Stéphane Chauvie
Pablo Cirrone
Giacomo Cuttone
Francesco Di Rosa
Susanna Guatelli
Sébastien Incerti
Anton Lechner (new)
Alfonso Mantero
Barbara Mascialino
Petteri Nieminen
Luciano Pandola
Sandra Parlati
Andreas Pfeiffer
MG Pia
Pedro Rodrigues
Giorgio Russo
Andreia Trindade
Paolo Viarengo
Valentina Zampichelli

Geant4 Low Energy Electromagnetic Physics

Maria Grazia Pia
On behalf of the LowE EM Working Group

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

Geant4 Japan-Taiwan Symposium
KEK, 12-15 December 2006

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
  - "very low" energy extensions in progress (eV scale)

- A set of processes based on detailed models
  - shell structure of the atom
  - precise angular distributions

- Complementary to the "standard" electromagnetic package
  - …but the Geant4 standard electromagnetic package recently copied various models from the LowE package
  - it would be fair to credit the original ideas and WG where they originated…

Vision

Driven by

User Requirements

+

Our own scientific background

Physics Modeling

High precision
Collaboration with theorists

Physics Validation

Rigorous method, quantitative

Technology

Advanced software technology
at the service of physics

Software process

For **quality**
For **productivity**
For **maintainability**

Analysis & Design

Transparency
Openness
Maintainability

Synergy with Advanced Examples

Experimental investigation
Requirements
Feedback

People

Internal training
Investment in the young
Geant4 generation

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

- In progress
  - Precision models for specific components
  - Validation
  - Extensions to the eV scale

- 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 specific projects

Huge effort invested into SPI

- *started from level 1 (CMM)*
- *in very early stages: chaotic, left to heroic improvisation*

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)

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:

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

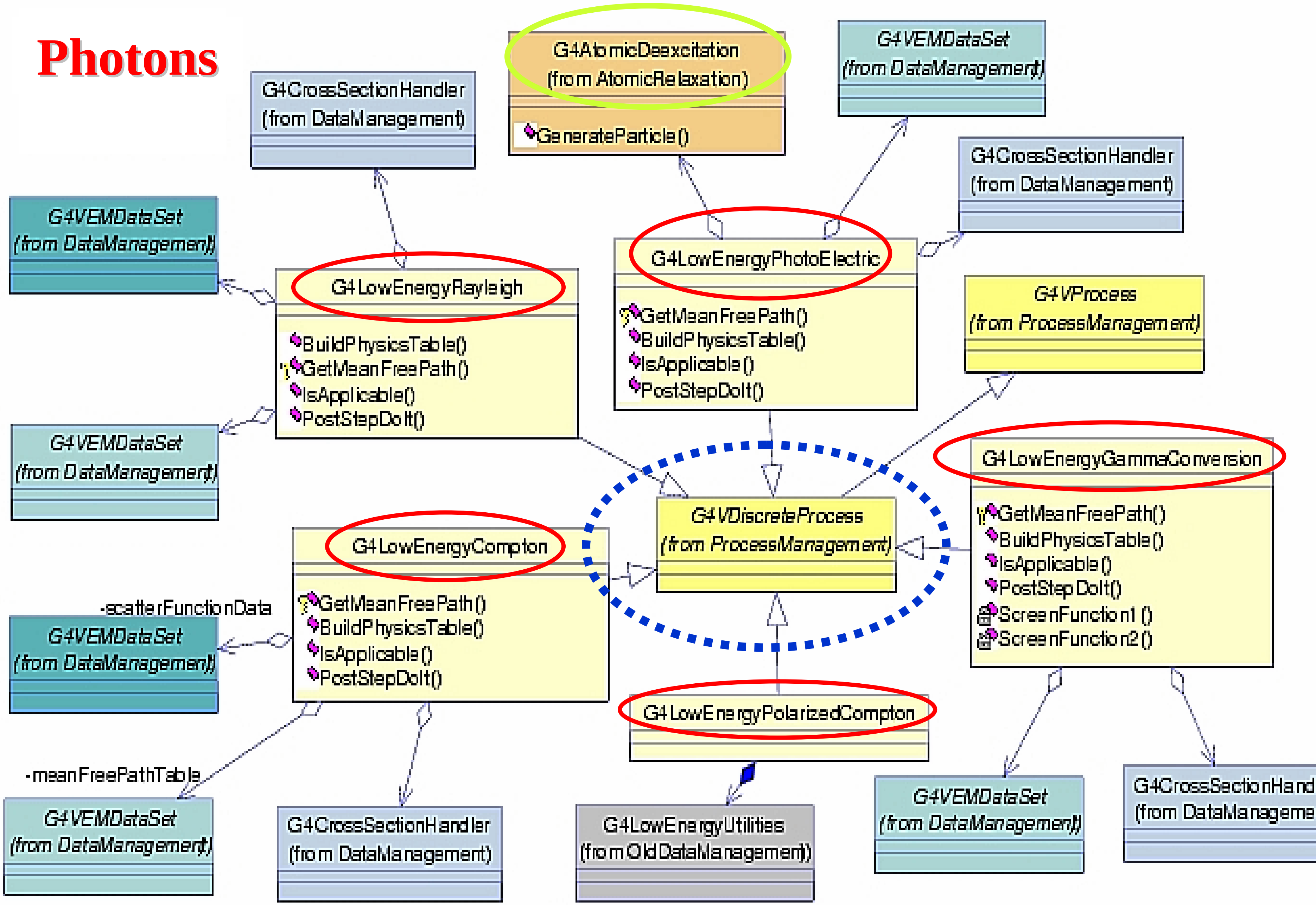
E_1 and E_2 are the lower and higher energy for which data (σ_1 and σ_2) are available

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



G4AtomicDeexcitation
(from AtomicRelaxation)
GenerateParticle()
G4CrossSectionHandler
(from DataManagement)
G4VEMDataSet
(from DataManagement)
G4CrossSectionHandler
(from DataManagement)
G4VEMDataSet
(from DataManagement)
G4LowEnergyRayleigh
BuildPhysicsTable()
GetMeanFreePath()
IsApplicable()
PostStepDoIt()
G4LowEnergyPhotoElectric
GetMeanFreePath()
BuildPhysicsTable()
IsApplicable()
PostStepDoIt()
G4VProcess
(from ProcessManagement)
G4VEMDataSet
(from DataManagement)
G4LowEnergyGammaConversion
GetMeanFreePath()
BuildPhysicsTable()
IsApplicable()
PostStepDoIt()
ScreenFunction1()
ScreenFunction2()
G4VDiscreteProcess
(from ProcessManagement)
G4LowEnergyCompton
GetMeanFreePath()
BuildPhysicsTable()
IsApplicable()
PostStepDoIt()
-scatterFunctionData
G4VEMDataSet
(from DataManagement)
G4LowEnergyPolarizedCompton
-meanFreePathTable
G4VEMDataSet
(from DataManagement)
G4CrossSectionHandler
(from DataManagement)
G4LowEnergyUtilities
(from OldDataManagement)
G4VEMDataSet
(from DataManagement)

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 recently released*

Photoelectric Angular Distributions

Geant4 LowE-EPDL *(until December 2005)* and **LowE-Penelope** processes

The incident photon is absorbed and one electron is emitted in the same direction as the primary photon

Geant4 Standard (*à la* GEANT3)

The polar angle of the photoelectron is sampled from an approximate Sauter-Gavrila cross-section (for K-shell)

PENELOPE

The polar angle is sampled from K-shell cross-section derived from Sauter

The same cross-section is used for other photoionization events

EGSnrc

Controlled by a master flag IPHTER

- IPHTER = 0 (similar to G4 LowE)
- IPHTER = 1 (Sauter distribution valid for K-shell)

Both assume that the azimuthal angle distribution is uniform (no polarization)

Photoelectric Angular Distribution

Sauter formalism is valid for **light-Z**, **K-shell photoelectrons** and **non-polarized** photons

New Geant4-LowE model:

use a more generalized approach based on Gavrila theory

Valid for **all-Z** elements, for photoelectrons emitted from **K and L shells** - also includes the effect of the **polarization** of the incident photon

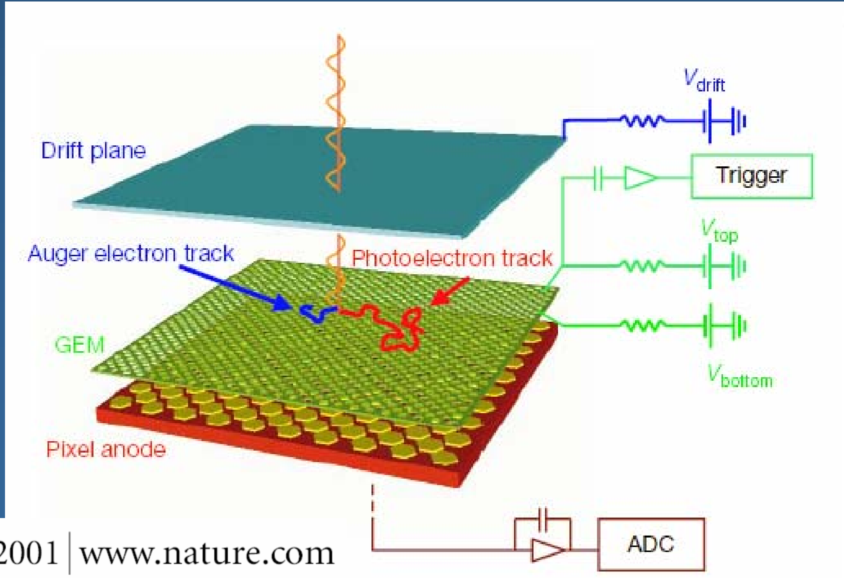
This enhancement is of significance importance for the design of experiments that aim to measure the polarization of X-rays emitted from black holes and neutron stars

letters to nature

An efficient photoelectric X-ray polarimeter for the study of black holes and neutron stars

Enrico Costa*, Paolo Soffitta*, Ronaldo Bellazzini†, Alessandro Brez†, Nicholas Lumb† & Gloria Spandre†

* *Istituto di Astrofisica Spaziale del CNR, Via Fosso del Cavaliere 100, 1-00133, Rome, Italy*
† *Istituto Nazionale di Fisica Nucleare-Sezione di Pisa, Via Livornese 1291, I-56010 San Piero a Grado, Pisa, Italy*



NATURE | VOL 411 | 7 JUNE 2001 | www.nature.com

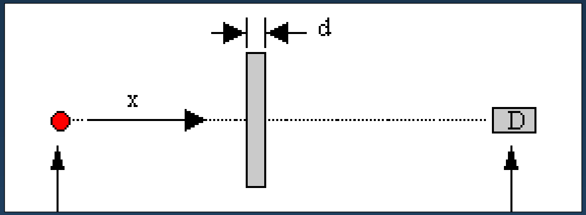
Geant4 LowE Photoelectric effect: current status

- New model for precise angular distribution
  - P. Rodrigues, A. Trindade and L. Peralta+ MGP integration
- Difficulties encountered because of errors(?) in the theoretical reference paper
  - Contacts with other theorists
- Released June 2006 (K-L shells)
  - Further improvements depending on clarification of the theoretical calculations

