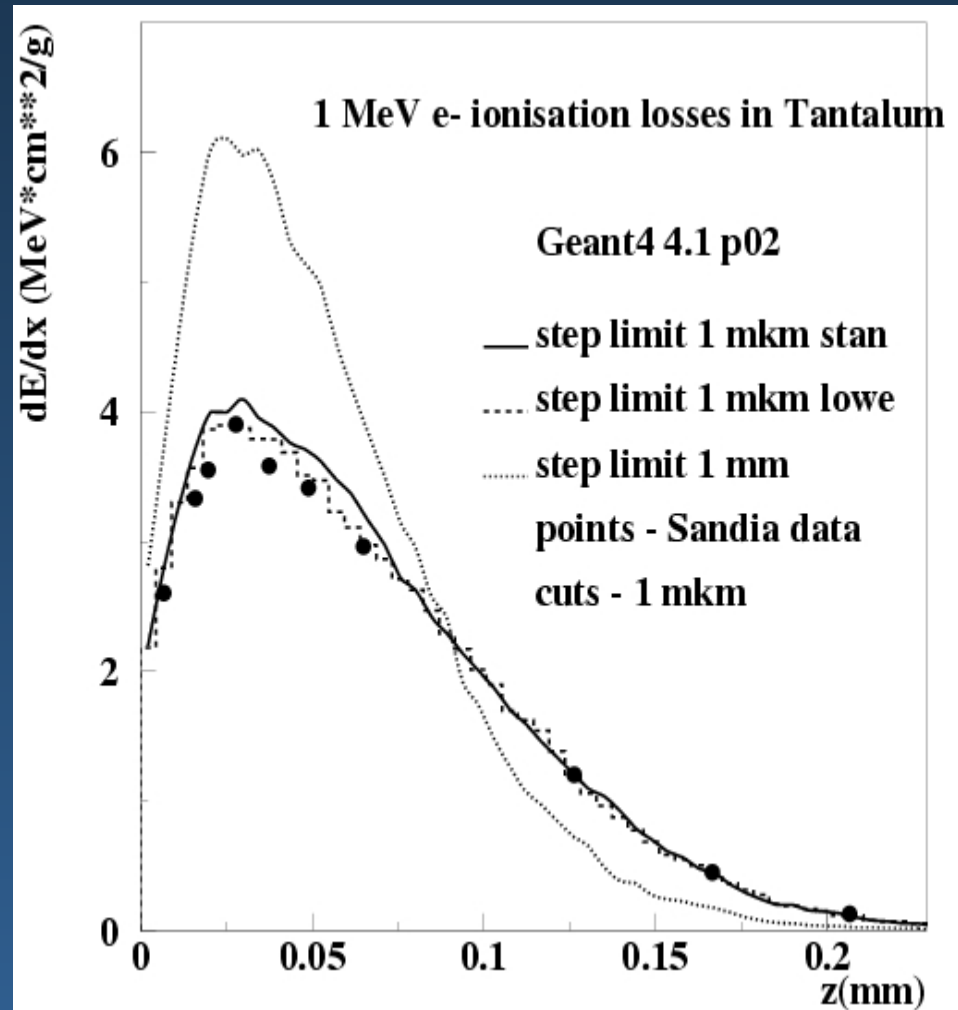


Electrons: dE/dx

Ionisation energy loss in various materials

Compared to Sandia database

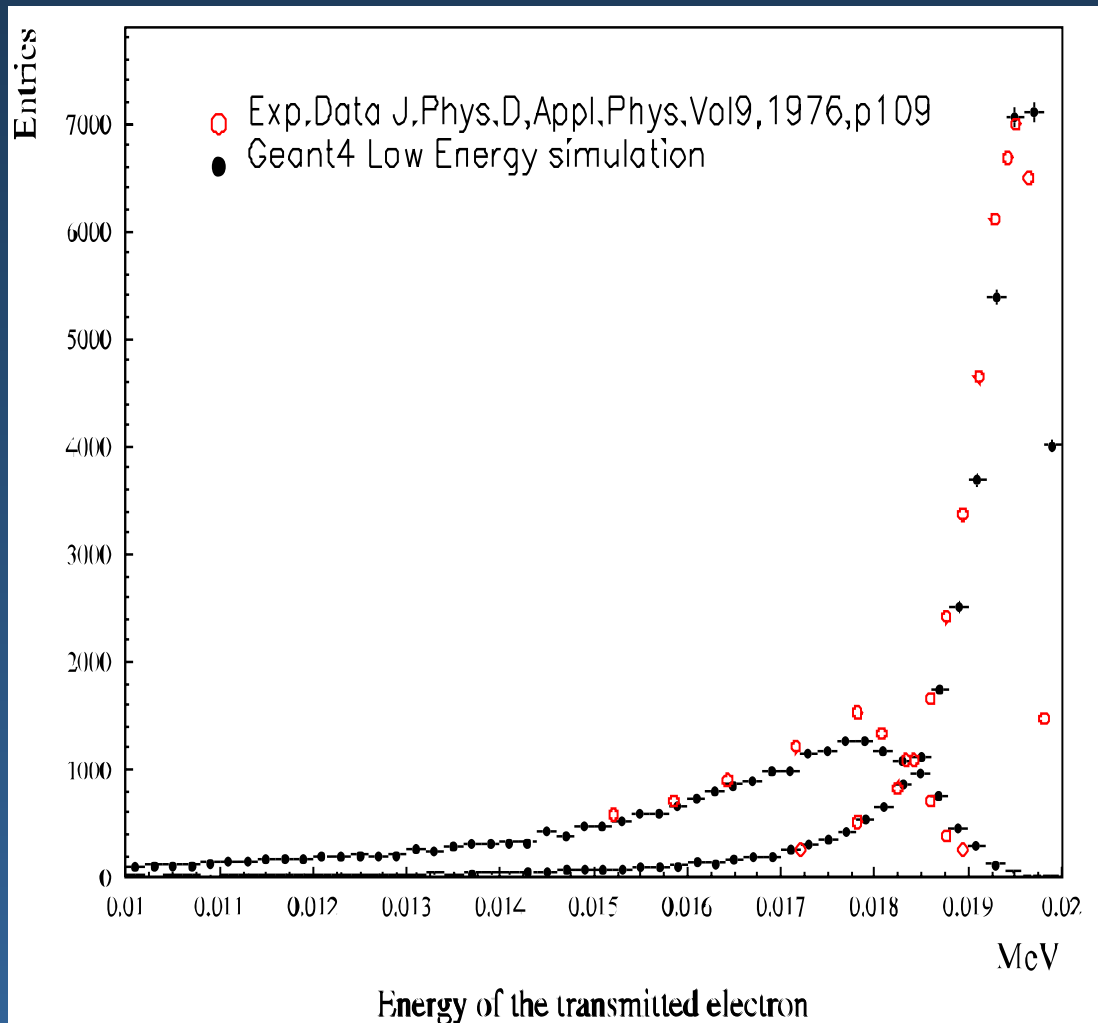
More systematic verification planned (for publication)



