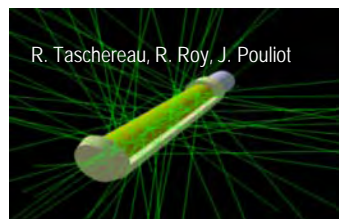
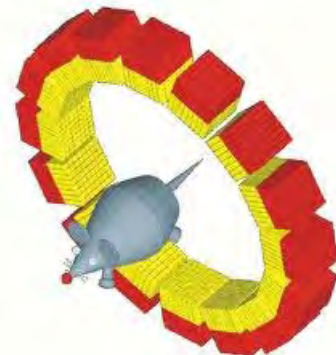


*Courtesy T. Ersmark, KTH Stockholm*



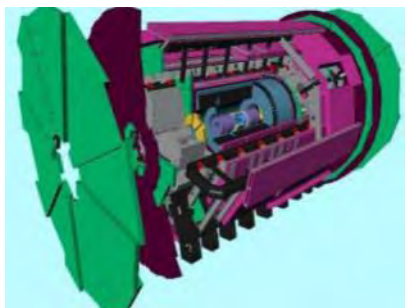
R. Taschereau, R. Roy, J. Pouliot

# Geant 4



*GATE Collaboration*

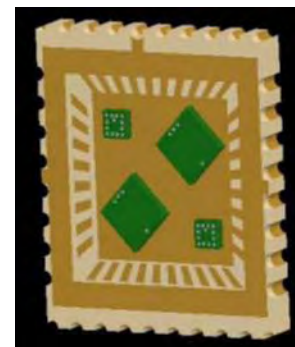
## Physics Modeling Capabilities



*Courtesy of ATLAS Collaboration*

Maria Grazia Pia

*INFN Genova, Italy*



**ANS Winter Meeting 2010**

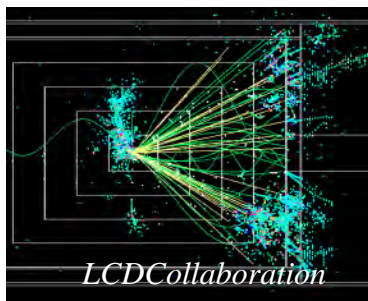
Thursday, 11 November 2010

Las Vegas, NV

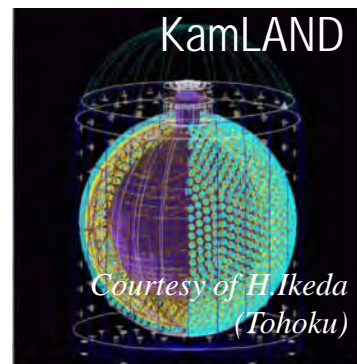
<http://cern.ch/geant4>



*Courtesy of H. Araujo,  
Imperial College London*



*LCDCollaboration*



**KamLAND**

*Courtesy of H. Ikeda  
(Tohoku)*

# Physics

“It was noted that experiments have requirements for **independent, alternative physics models**. In Geant4 these models, *differently from the concept of packages*, allow the user to **understand** how the results are produced, and hence improve the **physics validation**. Geant4 is developed with a modular architecture and is the ideal framework where existing components are integrated and new models continue to be developed.”

Minutes of LCB (LHCC Computing Board) meeting, 21/10/1997

# Physics: general features

- Ample variety of physics functionality
- **Abstract interface** to physics processes
  - Tracking **independent** from physics
- Open system
  - Users can easily create and use their own models
- Distinction between **processes** and **models**
  - often multiple models for the same physics process
  - complementary/alternative

# Outline

Geant4 physics in less than one hour...

- **A little bit of software**

- Basic concepts of Geant4 use: application, PhysicsList

- **Overview of Geant4 physics functionality**

- Electromagnetic and hadronic physics

- **Validation**

- Concepts and a few results

- **Outlook**

# Toolkit + User application

- Geant4 is a **toolkit**
  - i.e. one cannot “run” Geant4 out of the box
  - One must write an application, which uses Geant4 tools
- Consequences
  - There is no such concept as “**Geant4 defaults**”
  - One must provide the necessary information to configure one’s simulation
  - The user must deliberately **choose** which Geant4 tools to use
- Guidance: many **examples** are distributed with Geant4