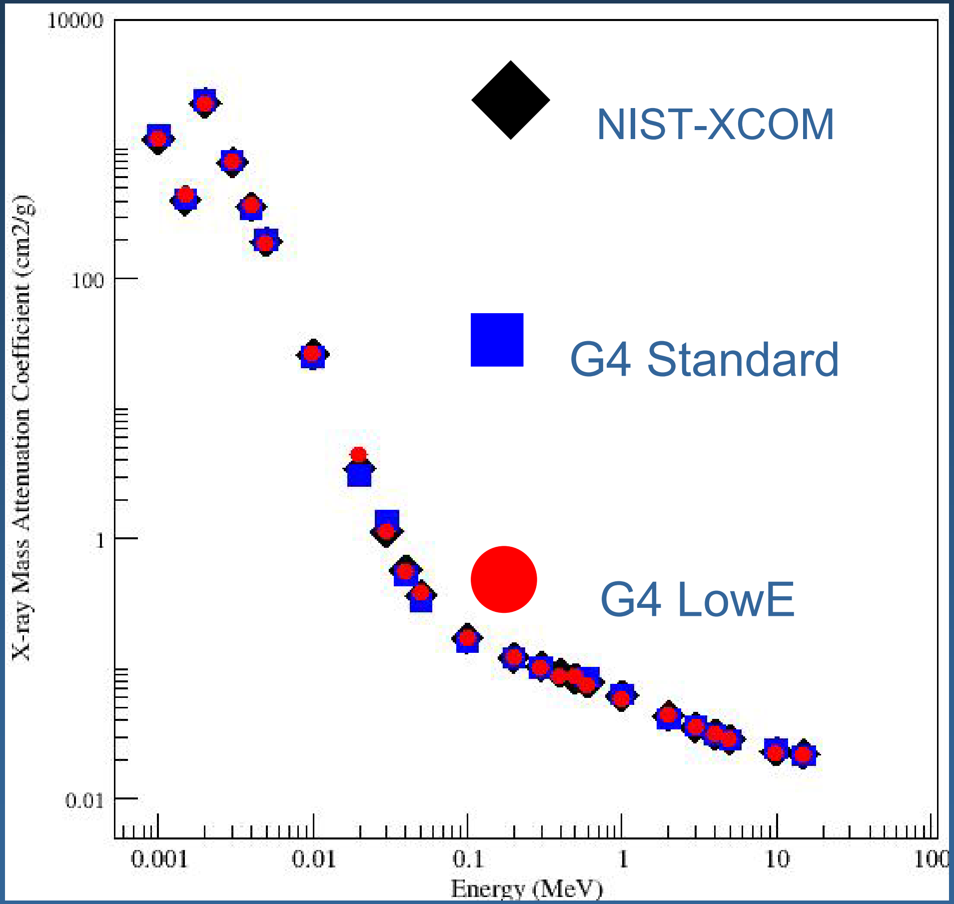
γ conversion

- 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



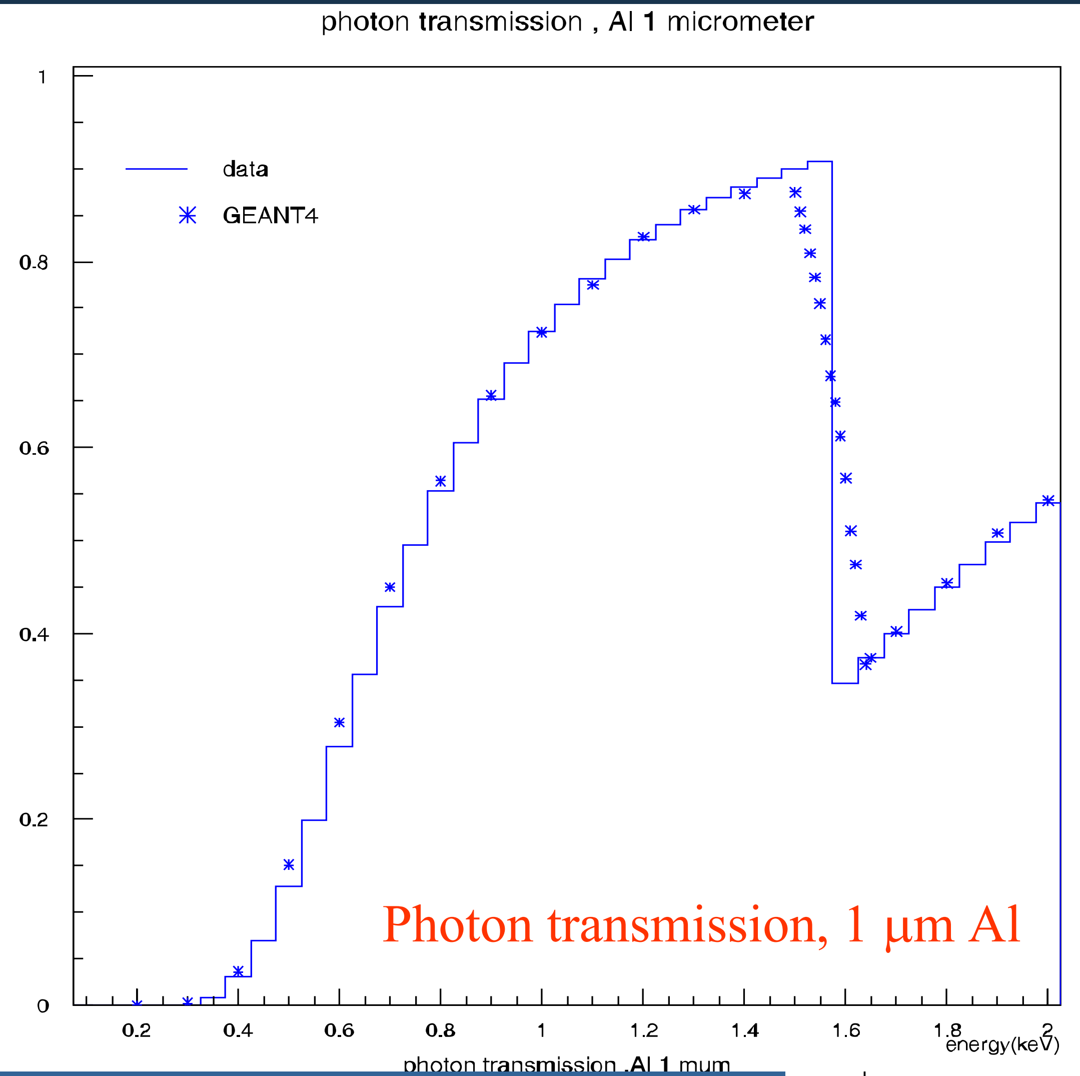
Comparison against NIST data

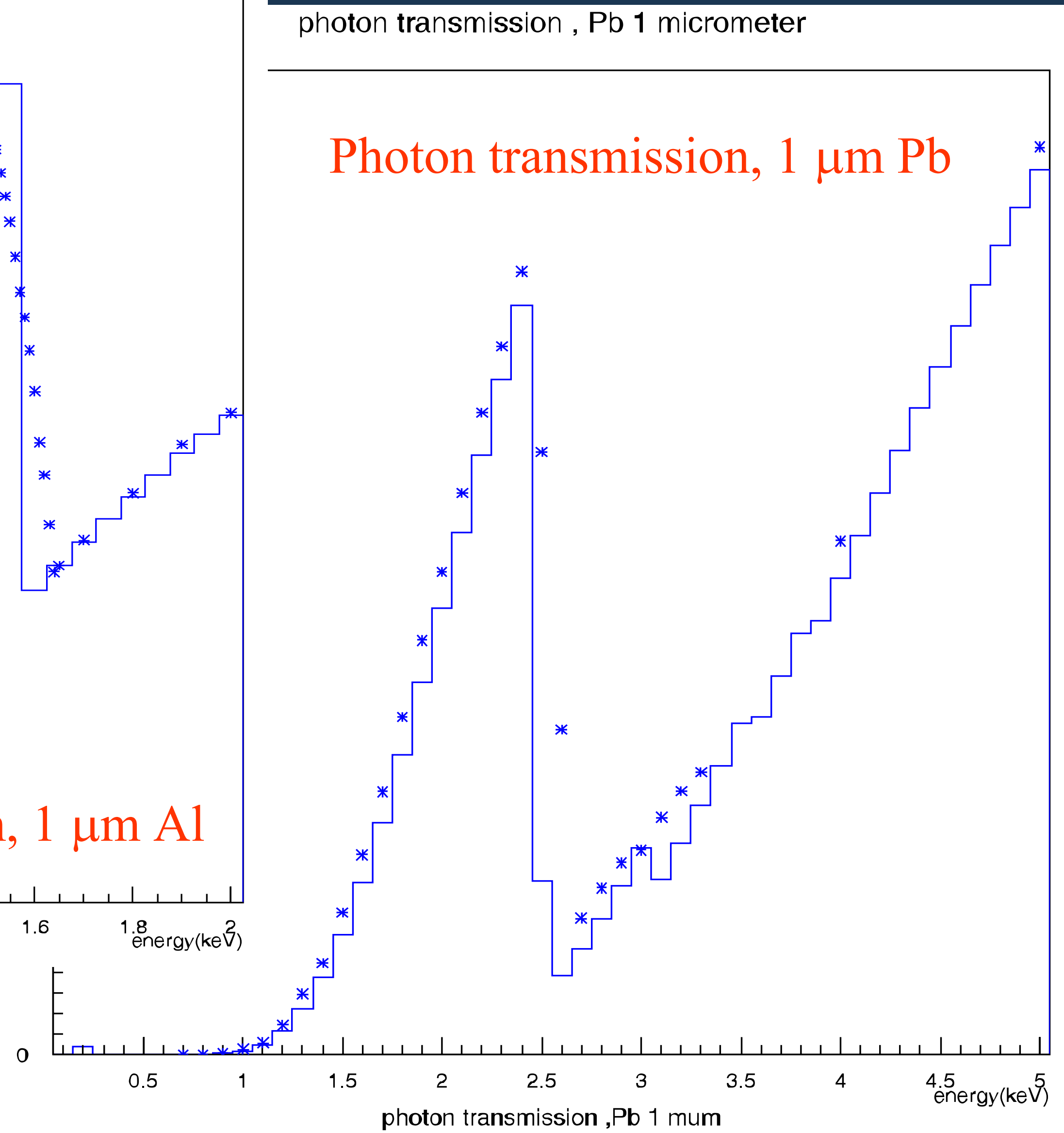


$\chi^2_{N\text{-}L}=13.1$ – $\nu=20$ - $p=0.87$

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

Photons, evidence of shell effects





Polarisation

Cross section:

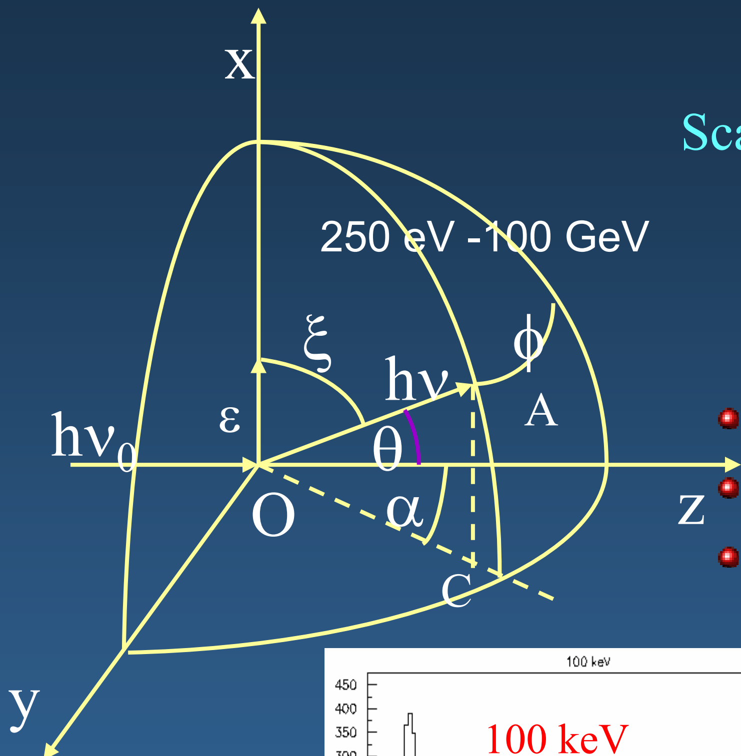
$$\frac{d\sigma}{d\Omega} = \frac{1}{2} r_0^2 \frac{h\nu^2}{h\nu_0^2}\left[\frac{h\nu_0}{h\nu} + \frac{h\nu}{h\nu_0} - 2\sin^2\theta\cos^2\phi\right]$$

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

Scattered Photon Polarization

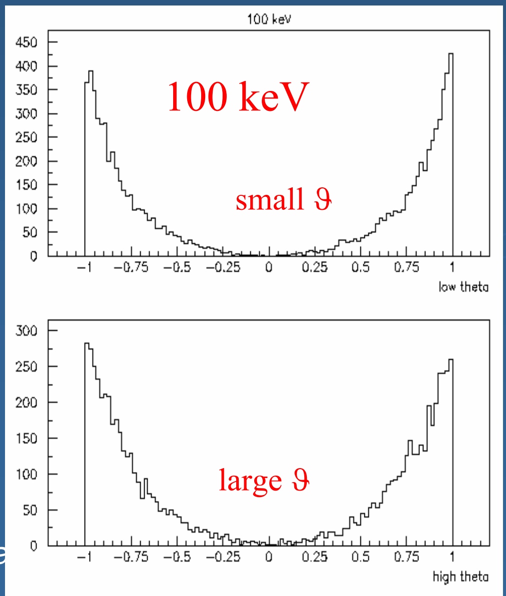
$$\overline{\varepsilon_\perp^{'}} = \frac{1}{N}\left(\cos\theta\,\hat{j} - \sin\theta\sin\phi\,\hat{k}\right)\sin\beta$$

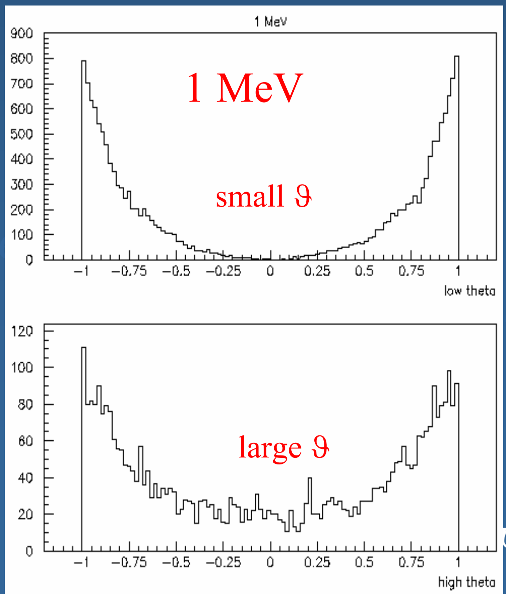
$$\overline{\varepsilon_\parallel^{'}} = \left(N\hat{i} - \frac{1}{N}\sin^2\theta\,\sin\phi\,\cos\phi\,\hat{j} - \frac{1}{N}\sin\theta\,\cos\theta\,\cos\phi\,\hat{k}\right)\cos\beta$$

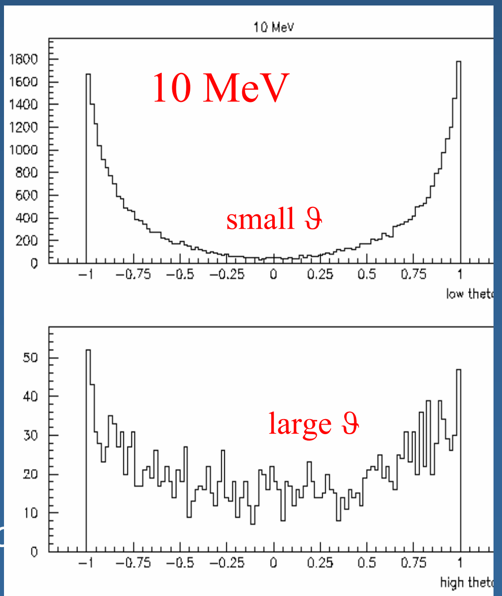


- θ Polar angle
- φ Azimuthal angle
- ε Polarization vector

Low Energy Polarised Compton

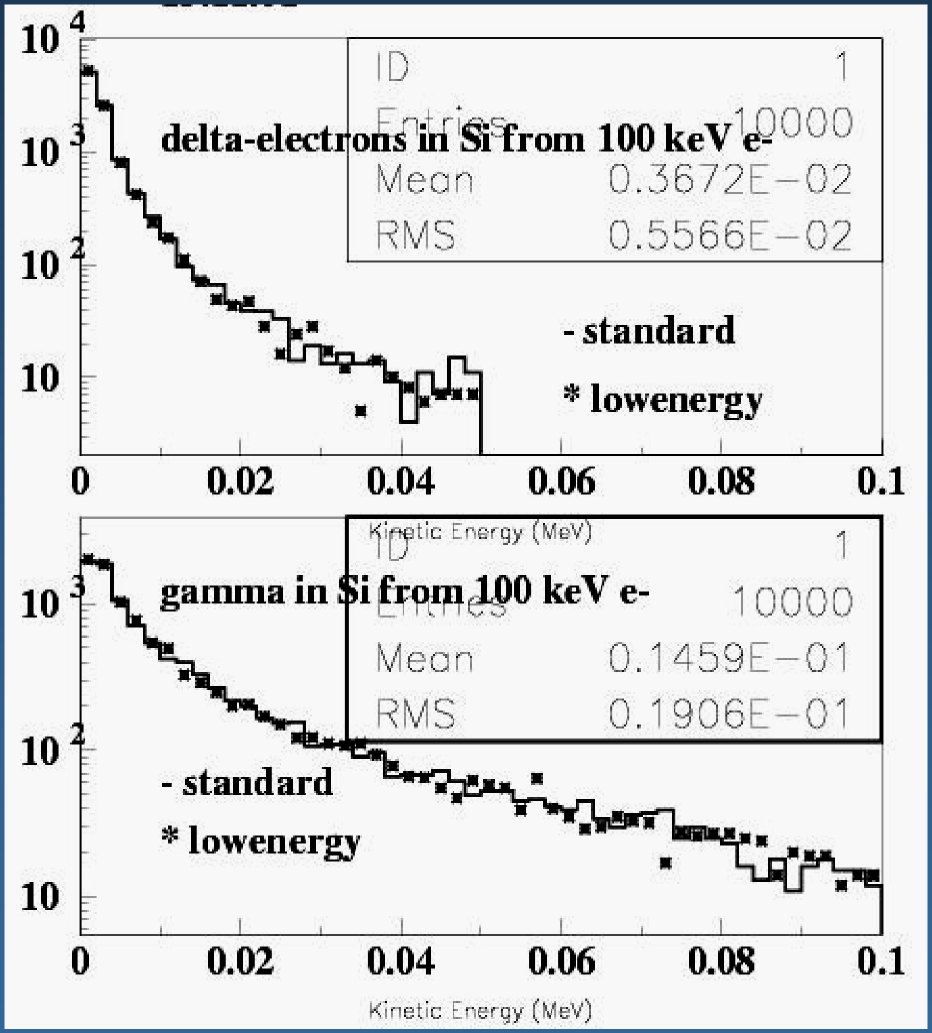






Electron Bremsstrahlung

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

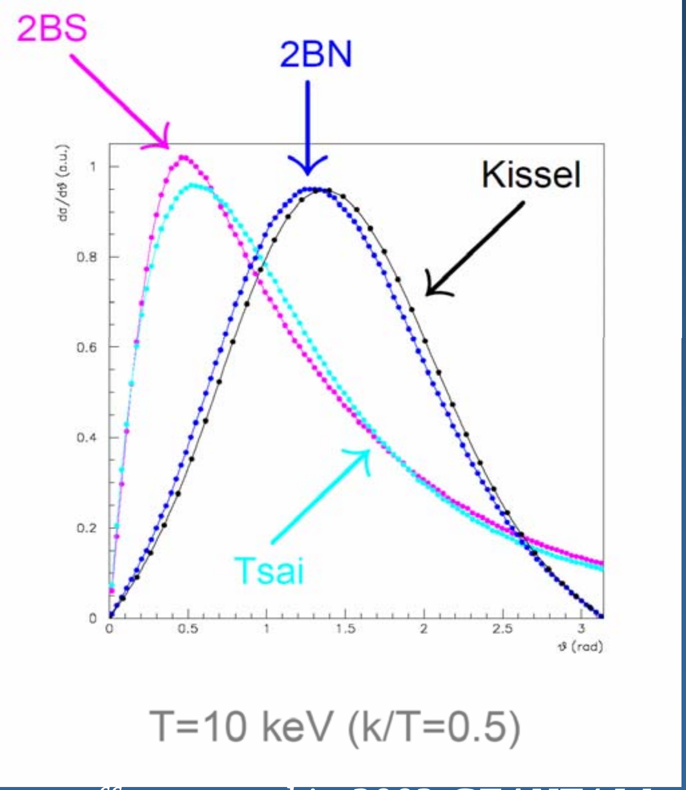


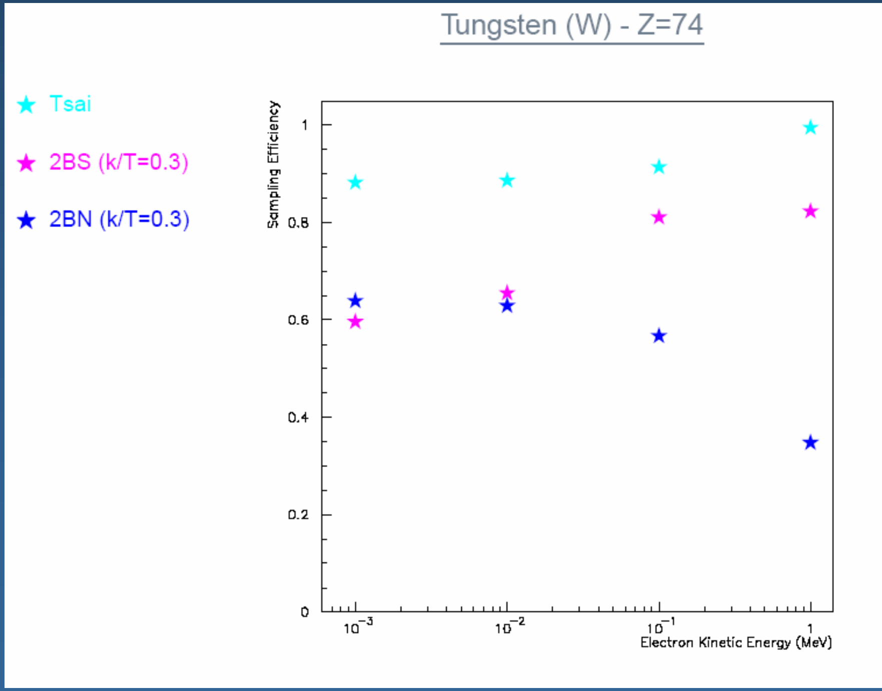
Bremsstrahlung Angular Distributions

Three LowE generators available in GEANT4 6.0 release:

G4ModifiedTsai, G4Generator2BS and G4Generator2BN

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

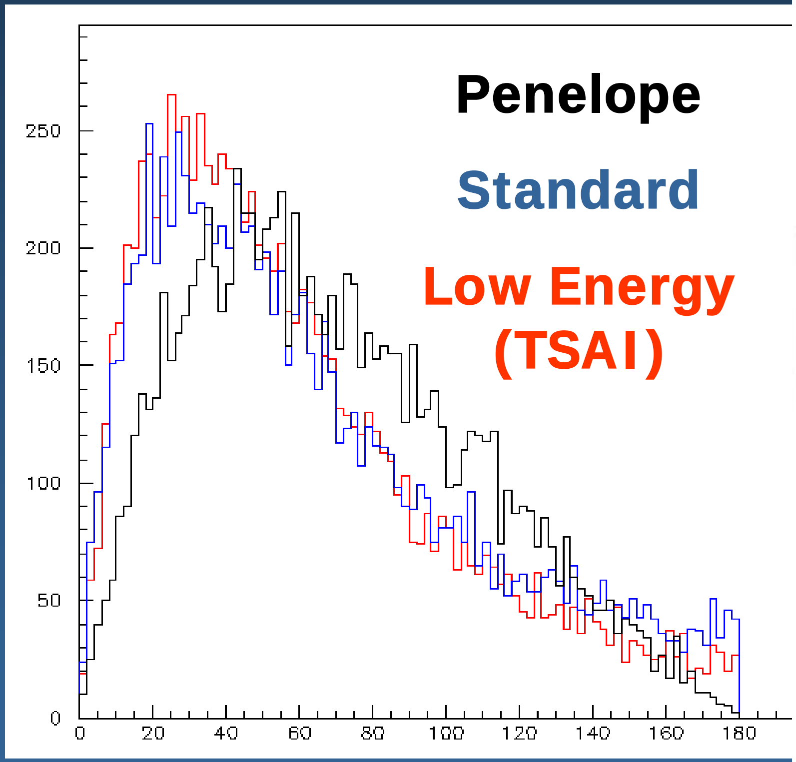


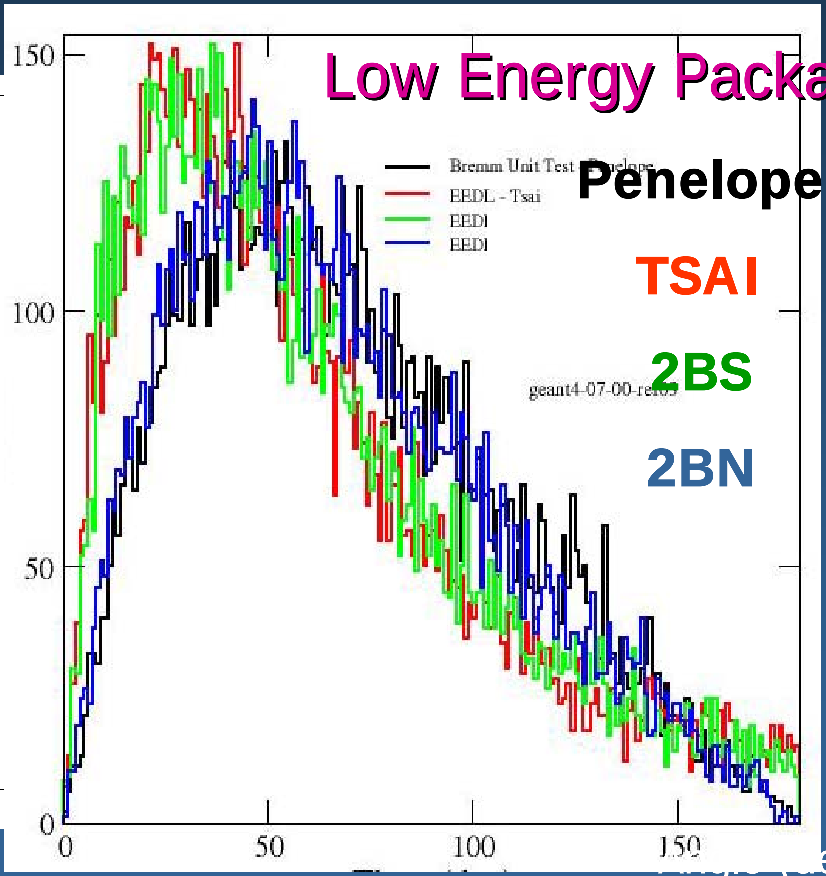


Most stuff presented in 2003 GEANT4 Workshop Vancouver

Maria Grazia Pia, *INFN Genova*

Angular distributions 70 keV



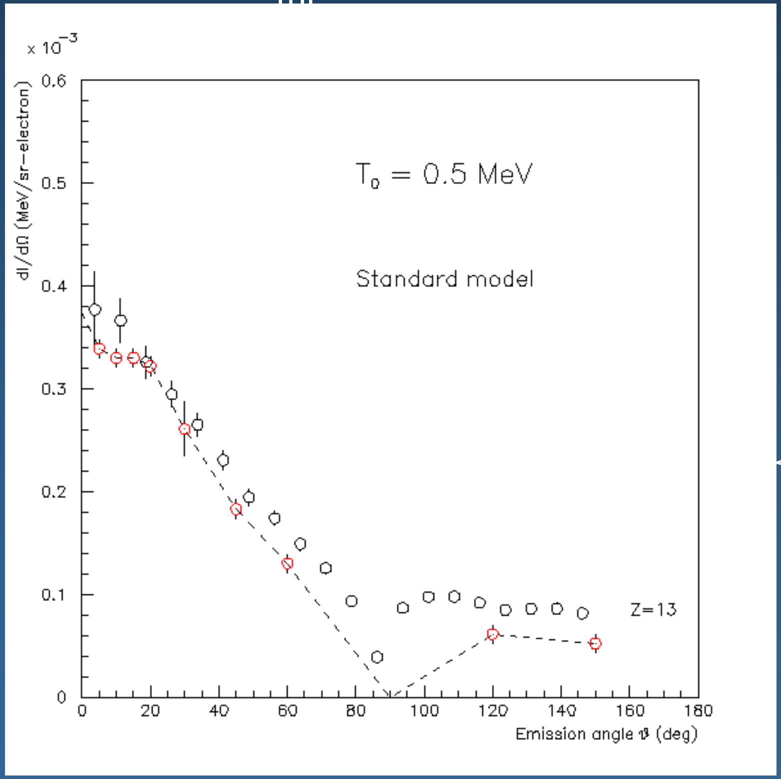


Angular distribution of photons is **strongly model-dependent**

Angular distribution

500 keV

E_{thr} = 46 keV



Absolute comparison

W.E. Dance et al., Journal of Applied Physics ***39*** *(1968) 2881*

500 keV electrons on
Al (0.548 g/cm²) *and Fe (0.257 g/cm²)*
Thick target experiment

Standard package

Red = data

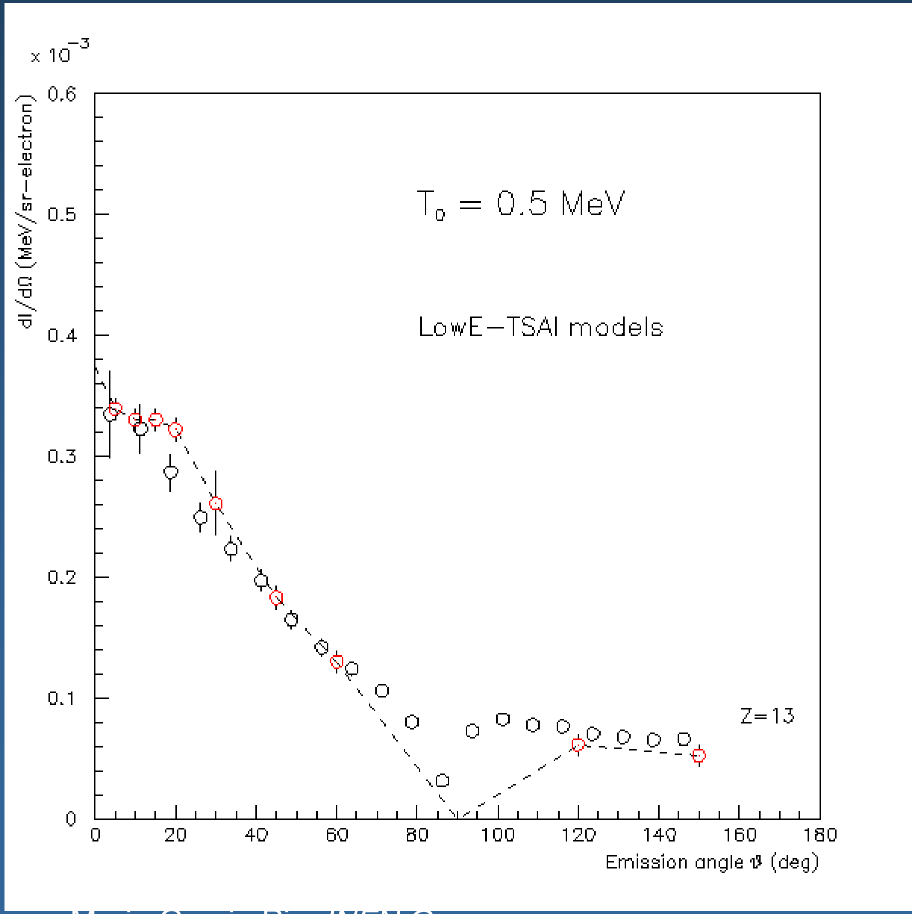
Black = simulation

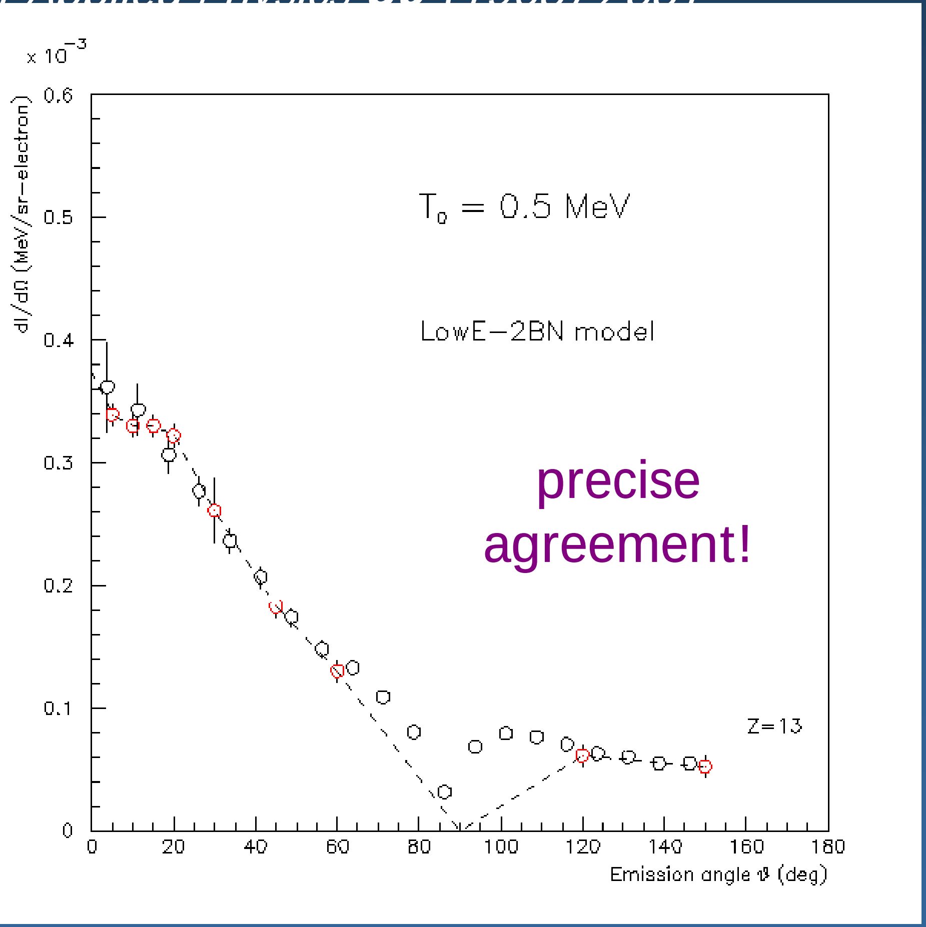
o → Al ● → Fe

Angular distribution

500 keV

*W.E. Dance et al., Journal of Applied Physics **39** (1968) 2881*

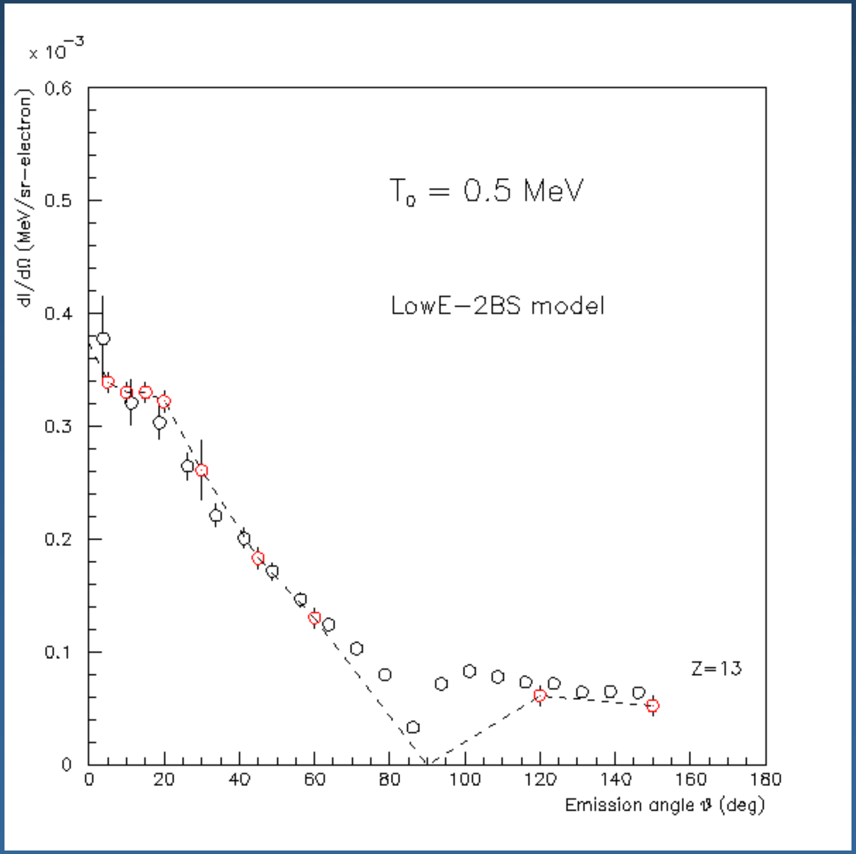


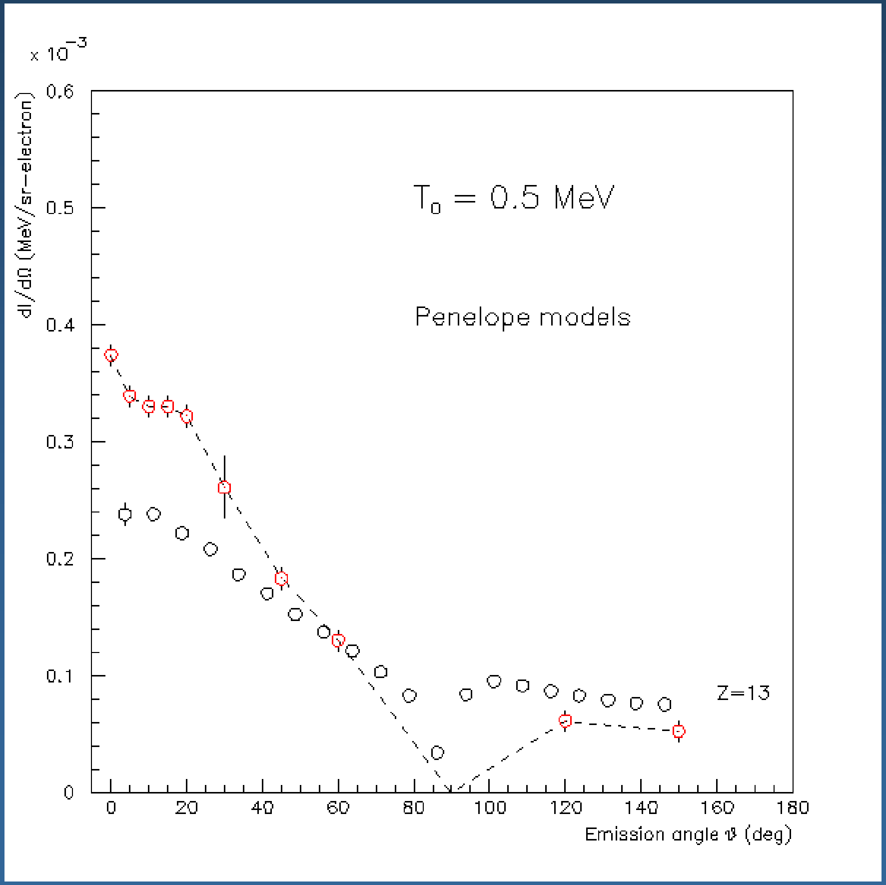


Angular distribution

500 keV

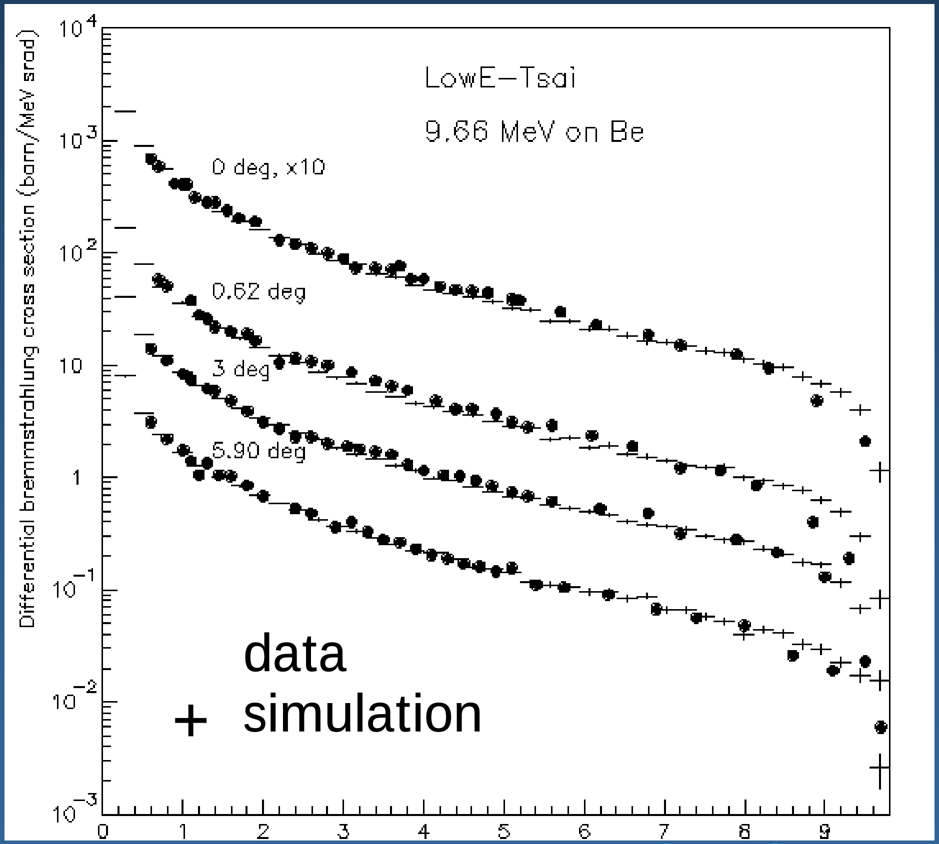
W.E. Dance et al., Journal of Applied Physics ***39*** *(1968) 2881*