Also Fe, Ur

Electrons, transmitted

20 keV electrons, 0.32 and 1.04 μm Al



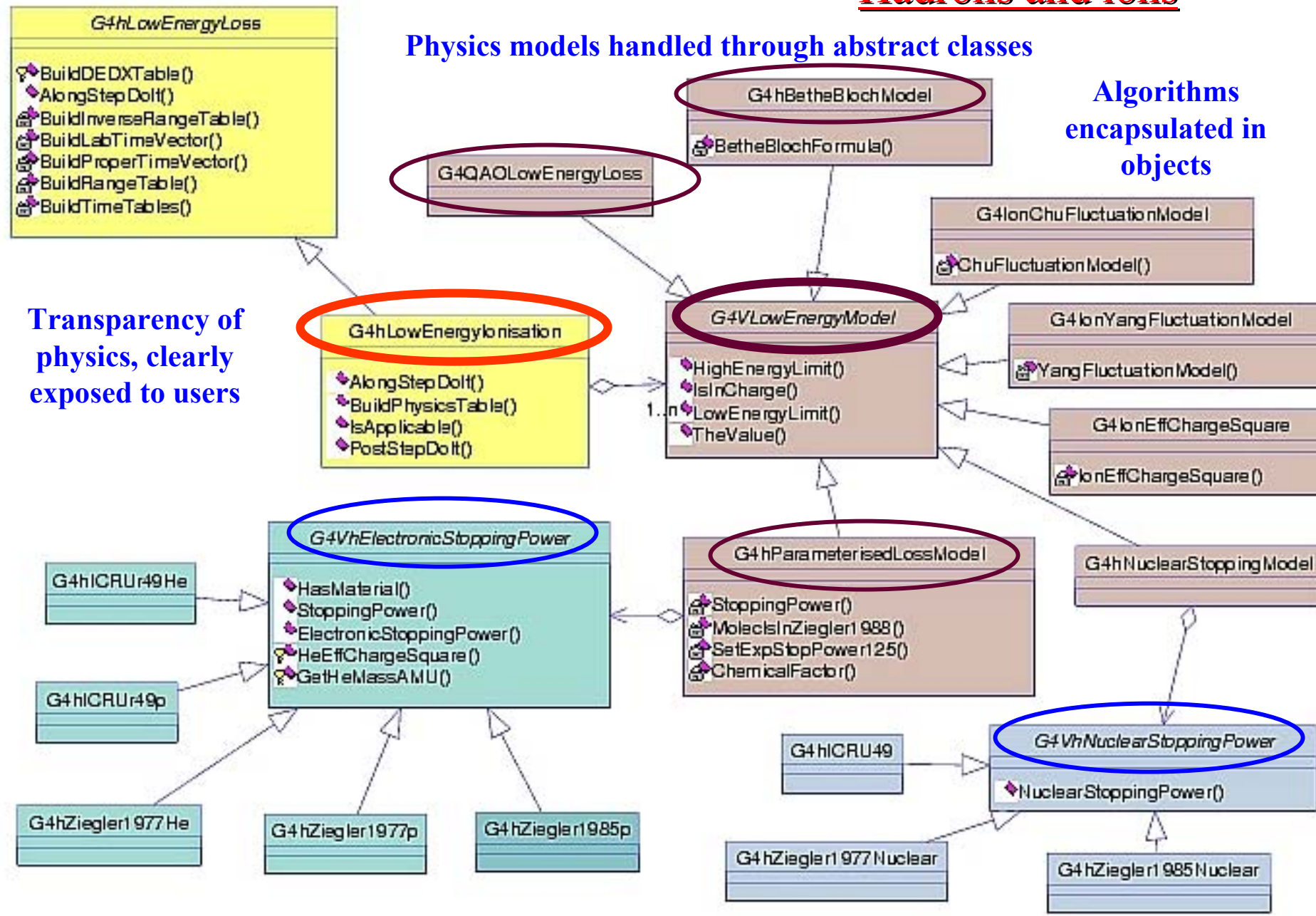
Hadrons and ions

- 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



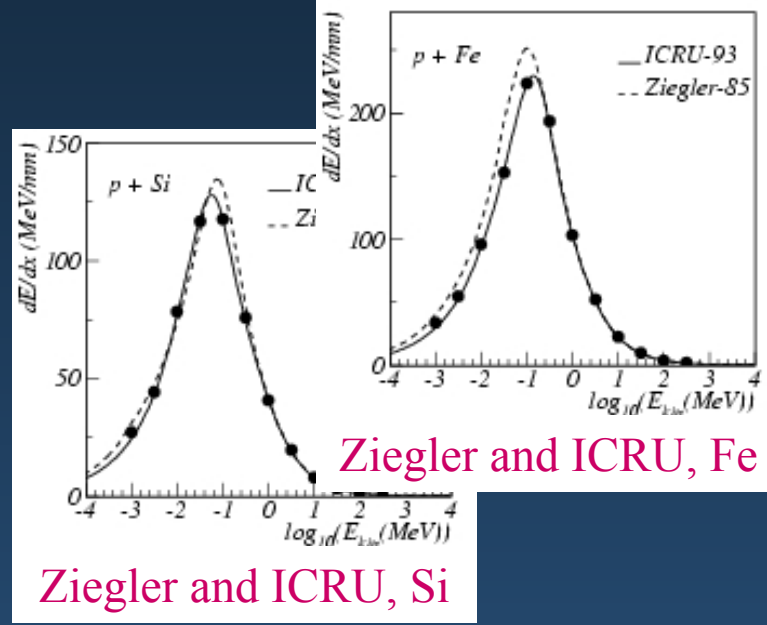
Transparency of physics, clearly exposed to users

Interchangeable and transparent access to data sets

Positive charged hadrons

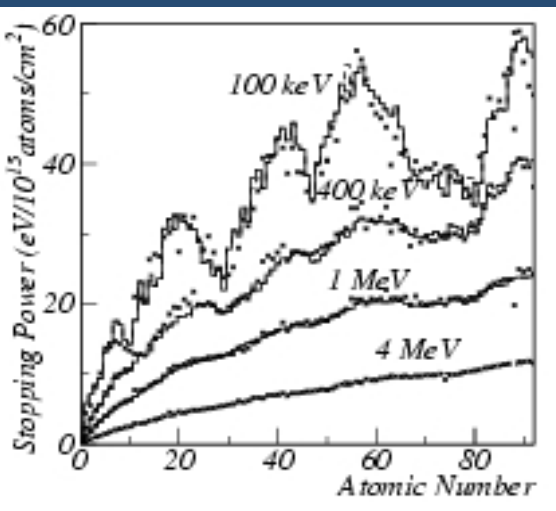
- Bethe-Bloch model of energy loss, $E > 2$ MeV
- 5 parameterisation models, $E < 2$ MeV
 - based on Ziegler and ICRU reviews
- 3 models of energy loss fluctuations