# Basic actions

- What a user **must** do:
  - Describe the **experimental set-up**
  - Provide the **primary particles** input to the simulation
  - Decide which **particles** and **physics models** one wants to use out of those available in Geant4 and the desired precision of the simulation (*cuts to produce and track secondary particles*)
- One may also **want**
  - To interact with Geant4 kernel to **control** the simulation
  - To **visualise** the simulation configuration or results
  - To produce **objects encoding simulation results** to be further analysed

# Interaction with Geant4 kernel

- Geant4 design provides **tools** for a user application
  - To tell the kernel about one's simulation configuration
  - To interact with Geant4 kernel itself
- Geant4 tools for user interaction are **base classes**
  - One creates **one's own concrete class** derived from the base classes
  - Geant4 kernel handles derived classes transparently through their base class interface (**polymorphism**)
- **Abstract base classes** for user interaction
  - User derived concrete classes are **mandatory**
- **Concrete base classes** (with *virtual* dummy methods) for user interaction
  - User derived classes are **optional**

# User classes

## Initialisation classes

*Invoked at initialization*


- *G4VUserDetectorConstruction*
- *G4VUserPhysicsList*

## Action classes

*Invoked during the execution*

- *G4VUserPrimaryGeneratorAction*
- *G4UserRunAction*
- *G4UserEventAction*
- *G4UserTrackingAction*
- *G4UserStackingAction*
- *G4UserSteppingAction*

## Mandatory classes:

- 
- *G4VUserDetectorConstruction*  
describe the experimental set-up
  - *G4VUserPhysicsList*  
select the physics one wants to activate
  - *G4VUserPrimaryGeneratorAction*  
generate primary events



# G4VUserPhysicsList

- It is one of the mandatory user classes (*abstract class*)
- It is the way one interacts with Geant4 kernel to tell it
  - which **particles** one intends to track in the simulation
  - which **processes** and models one decides to activate
  - the **thresholds** to produce secondary particles
- Pure virtual methods
  - ConstructParticles()
  - ConstructProcesses()
  - SetCuts()

to be implemented by the user in his/her concrete derived class

# Concepts

What is tracked

G4ParticleDefinition  
G4DynamicParticle  
G4Track

Process interface

G4VProcess  
Processes interacting with tracking

Production cuts

Why production cuts are needed  
The cuts scheme in Geant4

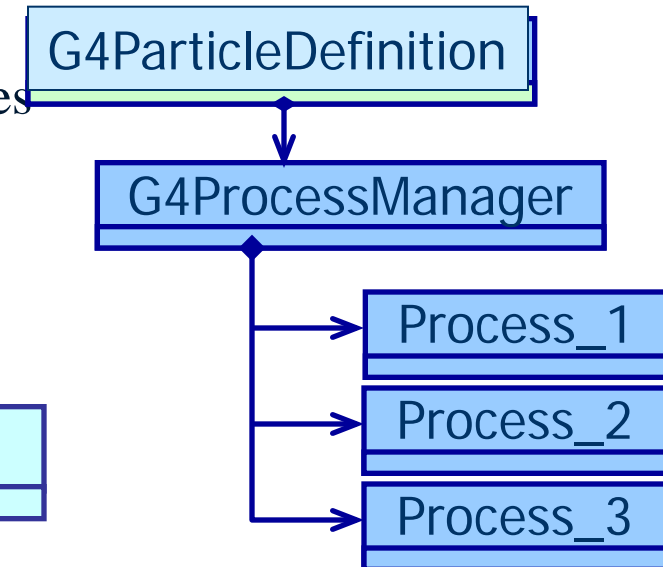
How the user  
interacts with  
Geant4 kernel