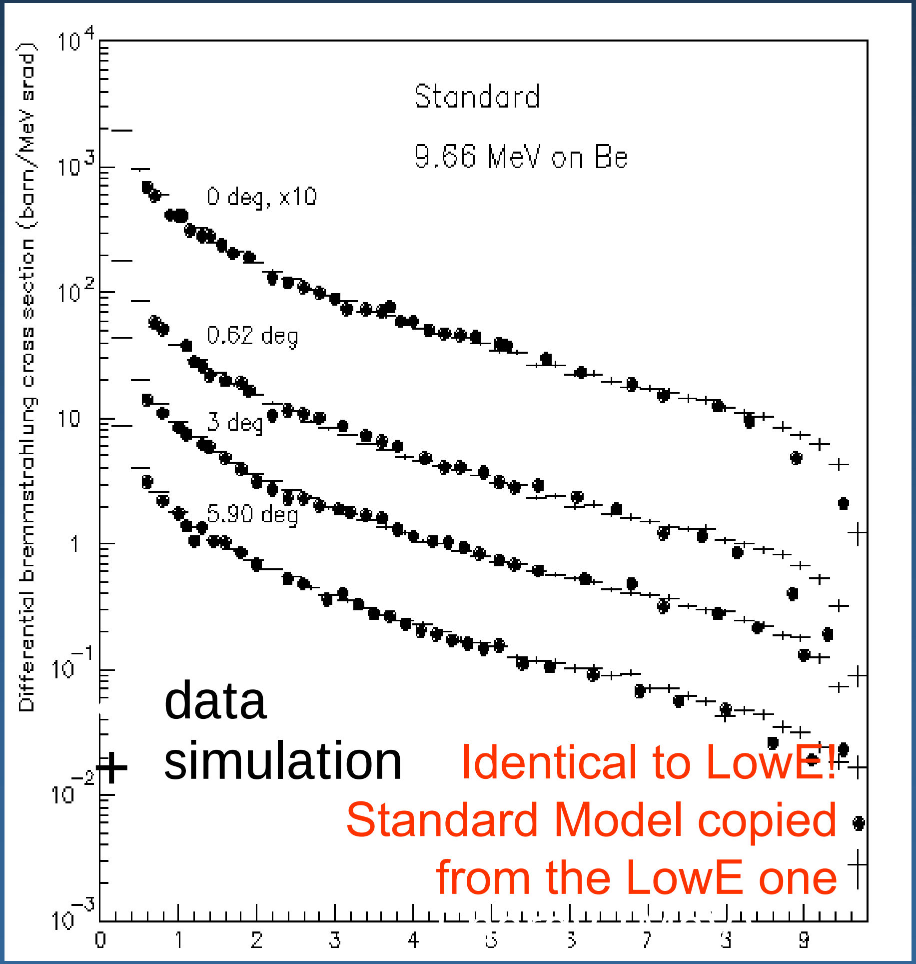




Double differential σ at 9.7 MeV on thin (2.63 mg/cm^2) Be target

N. Starfelt et al., Phys. Rev. ***102*** *(1956) 1598*

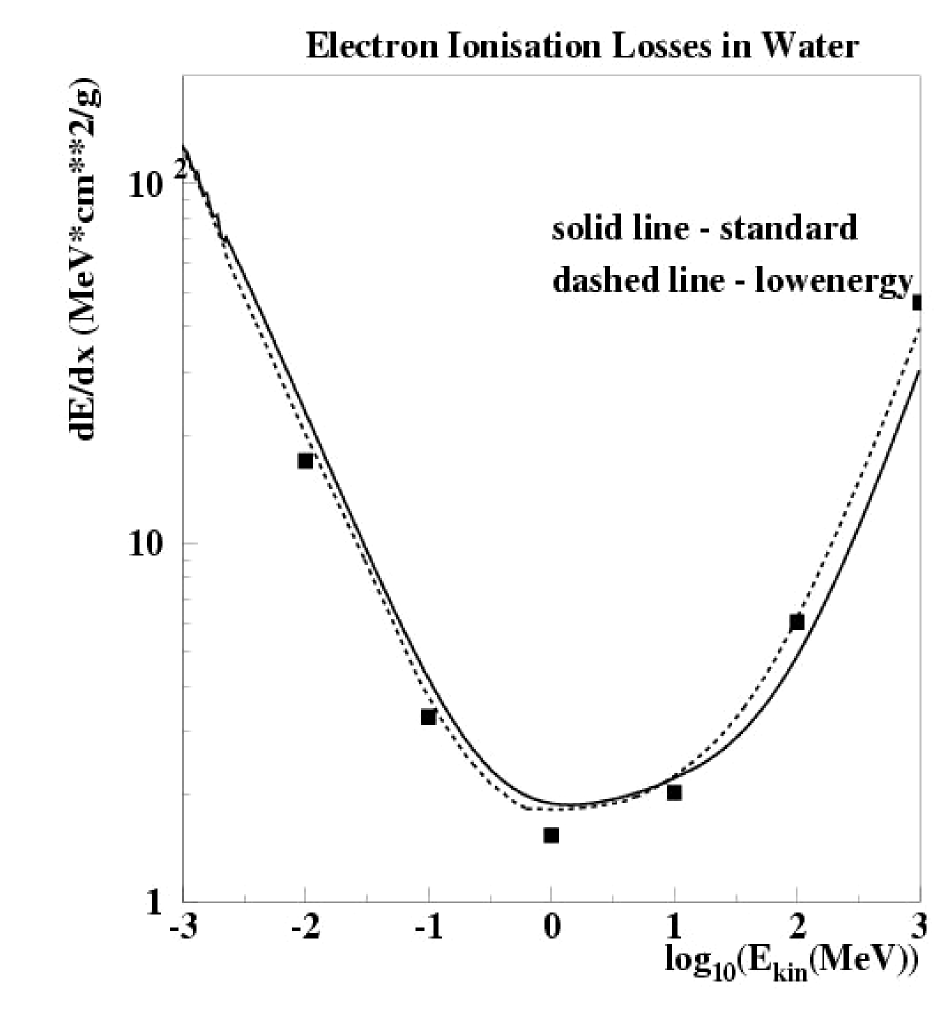




Energy (MeV)

Electron ionisation

- Parameterisation based on 5 parameters for each shell
- Precision of parametrisation is better then 5% for 50 % of shells, less accurate for the remaining shells
- Work in progress to improve the parameterisation and the performance



Electrons: range

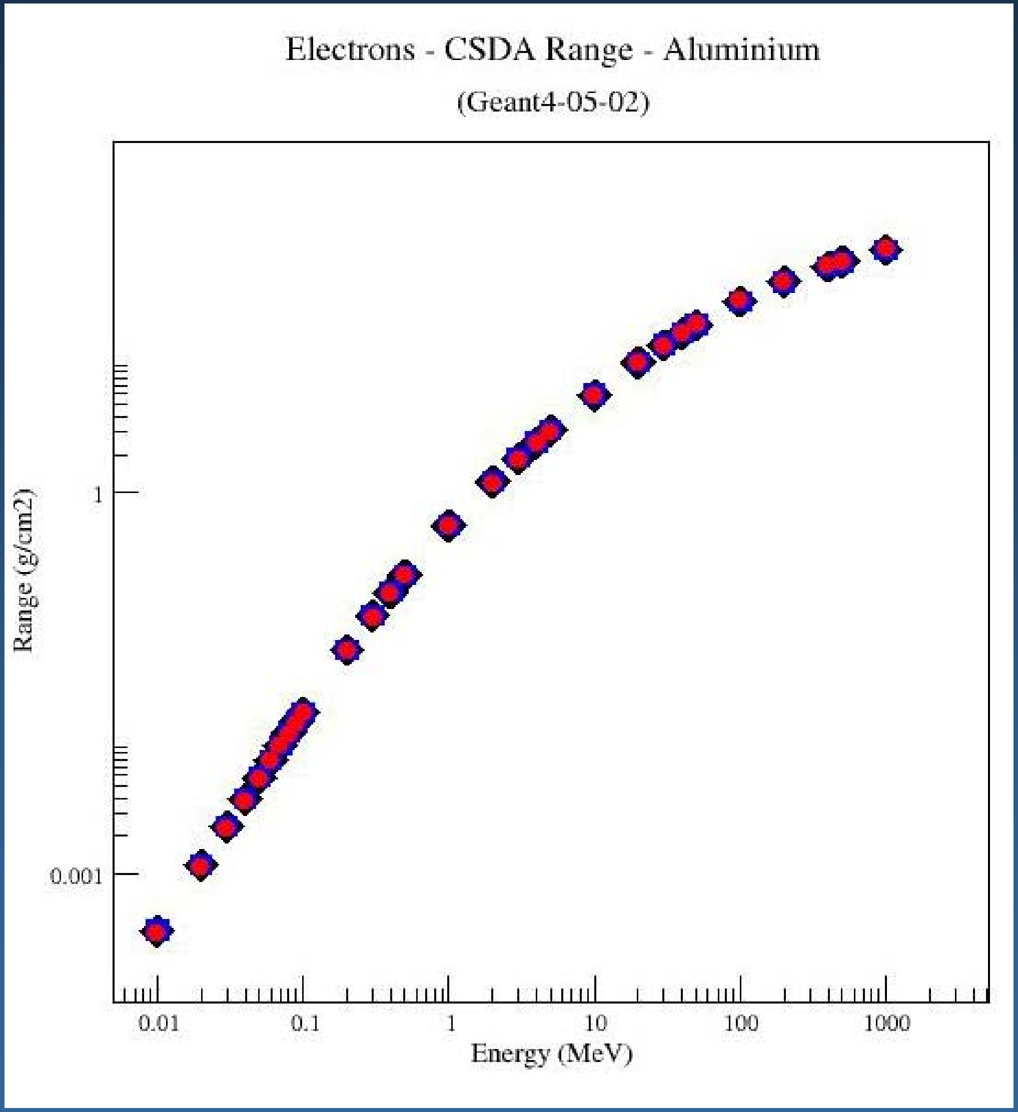
Range in various simple and composite materials

Compared to NIST database

NIST-ESTAR

G4 Standard

G4 LowE

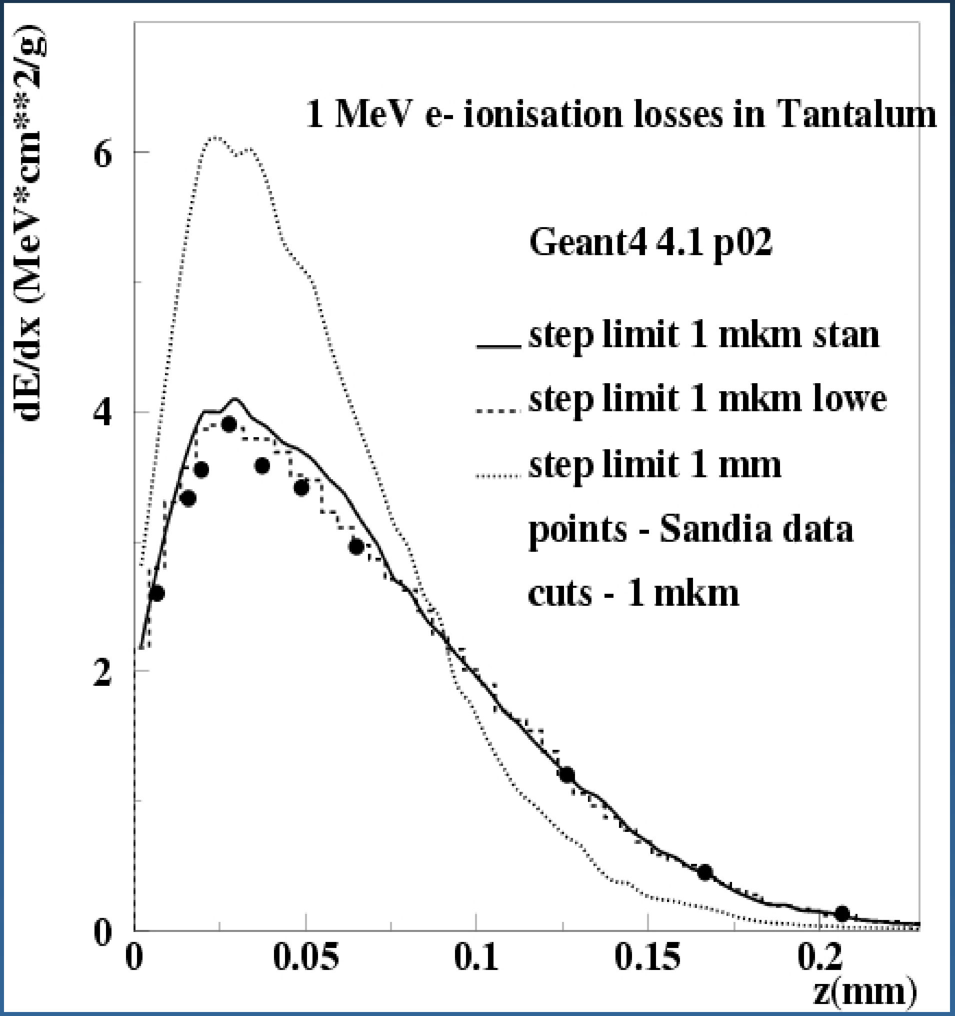


Electrons: dE/dx

Ionisation energy loss in various materials

Compared to Sandia database

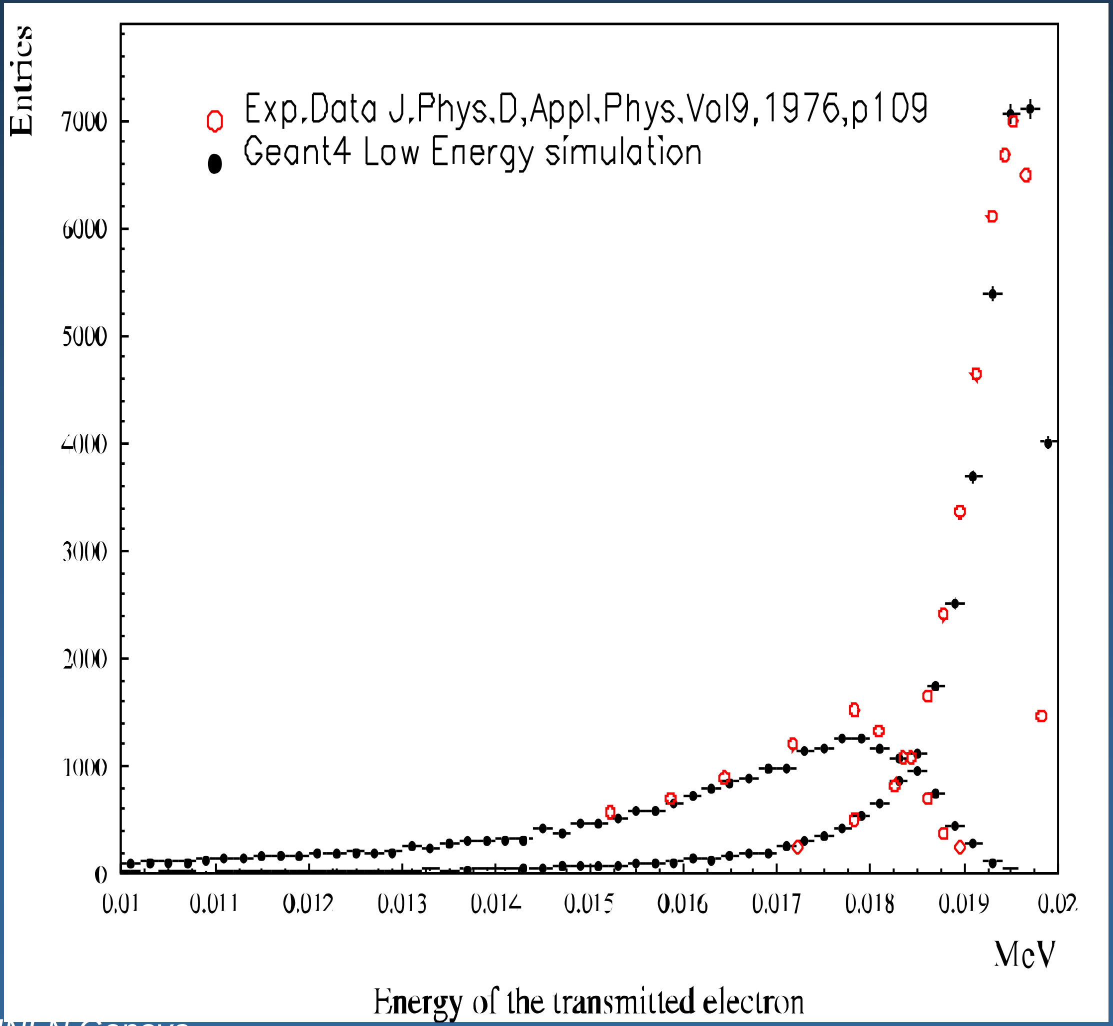
More systematic verification planned



Also Fe, Ur

Electrons, transmitted

20 keV electrons, 0.32 and 1.04 μm Al



Geant4 comparison vs. NIST database

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

Electromagnetic validation

K. Amako et al., Comparison of Geant4 electromagnetic physics models against the NIST reference data
IEEE Trans. Nucl. Sci., Vol. 52, Issue 4, Aug. 2005, 910-918