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

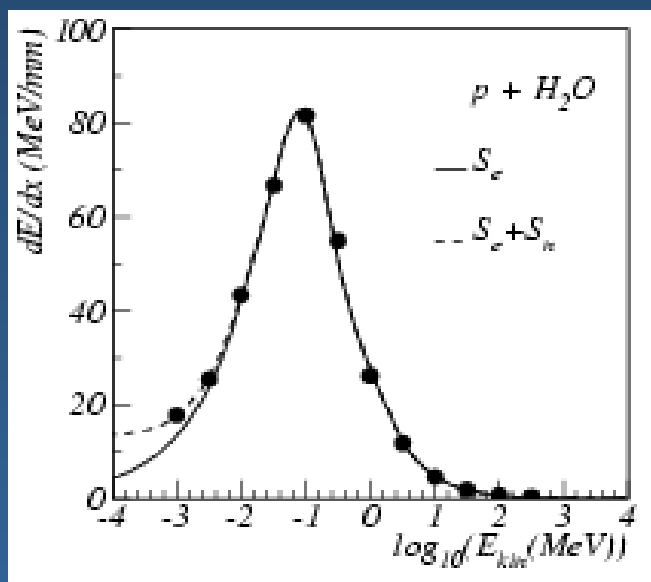
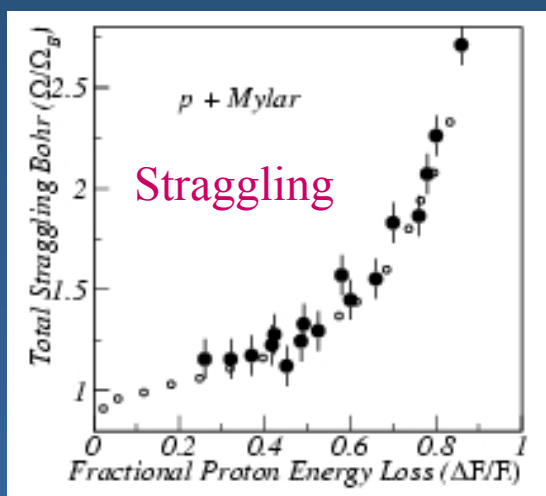


- Spin dependent term
- Barkas and Bloch terms

- Chemical effect for compounds
- Nuclear stopping power
- PIXE included (*preliminary*)

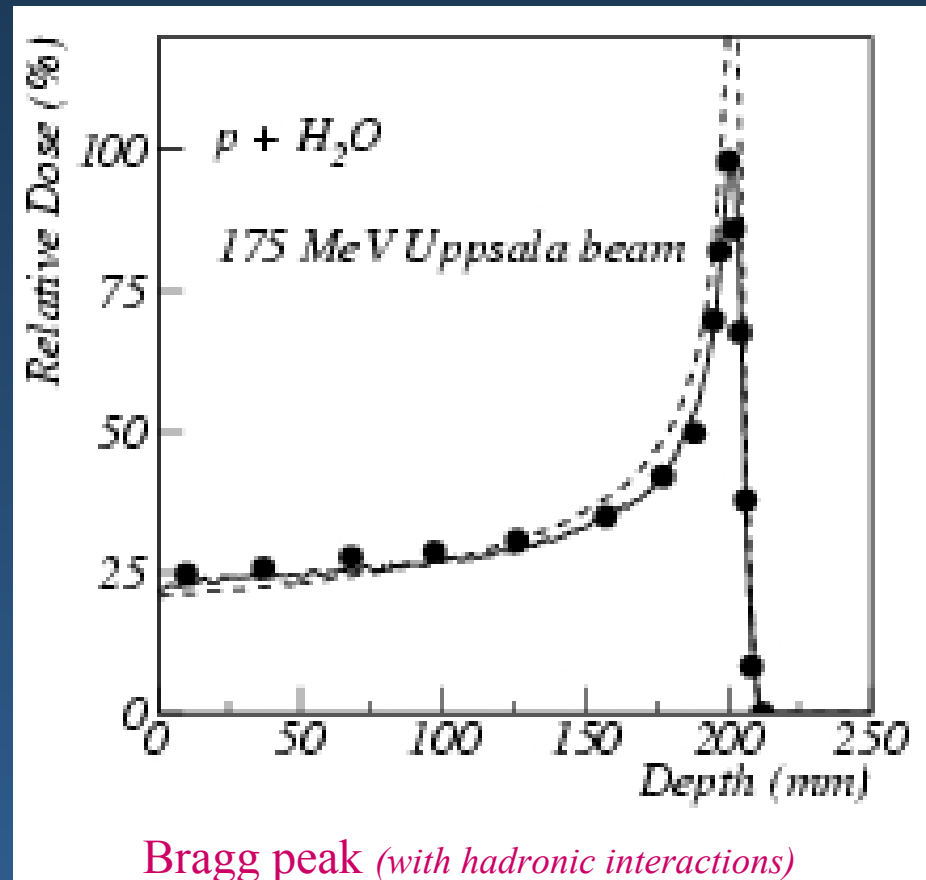


Stopping power
Z dependence for various energies
Ziegler and ICRU models



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



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
- $\beta < 0.01$: Free Electron Gas Model

- Effective charge model
- Nuclear stopping power

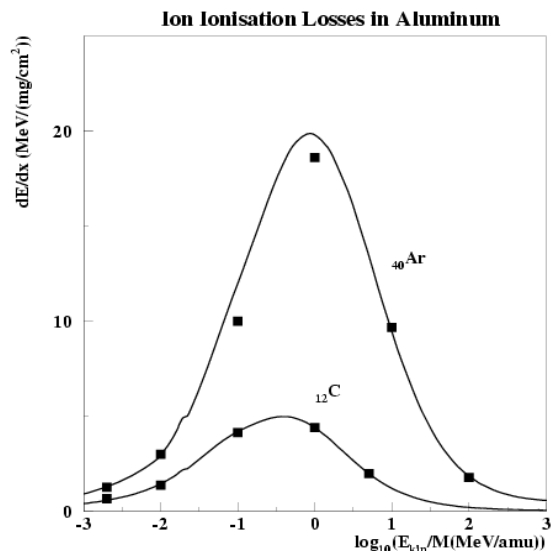
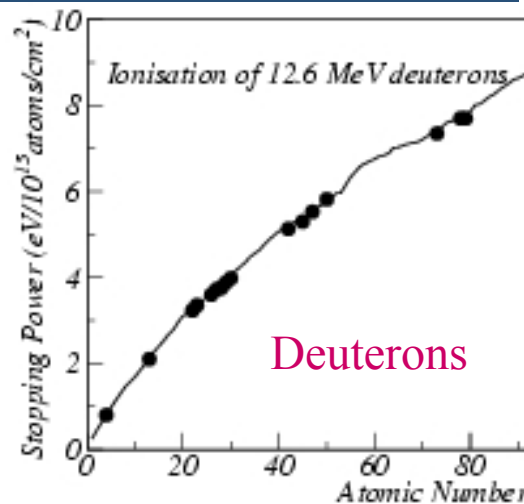
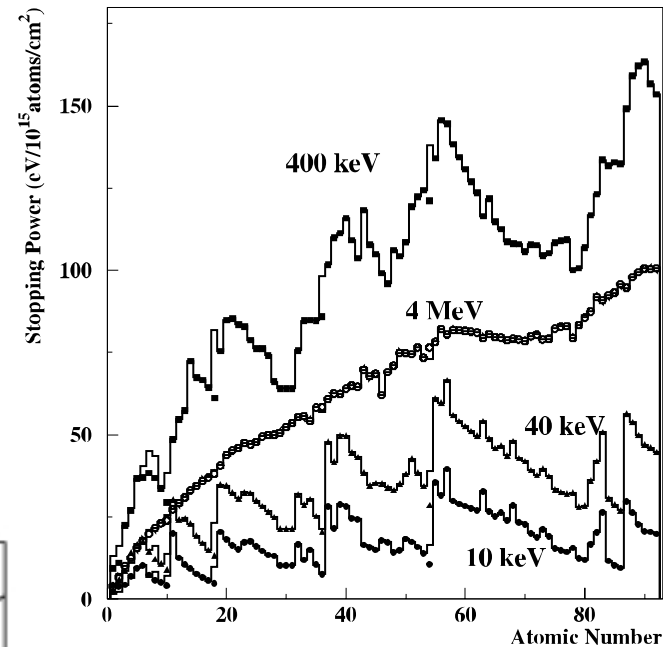