G4VUserPhysicsList  
Concrete physics lists

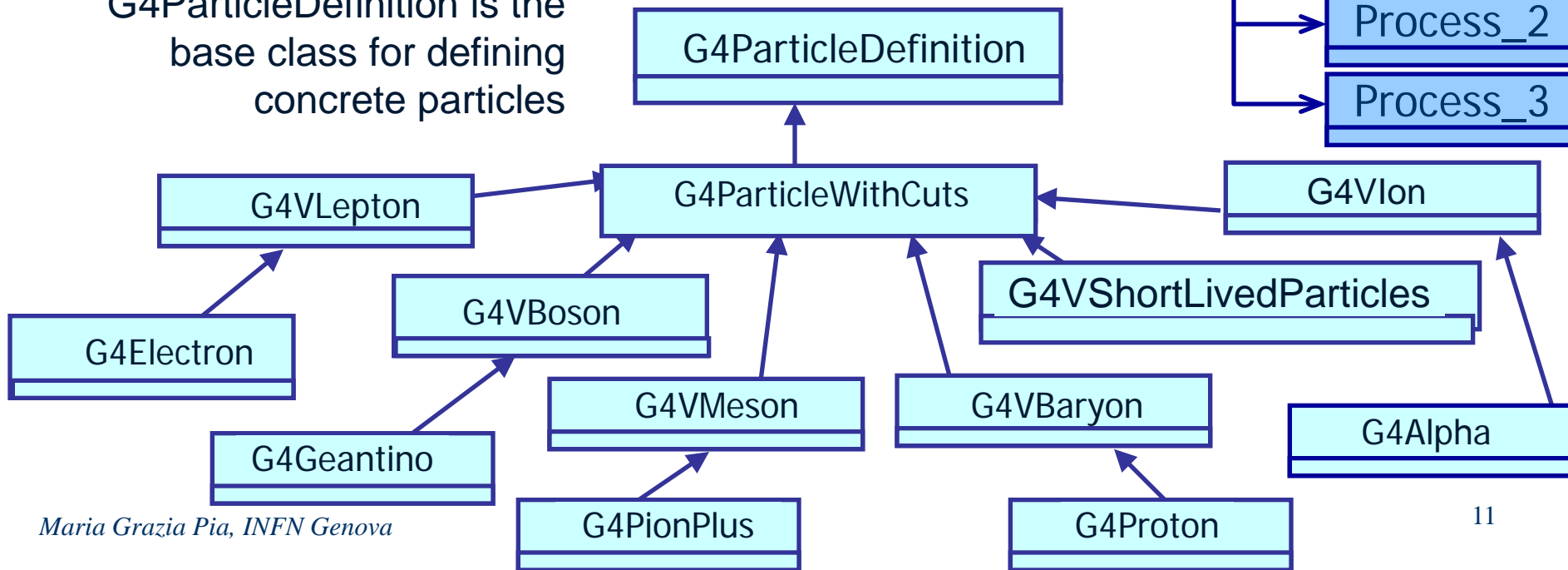
# G4ParticleDefinition

- ✓ intrinsic particle properties
  - *mass, width, spin, lifetime...*
- ✓ sensitivity to physics

- A **G4ProcessManager** object is attached to G4ParticleDefinition
- **G4ProcessManager** manages the list of processes the user wants the particle to be sensitive to
- **G4ParticleDefinition** does not know by itself its sensitivity to physics