Hadrons and ions

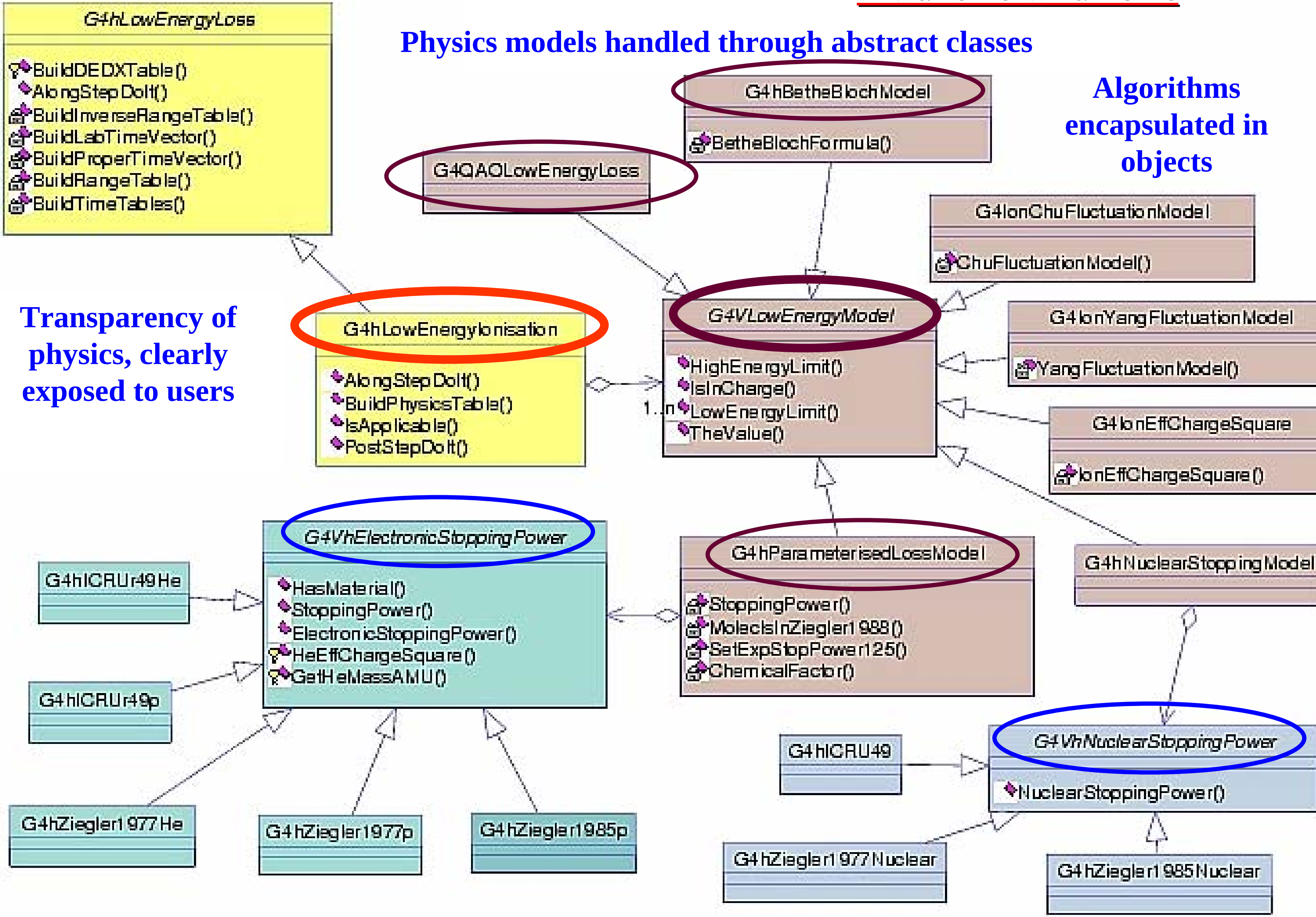
- Variety of models, depending on
  - energy range
  - particle type
  - charge
- Composition of models across the energy range, with different approaches
  - analytical
  - based on data reviews + parameterisations
- Specialised models for fluctuations
- Open to extension and evolution

Hadrons and ions

Physics models handled through abstract classes

Algorithms encapsulated in objects

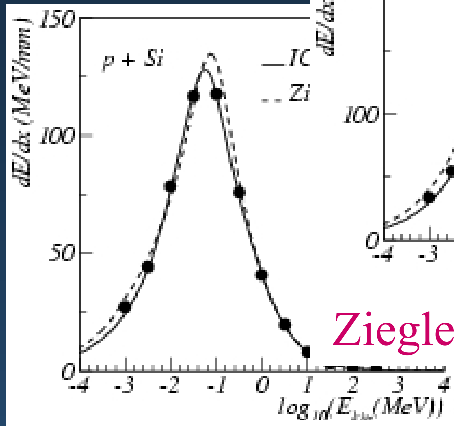
Transparency of physics, clearly exposed to users



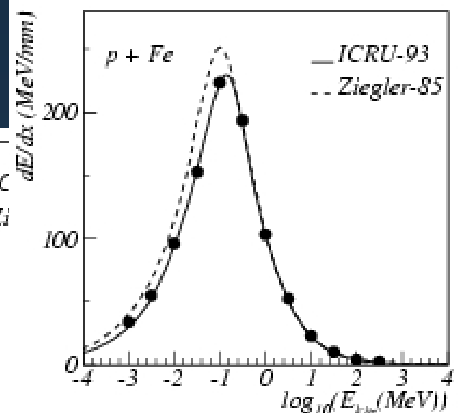
Interchangeable and transparent access to data sets

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



Ziegler and ICRU, Si

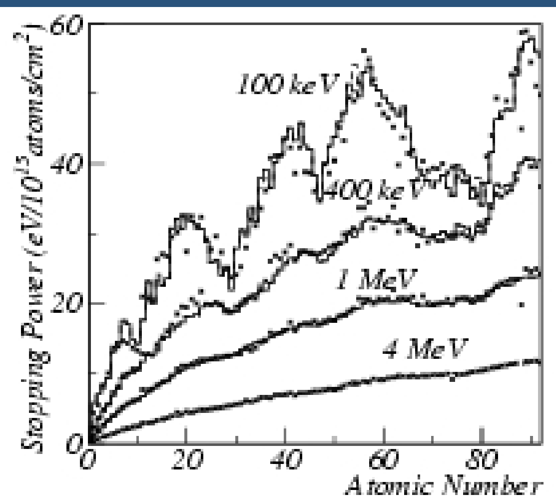


Ziegler and ICRU, Fe

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

- Spin dependent term
- Barkas and Bloch terms

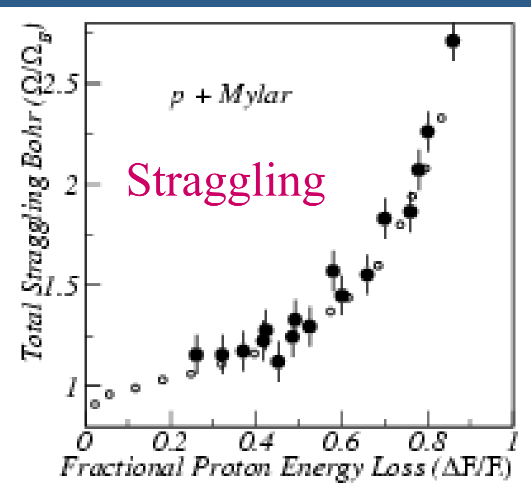
- Chemical effect for compounds
- Nuclear stopping power
- PIXE included

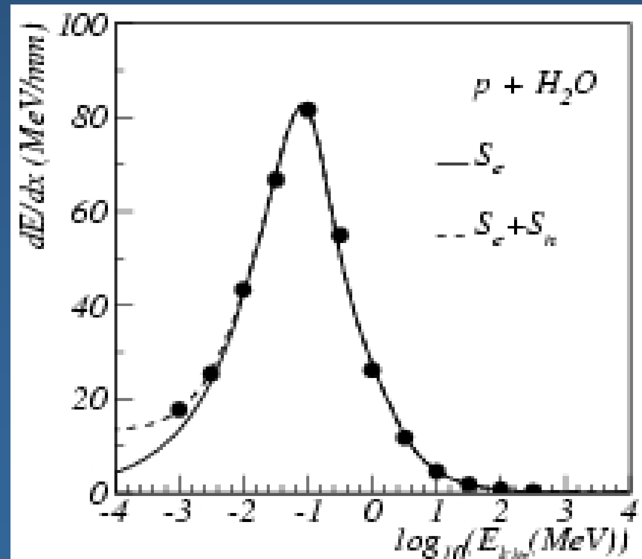


Stopping power

Z dependence for various energies

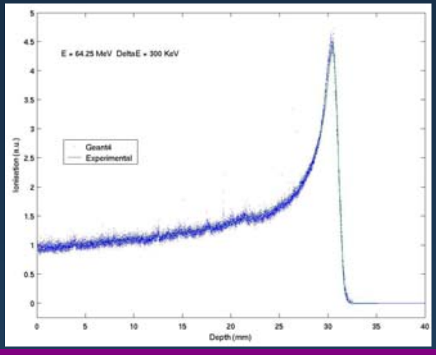
Ziegler and ICRU models





Nuclear stopping power

Bragg peak simulation



	p-value						
	Standard LElastic Precompound	LowE ICRU49 LElastic Precompound GEM	LowE ICRU49 LElastic Bertini Inelastic	LowE ICRU49 LElastic Precompound Fermi Break-up	LowE ICRU49 LElastic Precompound	LowE ICRU49 HadronElastic Precompound	LowE ICRU49 Bertini Elastic Bertini Inelastic
Left branch **(CvM)**	0.648	0.667	0.790	0.814	0.836	0.973	**0.977**
Right branch **(KS)**	0.760	0.985	0.985	0.985	0.985	0.985	**0.985**
Whole curve **(AD)**	0.666	0.858	0.936	0.945	0.946	0.982	**0.994**

Key ingredients

- Precise **electromagnetic** physics
- Good **elastic scattering** model
- Good **pre-equilibrium** model

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

- Effective charge model
- Nuclear stopping power

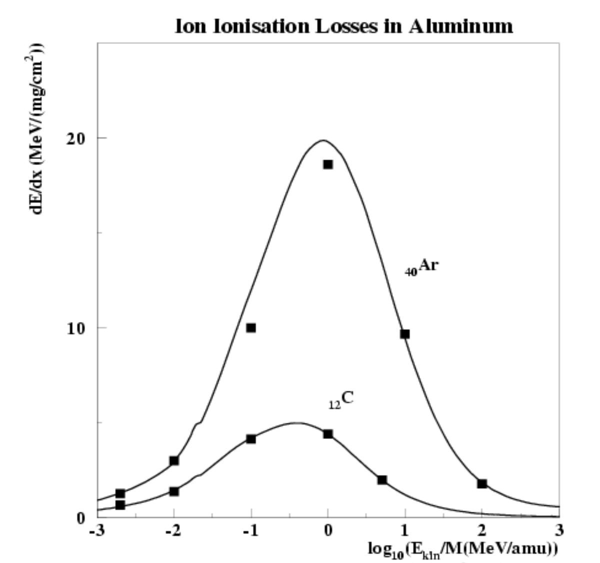
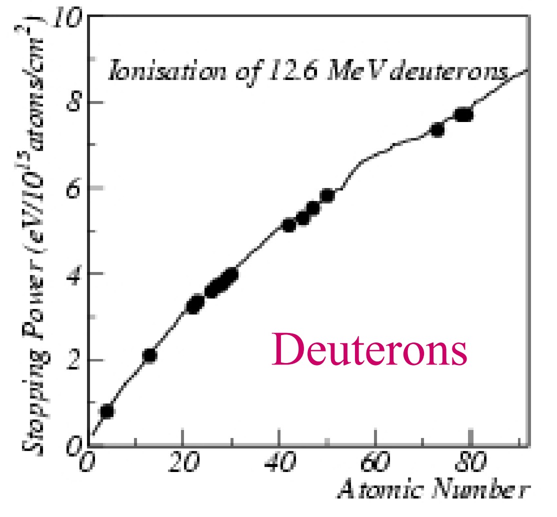
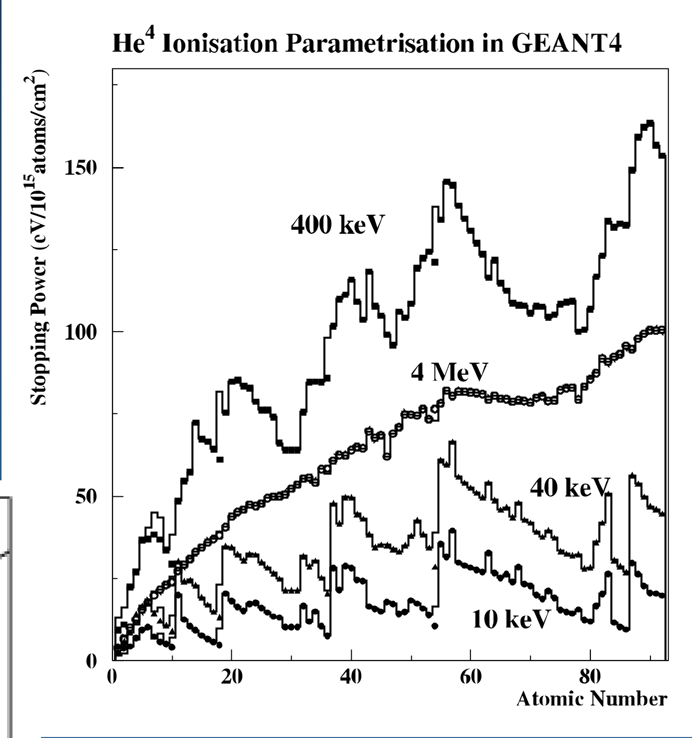


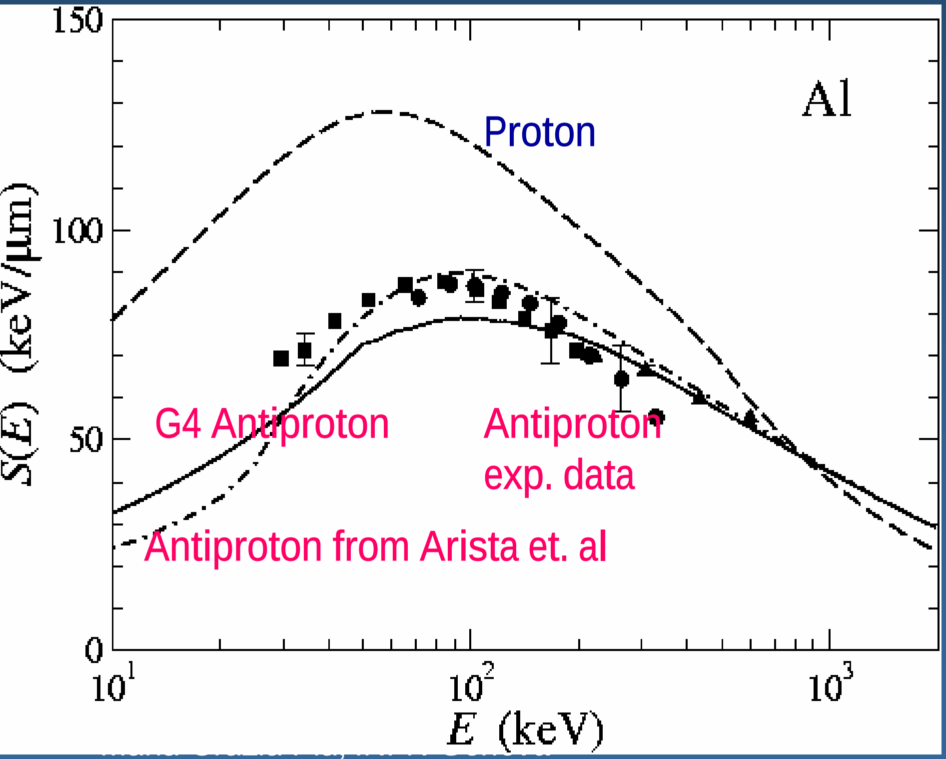
Figure 9: Ion electronic stopping power in aluminum. Points - the best fit on the data from Ref.[12], solid line - GEANT4 parameterisation. The accuracy of the data is about 5 %.