Figure 9: Ion electronic stopping power in aluminum. Points - the best fit to the data from Ref.[12], solid line - GEANT4 parameterisation. The accuracy of the data is about 5 %.



He⁴ Ionisation Parametrisation in GEANT4



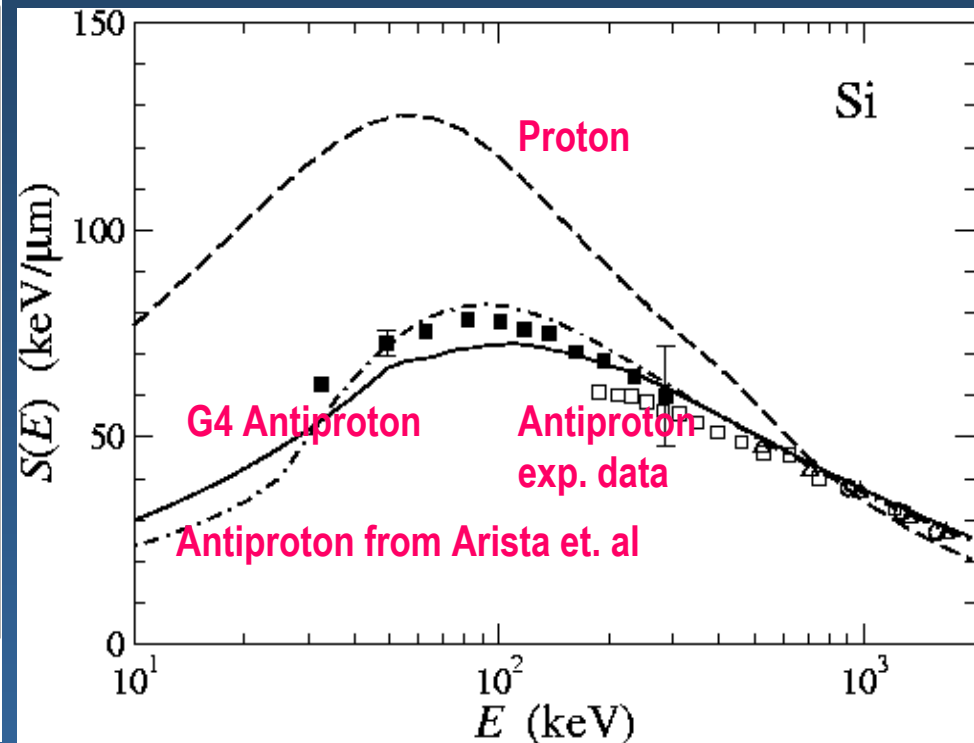
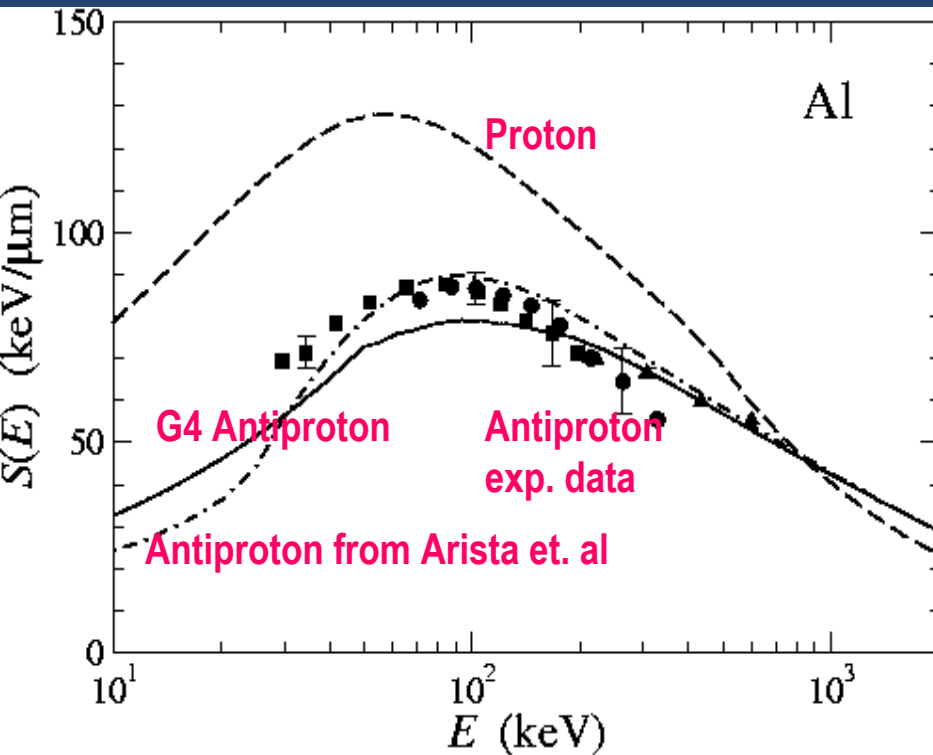
Models for antiprotons

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

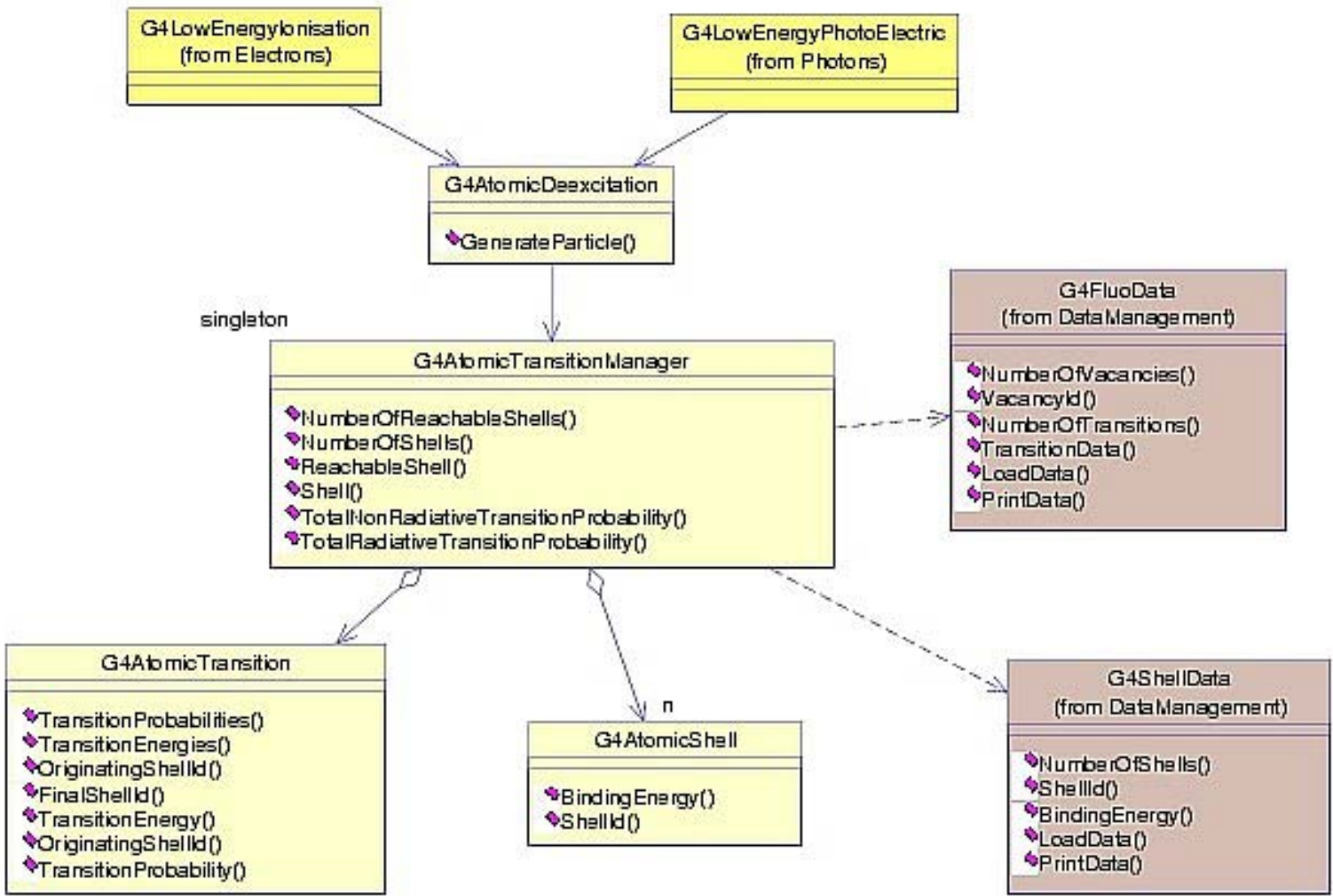
Bethe-Bloch formula

Quantum harmonic oscillator model

Free electron gas model



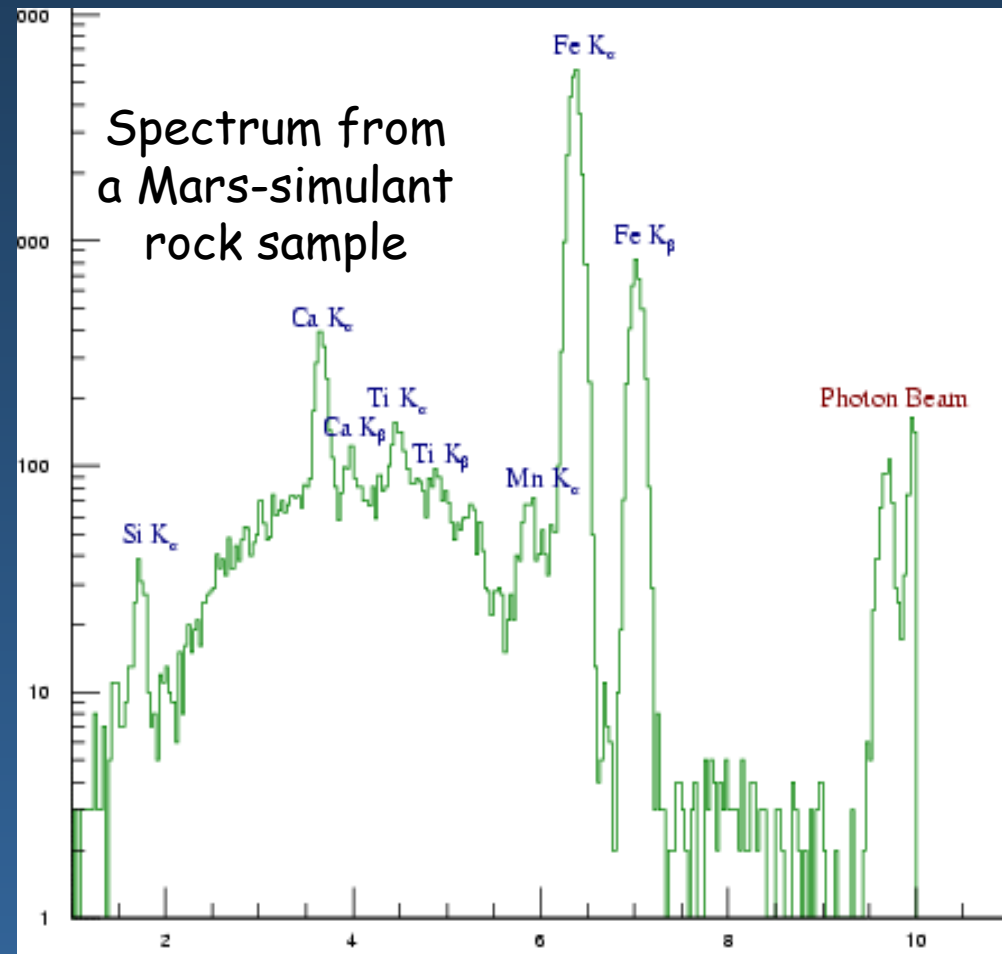
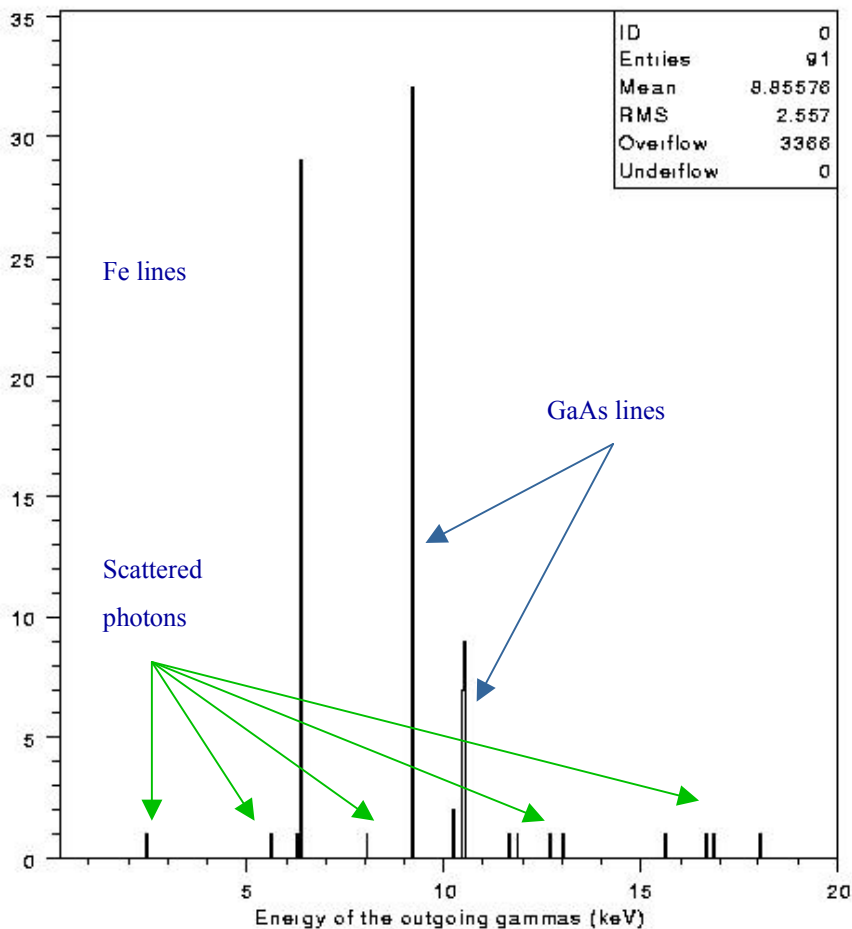
Atomic relaxation