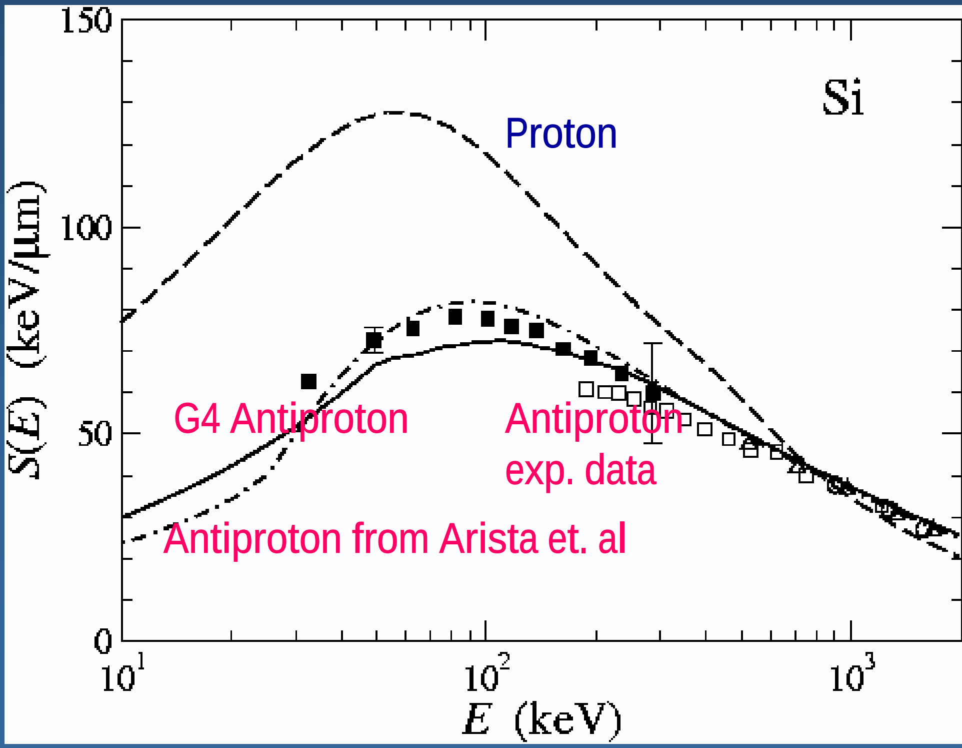




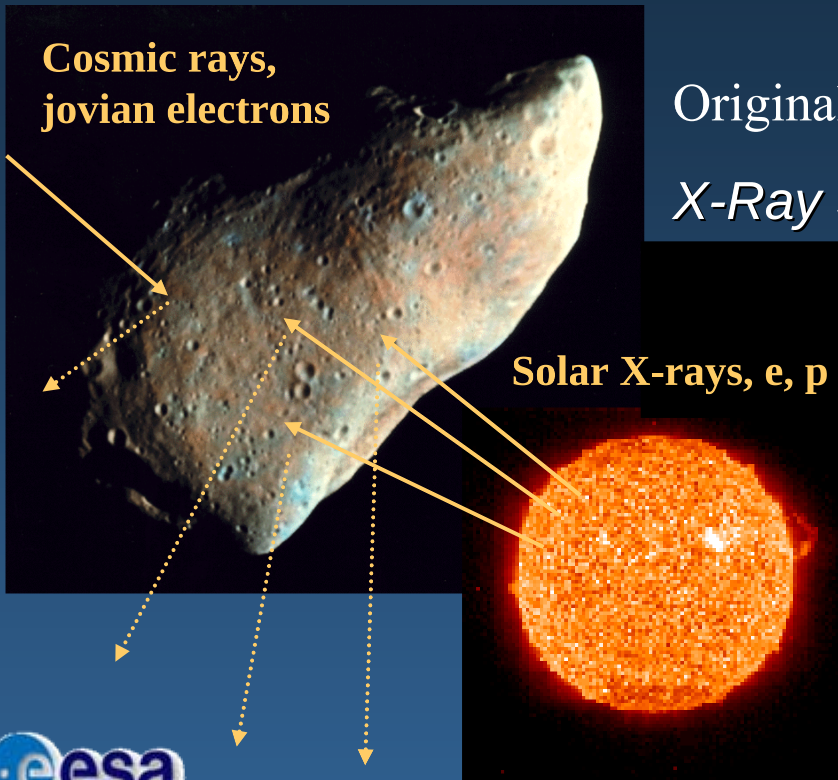
Models for antiprotons

- $\beta > 0.5$ — Bethe-Bloch formula
- $0.01 < \beta < 0.5$ — Quantum harmonic oscillator model
- $\beta < 0.01$ — Free electron gas mode





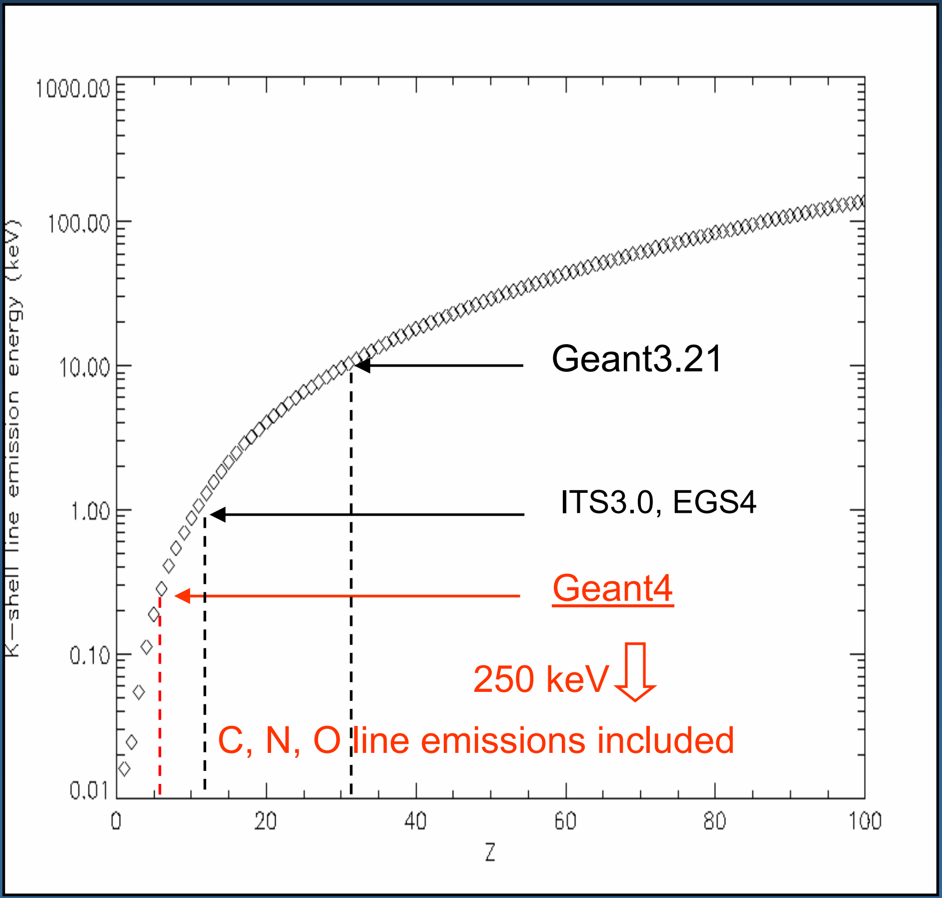
Geant4 Low Energy Electromagnetic package



Courtesy SOHO EIT

Original motivation from astrophysics requirements

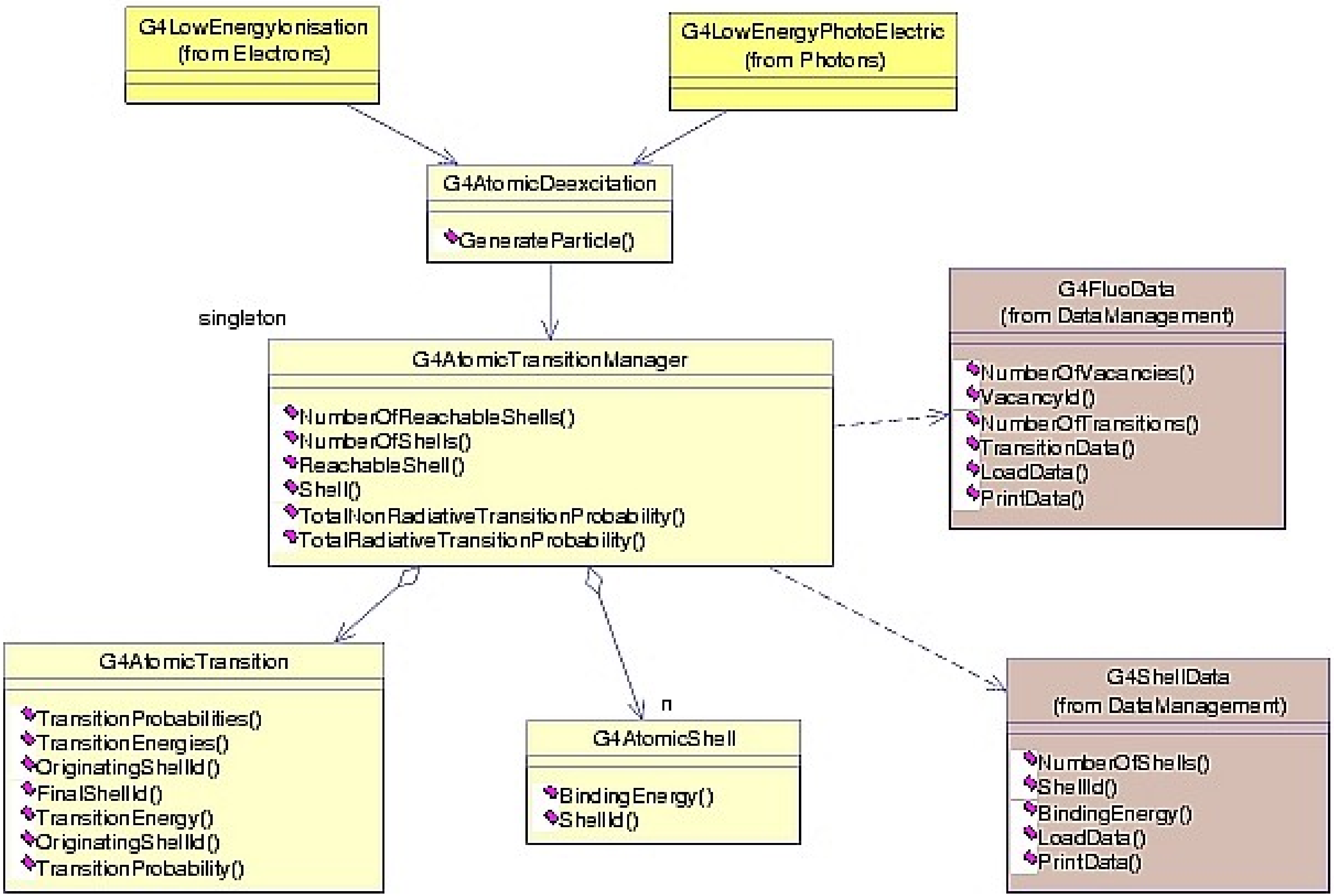
X-Ray Surveys of Asteroids and Moons



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

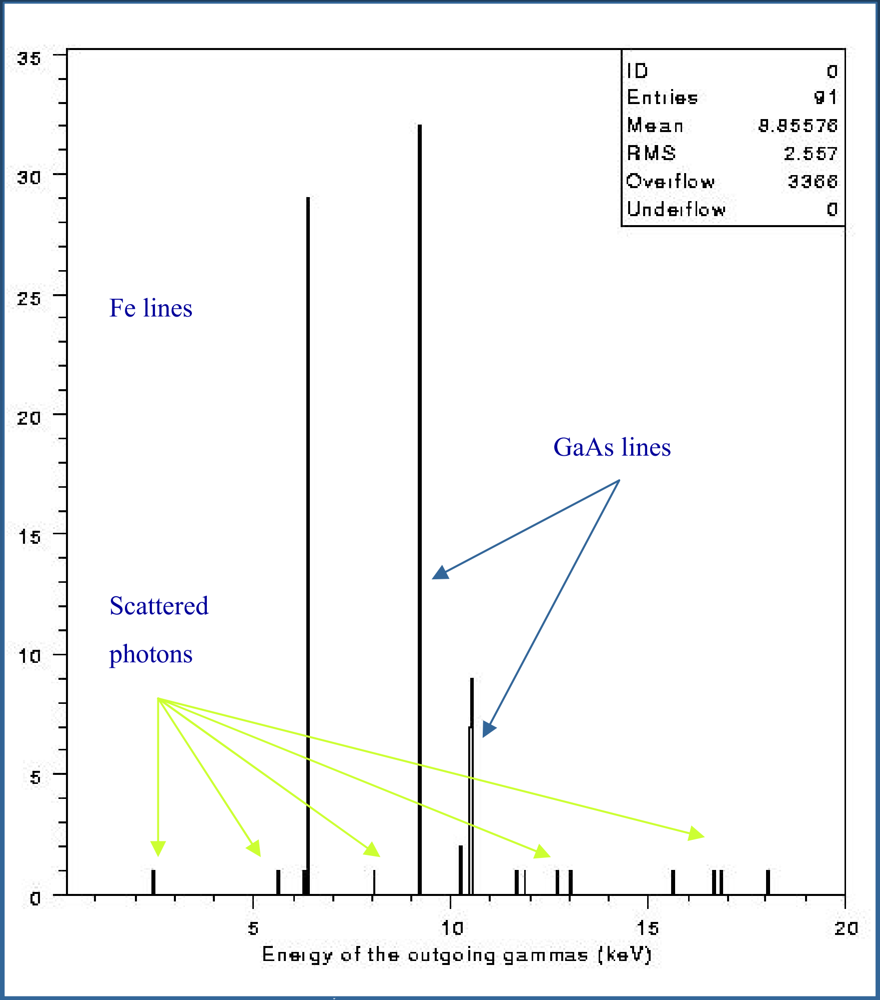
Wide field of applications beyond astrophysics

Atomic relaxation

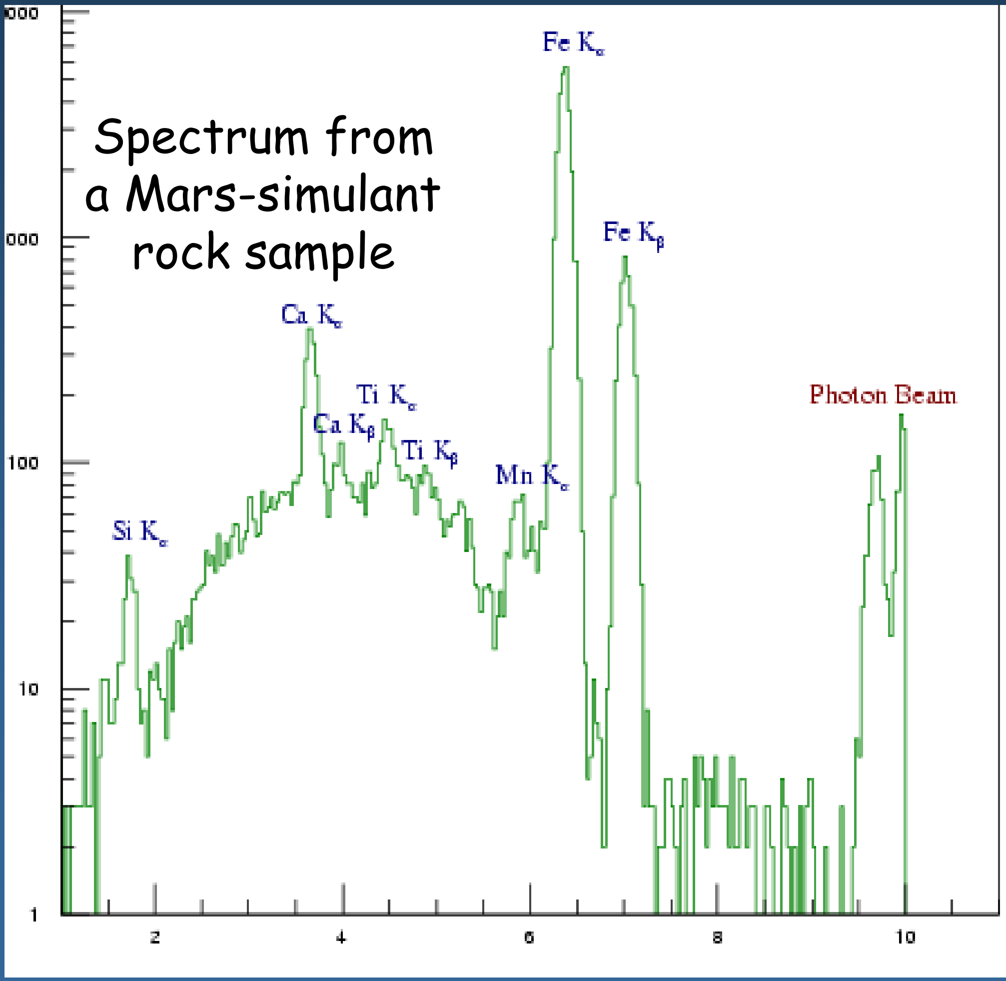


Fluorescence

Microscopic validation:
against reference data



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



Validation of Atomic relaxation against the NIST databases

Vacancy in K shell

Shell	Kolomogorov-Smirnov Distance	p-value
L2	0.0188	1
L3	0.0185	1
M2	0.0172	1
M4	0.0667	1
M5	0.0588	1
N2	0.0714	1
N3	0.0714	1

Vacancy in L1 shell

Shell	Kolomogorov-Smirnov Distance	p-value
M2	0.0192	1
M3	0.0175	1
M4	0.0250	1
M5	0.0256	1
N2	0.0294	1
N3	0.0312	1
N4	0.1429	0.997
N5	0.0588	1

etc.

REVIEWS OF MODERN PHYSICS, VOLUME 75, JANUARY 2003

X-ray transition energies: new approach to a comprehensive evaluation

Richard D. Deslattes* and Ernest G. Kessler, Jr.