Fluorescence

Microscopic validation:
against reference data

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



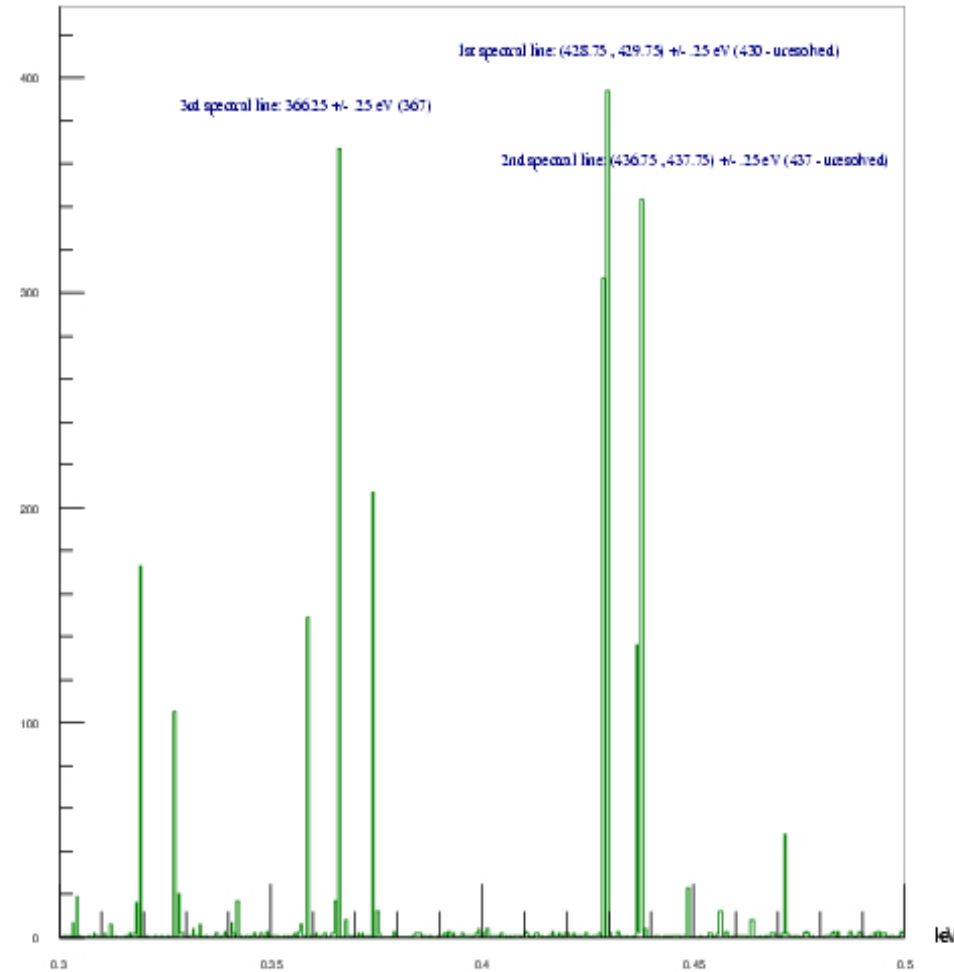
Auger effect

New implementation,
validation in progress

Auger electron emission
from various materials

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

Electron emission from Sn - 3 KeV photon Beam



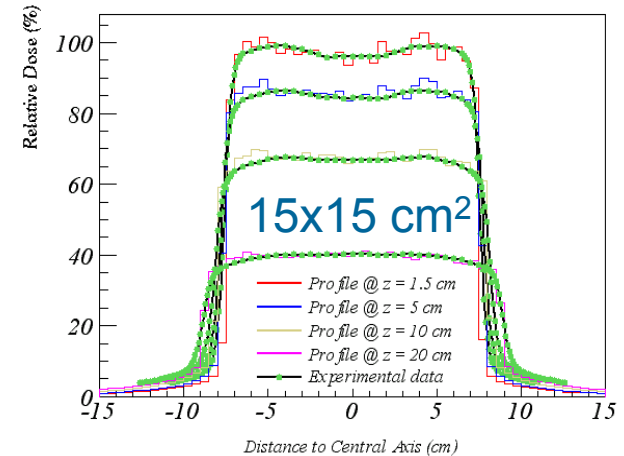
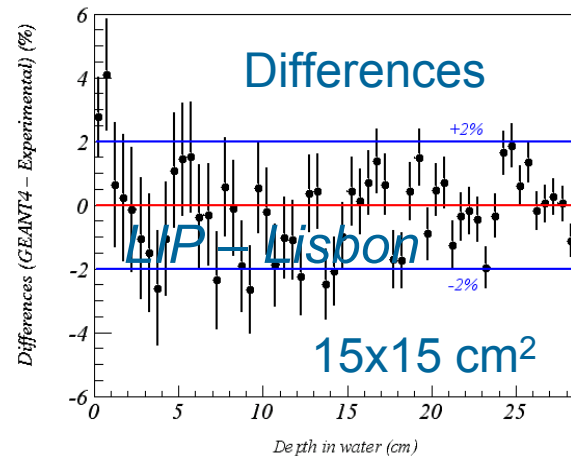
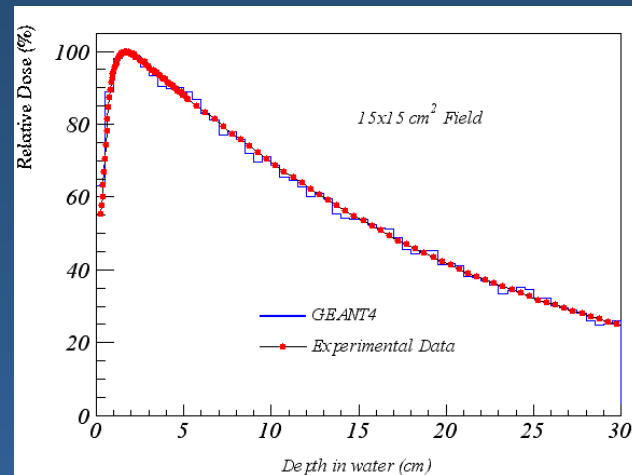
Contribution from users

- Many valuable contributions to the validation of LowE physics from users all over the world
 - excellent relationship with our user community
- User comparisons with data usually involve the effect of several physics processes of the LowE package
 - sometimes combining LowE + Standard e.m. processes
- A small sample in the next slides
 - no time to show all!

Homogeneous Phantom

P. Rodrigues, A. Trindade, L.Peralta, J. Varela, LIP

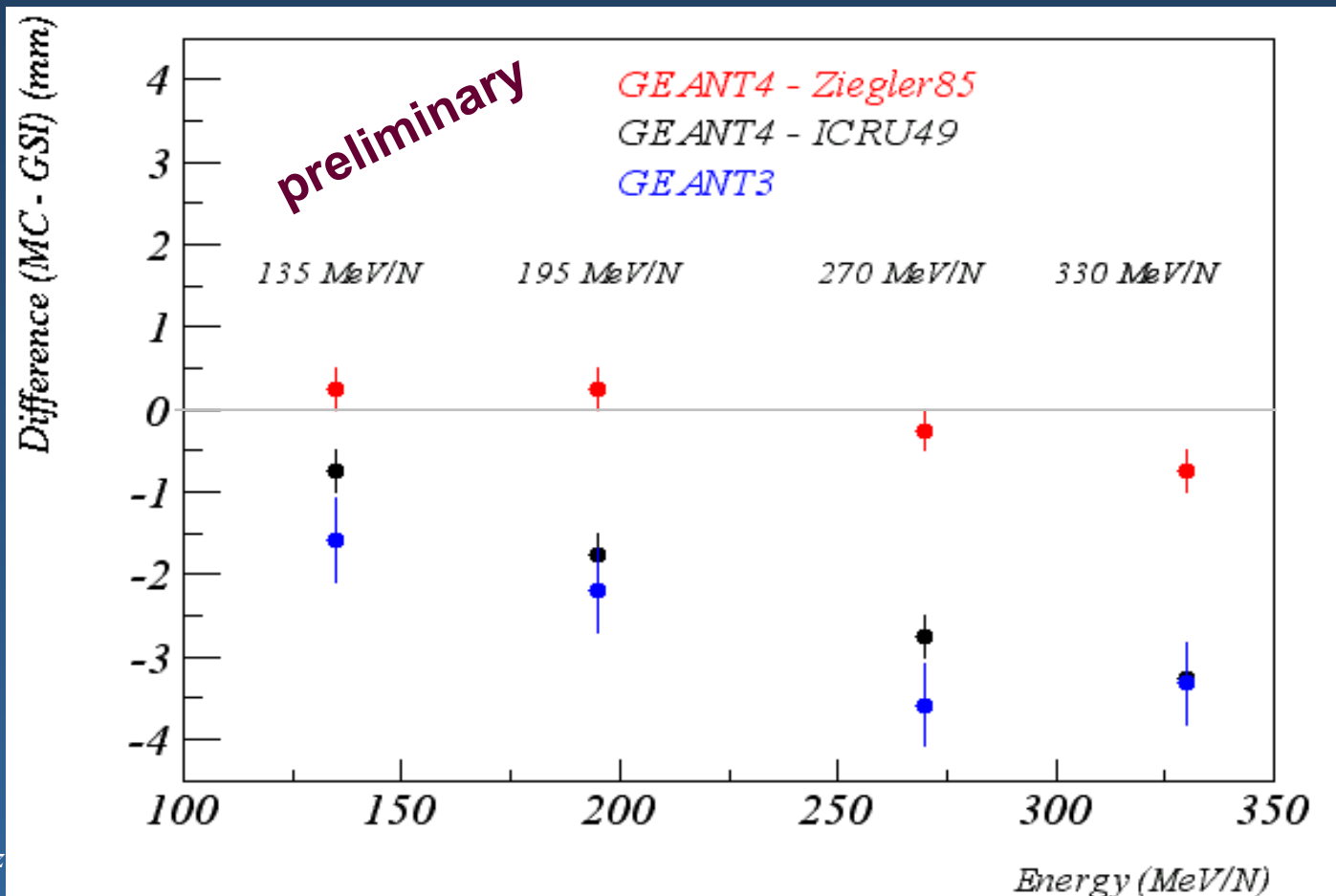
- Simulation of photon beams produced by a Siemens Mevatron KD2 clinical linear accelerator
- Phase-space distributions interface with GEANT4
- Validation against experimental data: depth dose and profile curves



Dose Calculations with ^{12}C

P. Rodrigues, A. Trindade, L.Peralta, J. Varela, LIP

- Bragg peak localization calculated with GEANT4 (stopping powers from ICRU49 and Ziegler85) and GEANT3 in a water phantom
- Comparison with GSI data



Uranium irradiated by electron beam

Jean-Francois Carrier, Louis Archambault, Rene Roy and Luc Beaulieu

Service de radio-oncologie, Hotel-Dieu de Quebec, Quebec, Canada
Departement de physique, Universite Laval, Quebec, Canada