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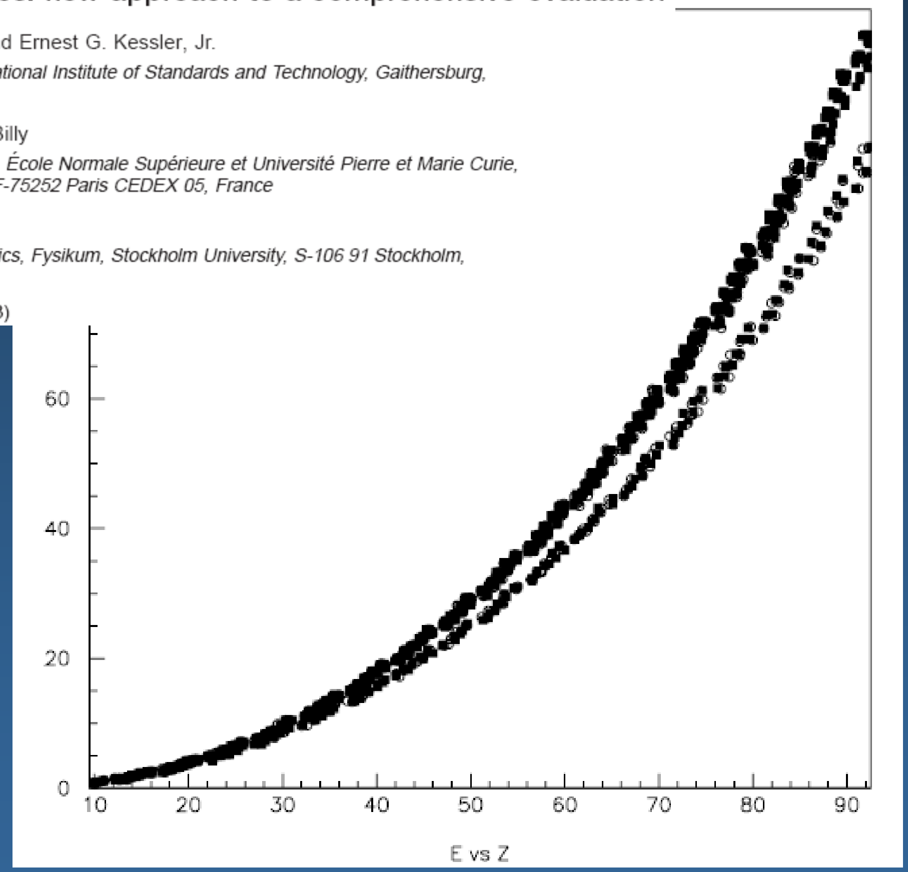
P. Indelicato† and L. de Billy

Laboratoire Kastler Brossel, École Normale Supérieure et Université Pierre et Marie Curie, Case 74, 4 place Jussieu, F-75252 Paris CEDEX 05, France

E. Lindroth and J. Anton

Department of Atomic Physics, Fysikum, Stockholm University, S-106 91 Stockholm, Sweden

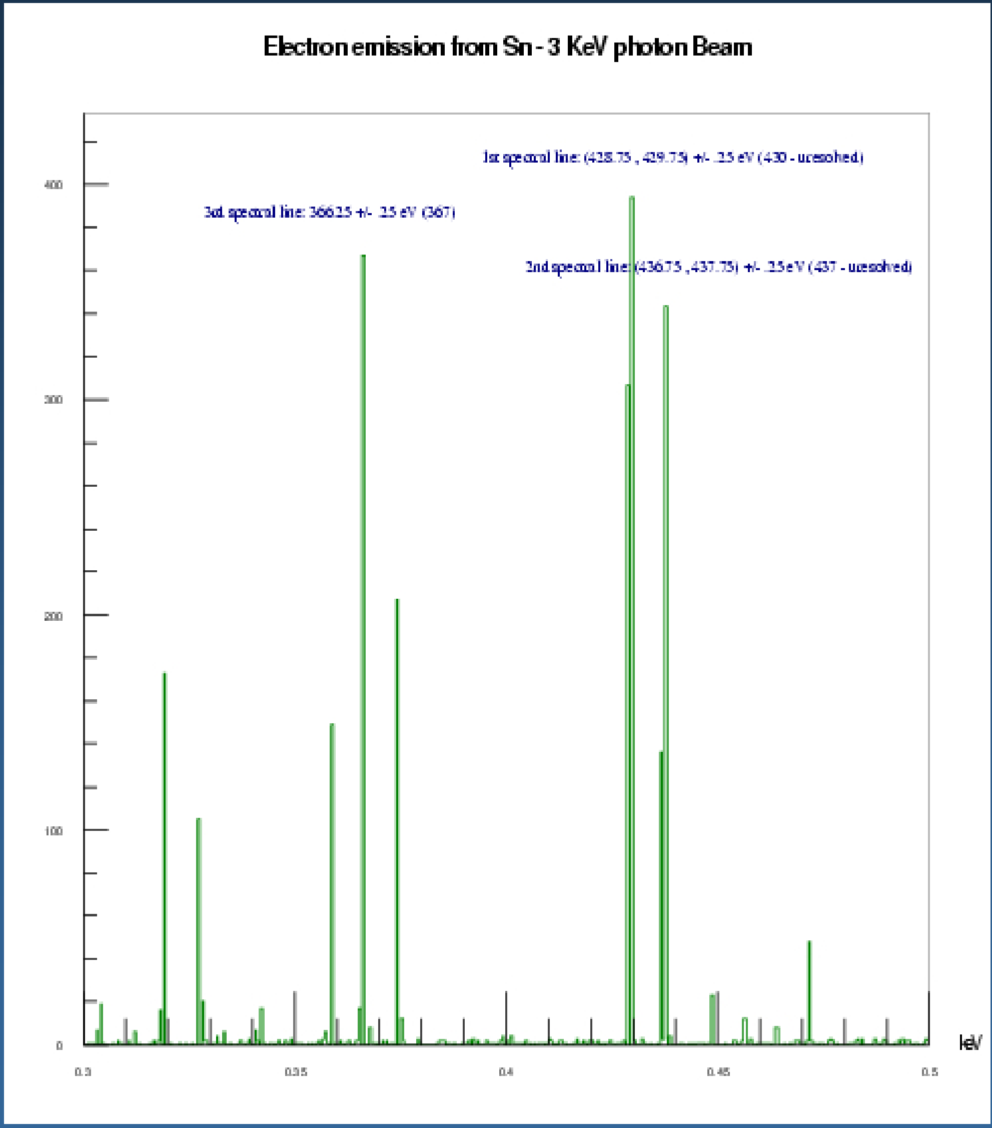
(Published 7 January 2003)



Publication in preparation (January 2006)

Auger effect

Also validated against NIST experimental data



Sn, 3 keV photon beam,

electron lines w.r.t. published experimental results

PIXE

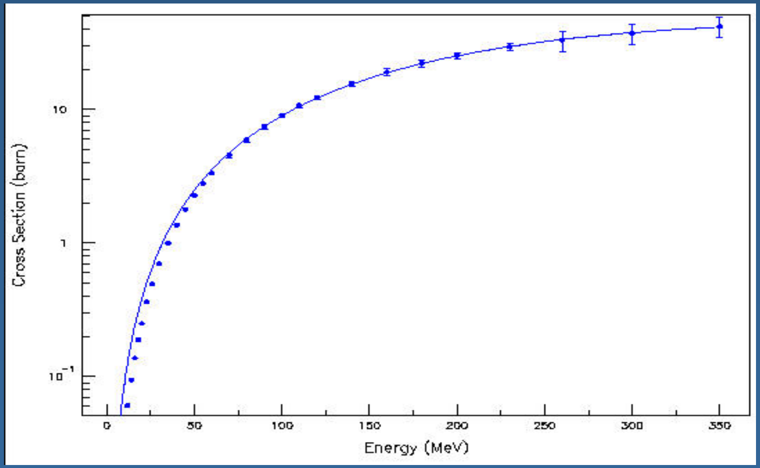
- New model based on experimental data
  - Parameterisation of Paul & Sacher data library for ionisation cross sections
  - Uses the EADL-based package of atomic deexcitation for the generation of fluorescence and Auger secondary products

- Current implementation: protons, K-shell
- Coming in future: protons, L-shell and α, K-shell

Example of p ionisation cross section, K shell

Geant4 parameterisation (solid line)

Experimental data



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

File Edit View Favorites Tools Help

http://www.ge.infn.it/geant4/dna

Go Links

esa

Geant 4 DNA

INFN Istituto Nazionale di Fisica Nucleare

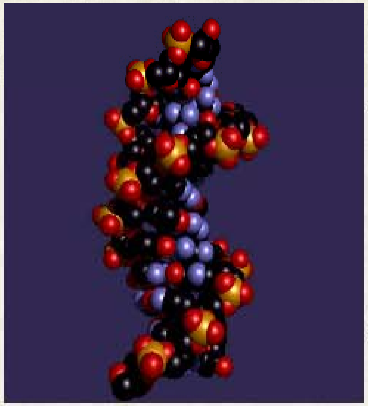
- [Home]

- [Requirements]
- [Documents]
- [Talks]
- [Papers]
- [Meetings]
- [Team]

- [Geant4]
- [Geant4-INFN]
- [Geant4 LowE Physics]

- [Useful links]

Simulation of Interactions of Radiation with Biological Systems at the Cellular and DNA Level

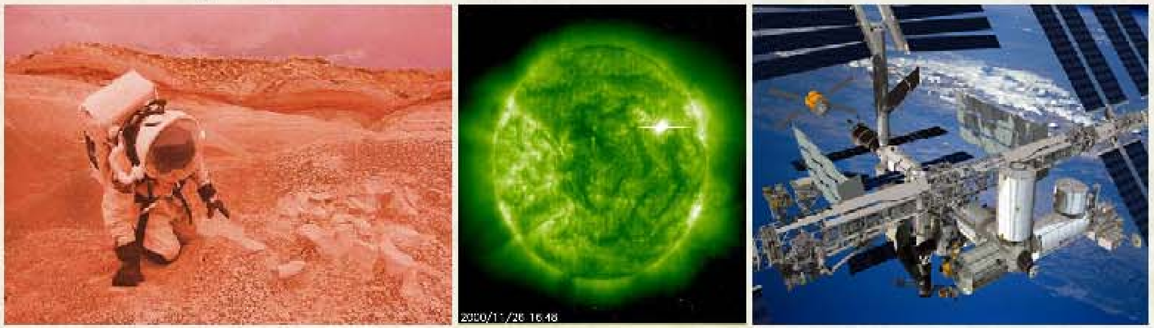


Estimating **cancer risk for human exposures to space radiation** is a challenge which involves a wide range of knowledge in physics, chemistry, biology and medicine.

Traditionally, the biological effects of radiation are analysed in top-bottom order, i.e. evaluation of the absorbed macroscopic radiation dose at a given location in the biological tissue is translated to the degree of danger it presents, and dose limits are consequently set that are considered to be acceptable.

A novel approach, based on the new-generation object-oriented **Geant4** Monte Carlo Toolkit, proceeds in a reverse order, from bottom to top, by analysing the nano-scale effects of energetic particles at the cellular and DNA molecule level.

This project is sponsored by the European Space Agency (ESA) and is pursued by a multidisciplinary European team of biologists, physicians, physicists, space scientists and software engineers.



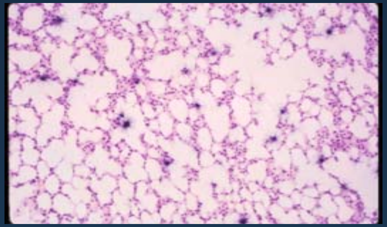
Pictures courtesy of ESA

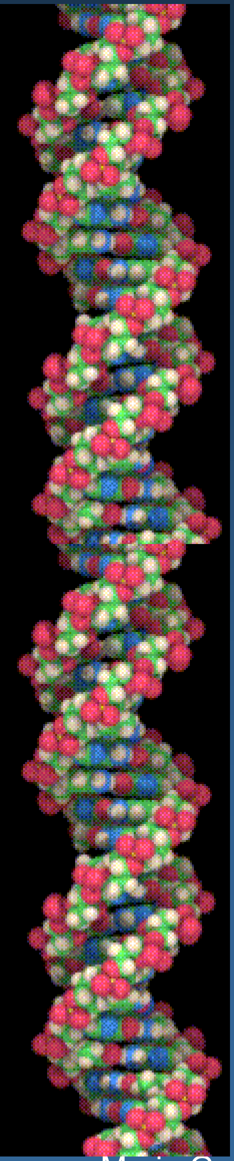
Biological models in Geant 4

Relevance for space:
astronaut and aircrew radiation hazards

esa

Geant 4 for radiation biology





- Several specialized Monte Carlo codes have been developed for radiobiology/microdosimetry
  - Typically each one implementing models developed by its authors
  - Limited application scope
  - Not publicly distributed
  - Legacy software technology (FORTRAN, procedural programming)

- Geant4-DNA
  - Full power of a general-purpose Monte Carlo system
  - Toolkit: multiple modeling options, no overhead *(use what you need)*
  - Versatility: from controlled radiobiology setup to real-life ones
  - Open source, publicly released
  - Modern software technology
  - Rigorous software process

Geant 4

Strategic vision

OO technology

Openness to extension and evolution

- new implementations can be added w/o changing the existing code

Robustness and ease of maintenance

- protocols and well defined dependencies minimize coupling

Toolkit

A set of compatible components

- each component is specialised for a specific functionality
- each component can be refined independently to a great detail
- components can be integrated at any degree of complexity
- it is easy to provide (and use) alternative components
- the user application can be customised as needed

Geant 4

Multiple domains in the same software environment

(advanced software technology)

- Macroscopic level
  - calculation of dose
  - already feasible with Geant4
  - develop useful associated tools
- Cellular level
  - cell modelling
  - **processes for cell survival**, damage etc.
- DNA level
  - DNA modelling
  - **physics processes at the eV scale**
  - bio-chemical processes
  - processes for DNA damage, repair etc.

Complexity of

software, physics and biology

addressed with an

iterative-incremental

software process

↓

Parallel development at all the three levels

(domain decomposition)

Low Energy Physics extensions

Z. Francis – S. Incerti - B. Mascialino – MG Pia

- Processes down to the eV scale
  - At this scale physics interactions depend on the detailed structure of the medium
  - Processes specialised by material
  - 1st cycle: processes in water
- Releases
  - β-version in Geant4 8.1 (June 2006)
  - Refined version in progress
  - Further extensions to follow
- Processes for other materials to follow
  - Interest for radiation effects on components
  - User requirements for gaseous materials

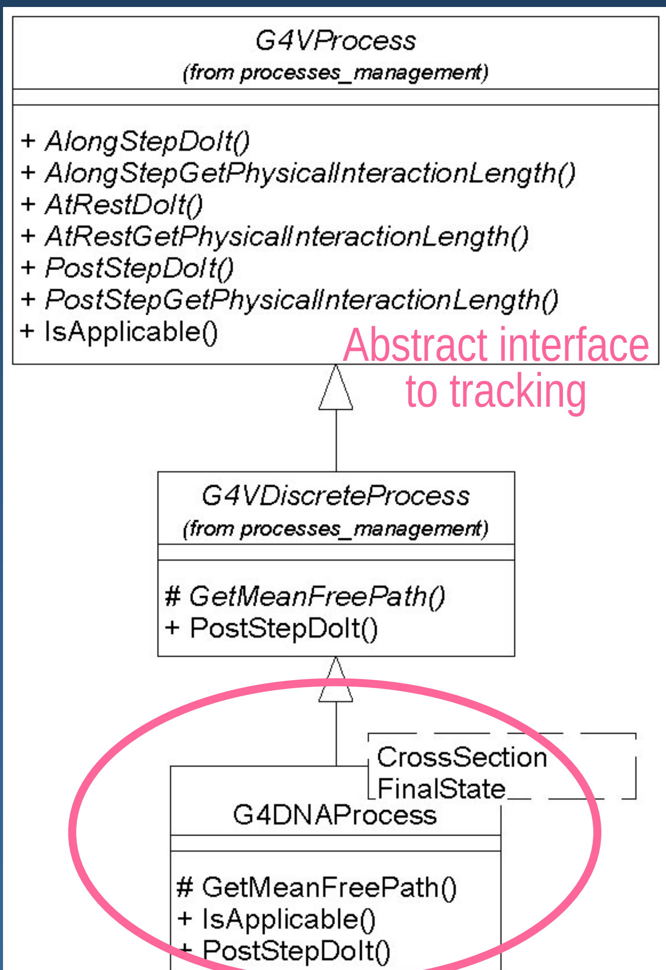
Particle	Processes
e	Elastic scattering Excitation Ionisation
p	Excitation Charge decrease Ionisation
H	Charge increase Ionisation
He++	Excitation Charge decrease Ionisation
He+	Excitation Charge decrease Charge increase Ionisation
He	Excitation Charge increase Ionisation

Software design

Playground for further applications of this design technique in the LowE EM package

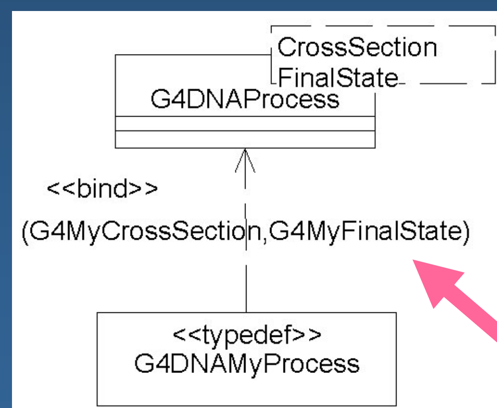
Innovative design introduced in Geant4: **policy-based class design**

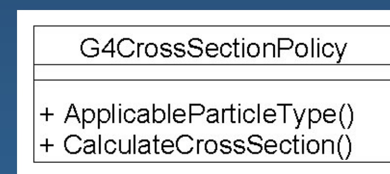
Flexibility of modeling + performance optimisation

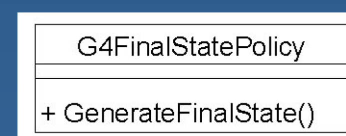


Policies

- cross section calculation
- final state generation







Parameterised class

The process can be configured with a variety of physics models by template instantiation

Policy based design

- Policy based classes are parameterised classes
  - classes that use other classes as a parameter
- Specialization of processes through template instantiation
  - The code is bound at compile time
- Advantages
  - Policies are not required to inherit from a base class
  - Weaker dependency of the policy and the policy based class on the policy interface
  - In complex situations this makes a design more flexible and open to extension
  - No need of virtual methods, resulting in faster execution
- Clean, maintainable design of a complex domain
  - Policies are orthogonal
- Open system
  - Proliferation of models in the same environment

Implementation

- First set of models implemented chosen among those available in literature
  - Direct contacts with theorists whenever possible
- Future extensions foreseen
  - Made easy by the design
  - Provide a wide choice among many alternative models
  - Different modeling approaches
  - Complementary models
  - Other materials than water
- Unit test in parallel with implementation

References of models implemented

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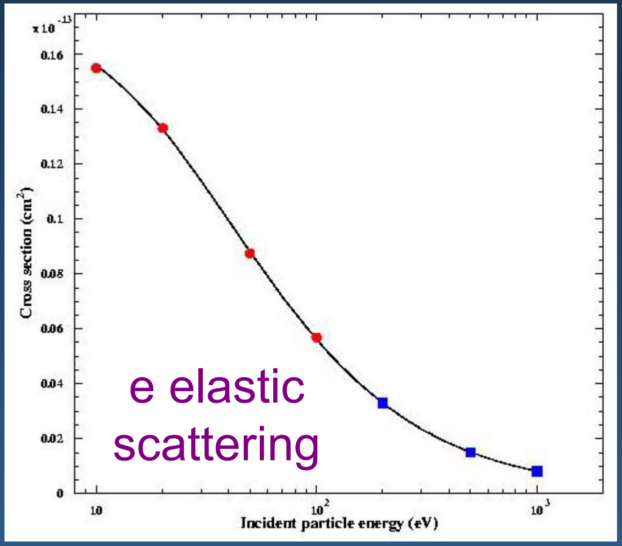
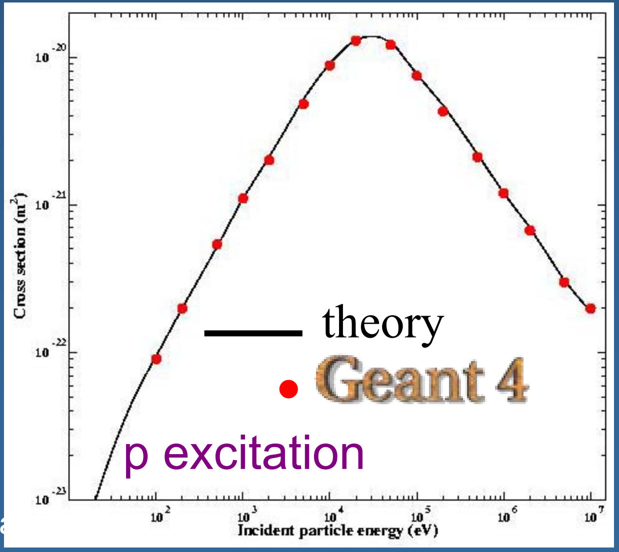
12. K. H. Berkner, R. V. Pyle, and J. W. Stearns, "Cross sections for electron capture by 0.3 to 70 keV deuterons in H2, H2O, CO, CH4, and C8F16 gases" , *Nucl. Fus*., vol. 10, pp. 145-149, 1970.
13. R. Dagnac, D. Blanc, and D. Molina, "A study on the collision of hydrogen ions H1+, H2+ and H3+ with a water-vapour target", *J. Phys. B: Atom. Molec. Phys*., vol. 3, pp.1239-1251, 1970.
14. L. H. Toburen, M. Y. Nakai, and R. A. Langley, "Measurement of high-energy charge transfer cross sections for incident protons and atomic hydrogen in various gases", *Phys. Rev*., vol. 171, no. 1, pp. 114-122, 1968.
15. P. G. Cable, Ph. D. thesis, University of Maryland, 1967.
16. M. E. Rudd, T. V. Goffe, R. D. DuBois, L. H. Toburen, "Cross sections for ionisation of water vapor by 7-4000 keV protons", *Phys. Rev. A*, vol. 31, pp. 492-494, 1985.

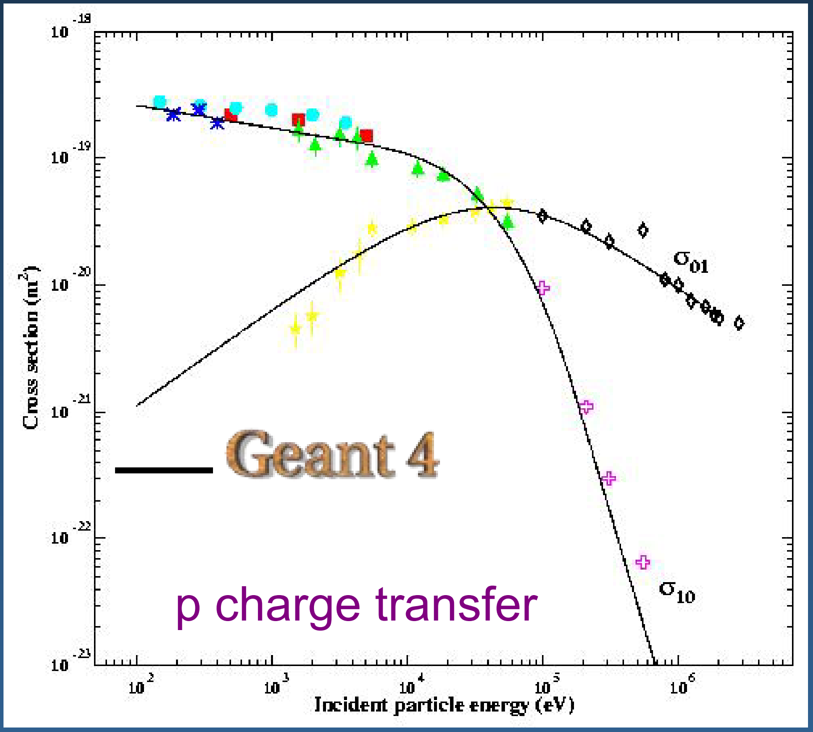
Test

Verification
against theoretical models





Comparison
against experimental data



Scarce experimental data

Large scale validation project planned

Outlook

- Publication
  - 1st software development cycle
- Validation
  - Scarce experimental data
  - 2nd publication
- New models for water
  - Some already identified
- **Models for other materials**
  - Facilitated by the design

In preparation

Geant4 Models for Low Energy Particle Interactions with Water

S. Chauvie, Z. Francis, S. Guatelli, S. Incerti, B. Mascialino, G. Montarou, P. Moretto, P. Nieminen, M. G. Pia

Abstract— **A set of processes specialized for the simulation of particle interactions with water has been developed in the Geant4 Low Energy Electromagnetic package. They address a physics domain relevant to the simulation of radiation effects in biological systems, where water represents an important component. The models cover the interactions of electrons, protons and light ions down to the electronVolt energy scale. The software design, the physics models implemented and a set of their tests are described.**

I. Introduction

THE simulation of radiation effects in biological systems is a critical concern in various domains, such as oncological radiotherapy and radiation protection. A common approach consists of describing the effects of the irradiation of a biological system in terms of the dose released to it. Nevertheless the concept of dose fails when the biological effects of radiation on cellular structures and on the DNA (deoxyribonucleic acid) molecule are the object of study.

The Geant4-DNA project addresses the extension of the Geant4 [1]-[2] simulation toolkit to deal with radiation effects at the cellular and DNA scale. It exploits the Geant4 architectural design to equip an open source, general purpose Monte Carlo system for particle transport for the first time with functionality specific to radiobiology simulation. This novel approach provides the user the opportunity to combine specialized tools for the study of the biological effects of radiation with the rich simulation functionality of a full Monte Carlo system for particle transport; nevertheless, thanks to the toolkit nature of Geant4, it does not imply any overhead for non essential functionality with respect to specialized Monte Carlo systems for radiobiology simulation: a user application only uses the toolkit components pertinent to it.

The Geant4-DNA software encompasses various domains: the extension of Geant4 physics processes down to the energy scale relevant to bio-molecular systems, the development of models to describe biological processes, and the description of biological entities, such as cells or the DNA molecule. The overall Geant4-DNA subsystem adopts a component-based architecture, where each domain is addressed by a software component.

This paper describes a new component of Geant4 physics developed in the context of the Geant4-DNA project: a set of specialized physics processes to model particle interactions in water, which is the main component of biological systems, down to the electronVolt energy scale. These new developments are identified in the following sections as the Geant4-DNA Physics Processes; they are part of the Geant4 Low Energy Electromagnetic Physics package [3]-[4].

The Geant4-DNA software is open-source; it is publicly released in the Geant4 Toolkit.

II. Software Process

The Geant4-DNA project addresses a very active scientific domain: the continuous progresses in biological research, as well as the availability of new accelerator facilities for cellular irradiation, contribute to a rapid evolution of the body of knowledge in fields pertinent to the project. The development of the Geant4-DNA software follows an iterative and incremental process. Such a process model is particularly suitable to address the complex, fast evolving research domain of radiation effects on biological systems: it allows building and refining the software taking into account the theoretical and experimental progresses in the field, at the same time producing concrete deliverables at each development cycle.

The software process of Geant4-DNA is based on the Unified Software Development Process [5] and adopts the Rational Unified Process™ (RUP) [6] as a process framework, tailored to the specific characteristics of the project and its scientific environment [7]. The rigorous software process,

Manuscript received September 20, 2006. Work partly supported through ESA/ESTEC Contract No. 14402/00/NL/MV.

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Biological models

Geant4-DNA

S. Chauvie – S. Guatelli – B. Mascialino – MG Pia

In progress

TARGET THEORY	Single-hit	$S = e^{-D/D_0}$
TARGET THEORY	Multi-target Single-hit	$S = 1-(1-e^{-qD})^n$ *Revised model*: $S = e^{-q_1 D}\,[\,1-(1-e^{-q_n D})^n\,]$
MOLECULAR THEORY	Radiation Action	$S = e^{-p(\alpha D + \beta D^2)}$
MOLECULAR THEORY	Dual Radiation Action	$S = S_0\, e^{-k(\xi D + D)^2}$
MOLECULAR THEORY	Repair-misrepair Lin Rep / Quadmis	$S = e^{-\alpha D}[1 + (\alpha DT / \varepsilon)]^{\varepsilon}$
MOLECULAR THEORY	Repair-misrepair Lin Rep / Mis	$S = e^{-\alpha D}[1 + (\alpha D / \varepsilon)]^{\varepsilon\Phi}$
MOLECULAR THEORY	Lethal-Potentially Lethal	$S = \exp[\,-N_{TOT}[1 + \frac{N_{PL}}{\varepsilon(1-e^{-\varepsilon BAtr})}\,]^{\varepsilon}\,]$
MOLECULAR THEORY	Lethal-Potentially Lethal – Low Dose	$S = e^{-\eta_{AC} D}$
MOLECULAR THEORY	Lethal-Potentially Lethal – High Dose	$-\ln[S(t)] = (\eta_{AC} + \eta_{AB}) D - \varepsilon \ln[1 + (\eta_{AB} D/\varepsilon)(1 - e^{-\varepsilon BA\, tr})]$
MOLECULAR THEORY	Lethal-Potentially Lethal – LQ Approx	$-\ln[S(t)] = (\eta_{AC} + \eta_{AB}\, e^{-\varepsilon BAtr})\, D + (\eta^2_{AB}/2\varepsilon)(1 - e^{-\varepsilon BA\, tr})^2 D^2]$

Not only for biology...

- The significant effort invested in a general design makes the system suitable to very low energy physics extensions relevant to other domains too
  - Radiation effects on components
  - Gaseous detectors
  - etc.
  - Only limitation: womanpower

- Collaboration with interested parties
  - No work duplication!
  - Sound software design

Validation

A large amount of activity is invested in validation

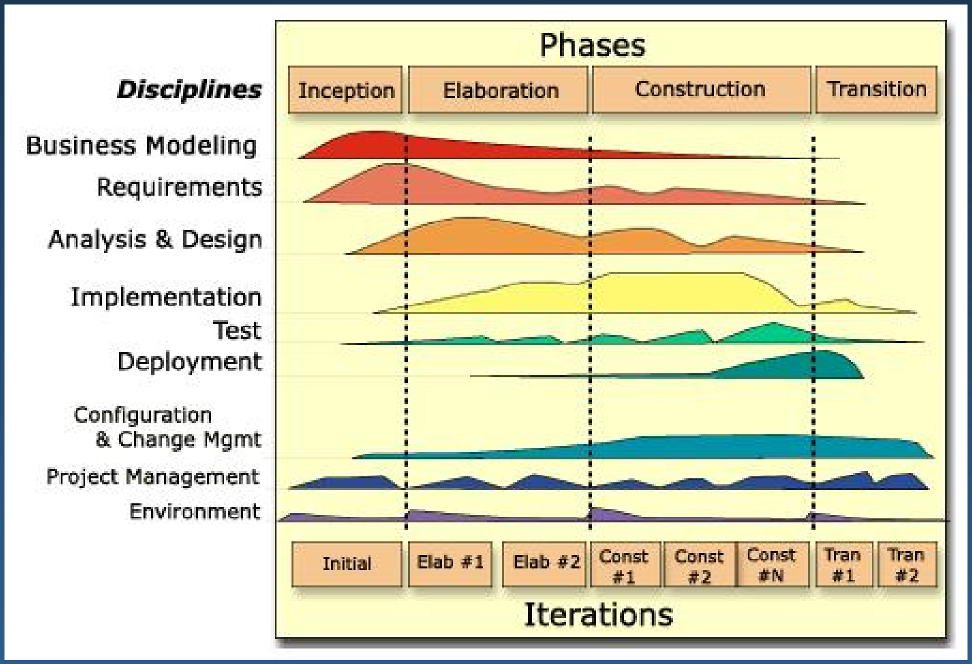
Essential also for further development cycles and design iterations

- Atomic relaxation
- Bremsstrahlung
- Proton Bragg peak
- + other validation activities in Advanced Examples

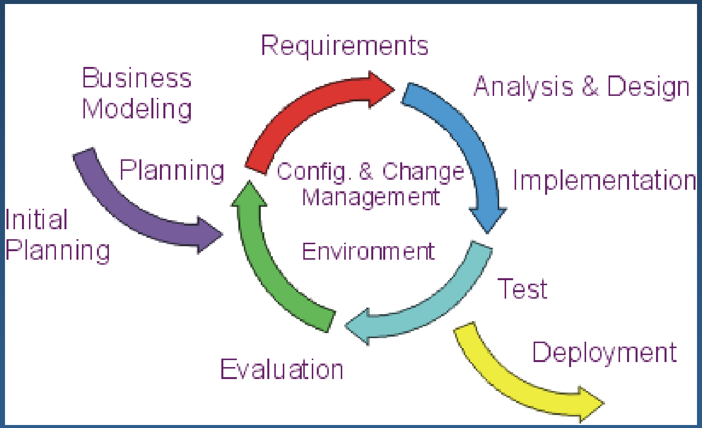
- Statistical Toolkit

- Common features of the validation activities
  - **Collaborative, open, transparent work environment**
  - Rigorous, quantitative analysis
  - Publication-quality methods and results

...and behind everything



Unified Process



A rigorous software process

Incremental and iterative lifecycle

RUP™ as process framework, tailored to the specific project

Mapped onto ISO 15504

Stéphane Chauvie
Pablo Cirrone
Giacomo Cuttone
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Geant4
Advanced Examples

http://www.ge.infn.it/geant4/examples

M.G. Pia
On behalf of the Advanced Examples Working Group

Mission

Investigate, **evaluate** and **demonstrate Geant4 capabilities** in various **experimental environments**

Provide **guidance** to Geant4 **users** in **realistic experimental applications**

Provide **feedback** to Geant4 **developers** about successful results, problems etc.

Identify **requirements** for further Geant4 **improvements** and **extensions** to address new experimental domains

Advanced Examples

1. air_shower
2. **brachytherapy**
3. ***cell_irradiation***
4. composite_calorimeter
5. cosmicray_charging
6. gammaray_telescope
7. **hadrontherapy**
8. **human_phantom**
9. lAr_calorimeter
10. **medical_linac**
11. **microbeam**
12. *nanotechnology*
13. **purging_magnet**
14. *radiation_monitor*
15. **radioprotection**
16. raredecay_calorimetry
17. RICH
18. Tiara
19. underground_physics
20. xray_fluorescence
21. xray_telescope

- Released
- *In preparation*

- Wide experimental coverage
  - HEP
  - Space science/astrophysics
  - **Medical physics**
  - Radiobiology
  - Detector technologies

- Wide Geant4 coverage
  - Geometry features
  - Magnetic field
  - Physics (EM and hadronic)
  - Biological processes
  - Hits & Digis
  - Analysis
  - Visualisation, UI

Validation

- **Goal:** document **quantitatively** the validation of the physics selections of all advanced examples
  - Objectively supported physics options rather than "educated guess" PhysicsLists
- Strategy
  - **Generic** validation studies of processes/models used
    Collaboration with Geant4 Physics Working Groups desirable
  - **Specific** validation studies with ad hoc experimental data
    Collaboration with experimental teams

Conclusion

- Emphasis on rigorous software process
- Significant investment in **Analysis & Design** process
- **Advanced design techniques**
- Rich physics functionality
- Precision modeling
- Extensions to the eV scale
- Biological processes
- **Validation** of existing models is a major activity in the Group
- Guidance to users through **Advanced Examples**