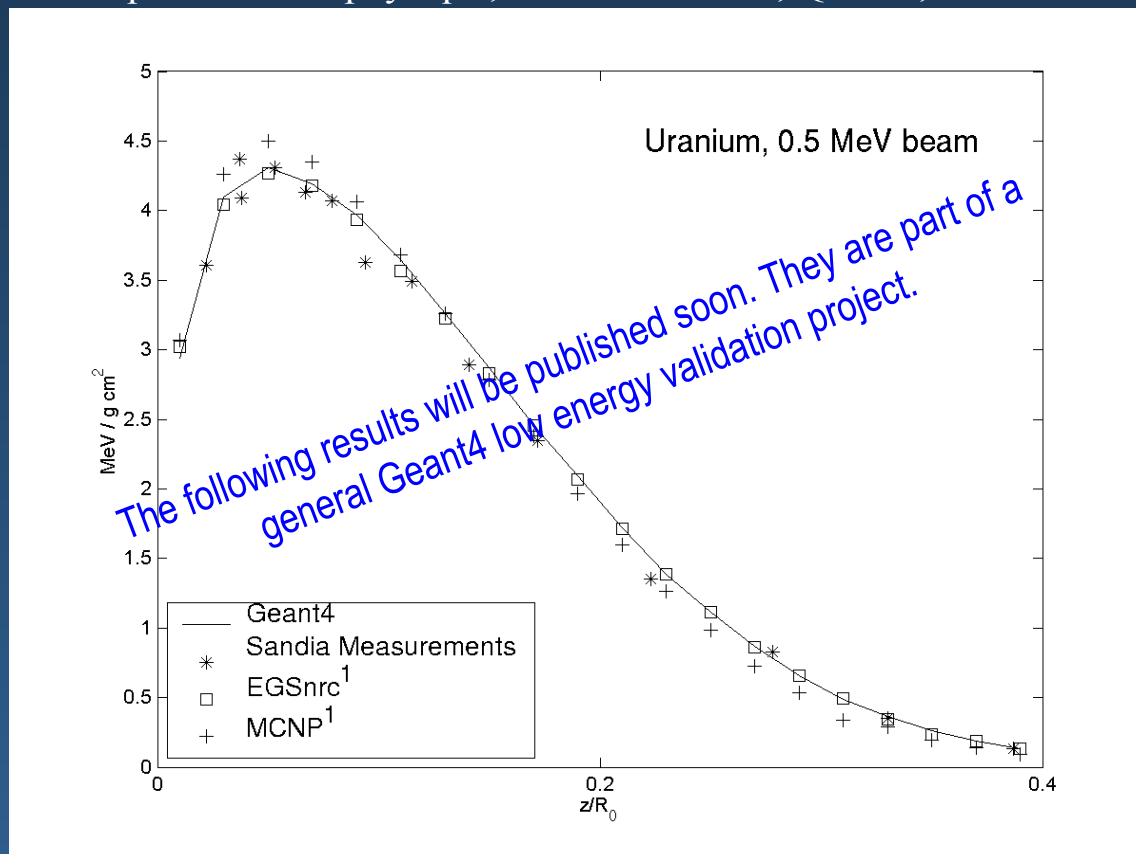
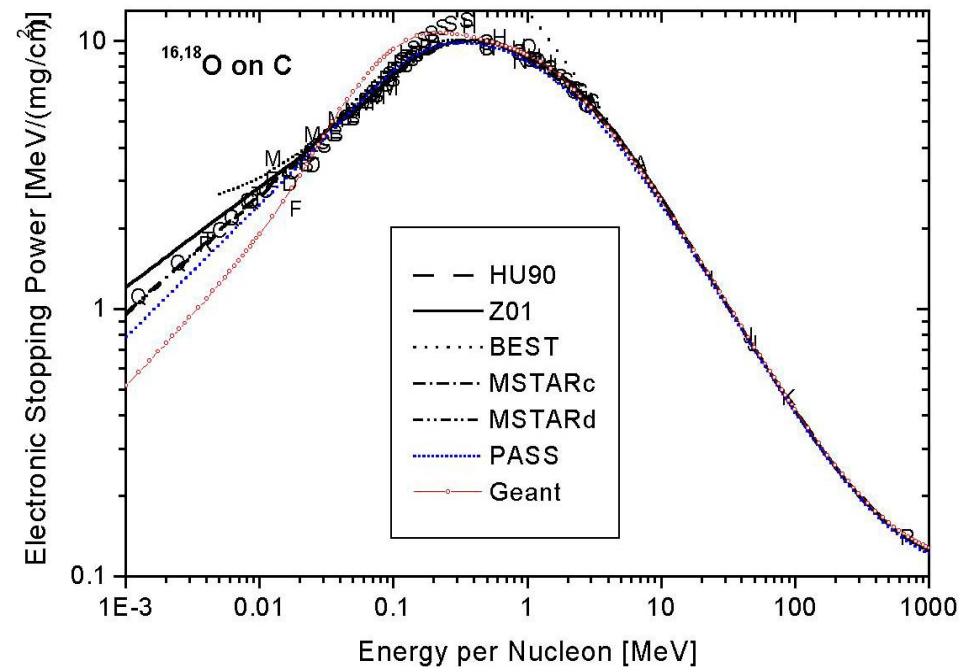
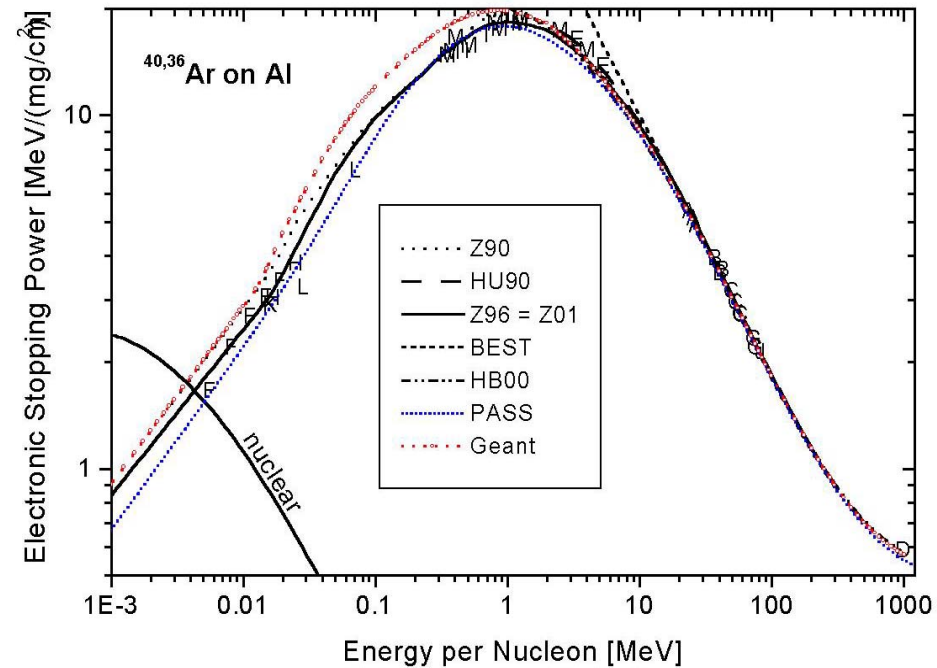


Fig 1. Depth-dose curve for a semi-infinite uranium slab irradiated by a 0.5 MeV broad parallel electron beam

Ions

Independent validation at
Univ. of Linz (H. Paul et al.)

Geant4-LowE reproduces the right
side of the distribution precisely,
but about 10-20% discrepancy is
observed at lower energies



To learn more

- Geant4 Physics Reference Manual
- Application Developer Guide
- User Forum: Electromagnetic

<http://www.ge.infn.it/geant4/lowE>

- Next lecture:
 - How to use Geant4 LowE electromagnetic processes
 - A guided tour of some examples
 - A selection of real-life applications