G4ParticleDefinition is the base class for defining concrete particles



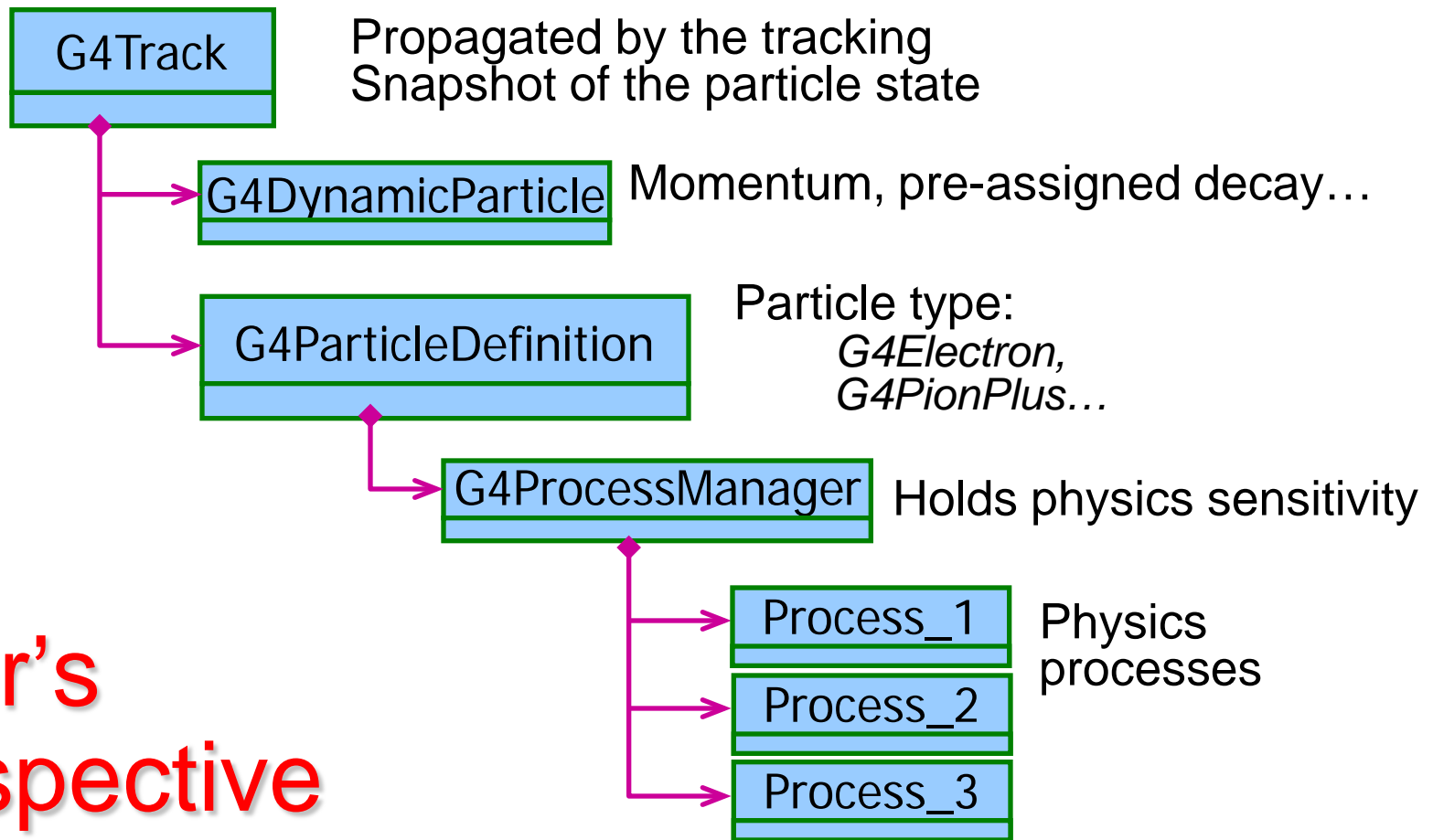
# G4DynamicParticle

- Describes the purely dynamic part of the particle state:
  - momentum, energy, polarization
- Holds a G4ParticleDefinition pointer
- Retains eventual pre-assigned decay information
  - decay products, lifetime

# G4Track

- Defines the class of objects propagated by Geant4 tracking
- Represents a snapshot of the particle state
- Aggregates
  - a G4ParticleDefinition
  - a G4DynamicParticle
  - geometrical information: *position, current volume etc.*
  - track ID, parent ID
  - process which created it
  - weight, used for event biasing

# User's perspective

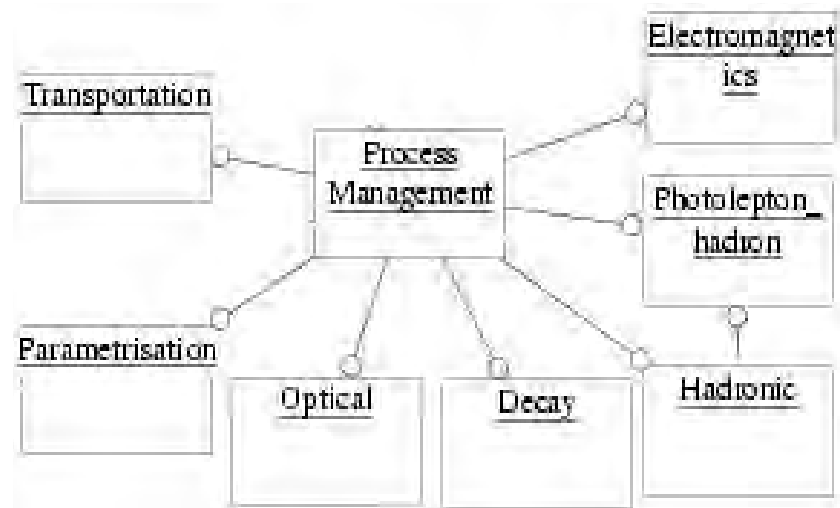


The classes involved in implementing a **PhysicsList** are:

- G4ParticleDefinition concrete classes
- G4ProcessManager
- the processes

# Processes

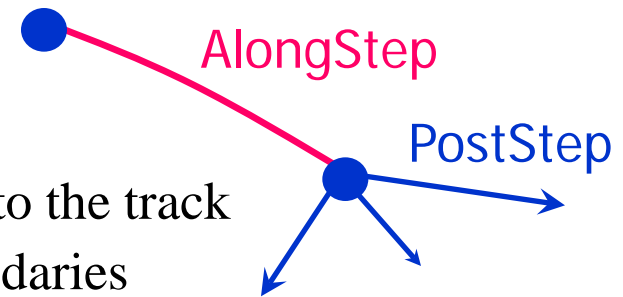
- Processes describe how particles interact with material or with a volume
- Three basic types
  - **At rest** process  
(eg. *decay at rest*)
  - **Continuous** process  
(eg. *ionisation*)
  - **Discrete** process  
(eg. *Compton scattering*)
- Transportation** is a process
  - interacting with volume boundary
- A process which requires the shortest interaction length limits the step



# G4VProcess

Abstract class defining the common interface of all processes in Geant4

- Defines three kinds of actions:
  - **AtRest** actions: decay, annihilation ...
  - **AlongStep** actions: continuous interactions occurring along the path, like ionisation
  - **PostStep** actions: point-like interactions, like decay in flight, hard radiation...
- A process can implement *any combination* of the three actions
- Each action defines two methods:
  - **GetPhysicalInteractionLength**
    - used to limit the step size
  - **Dolt**
    - implements the actual action to be applied to the track
    - implements the related production of secondaries
- **Geant4 stepping treats processes generically**
  - it does not know which process it is handling
- Geant4 stepping lets the processes
  - cooperate for **AlongStep** actions
  - compete for **PostStep** and **AtRest** actions



# Cuts in Geant4

- In Geant4 there are **no tracking cuts**
  - particles are tracked down to a zero range/kinetic energy
- Only **production cuts** exist
  - i.e. thresholds allowing a particle to be born or not

## *Why are production cuts needed ?*

- Some electromagnetic processes involve **infrared divergences**
  - This leads to an infinity [huge number] of smaller and smaller energy photons/electrons (*such as in Bremsstrahlung,  $\delta$ -ray production*)
  - Production cuts limit this production to particles above a threshold
  - The remaining, divergent part is treated as a continuous effect (*AlongStep* action)
- Secondary production thresholds are defined in terms of **range**
  - The production of a secondary particle is relevant if it can generate visible effects in the detector, otherwise “*local energy deposit*”
  - A range cut allows one to easily define such visibility: “*I want to produce particles able to travel at least 1 mm*”
  - criterion which can be applied uniformly across the detector (whole or “region”)



# Electromagnetic packages in Geant4

- Standard
- Low energy
- High energy
- Optical
- Muons
- X-rays *(but most X-ray physics is elsewhere)*
- Polarisation *(but some polarised processes are elsewhere)*
- Different modeling approach
- Specialized according to particle type, energy scope

Recent software design evolutions  
Improvements and drawbacks documented in  
conference proceedings  
(e.g. CHEP 2009, NSS 2009, Monte Carlo 2010)

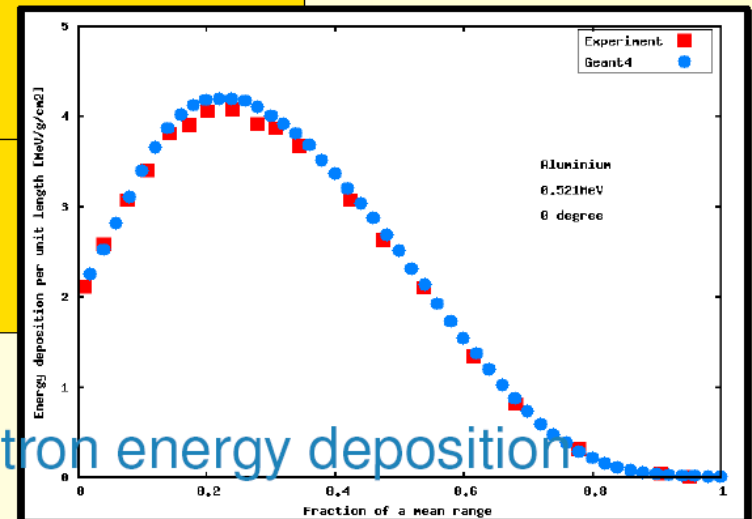
# Standard electromagnetic physics

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
<b>Photons</b>	Gamma conversion into $e^+e^-$ pair Compton scattering Photoelectric effect
<b>Electrons, Positrons</b>	Ionization Coulomb scattering Bremsstrahlung
<b>Positrons</b>	Annihilation

Example: Electron energy deposition



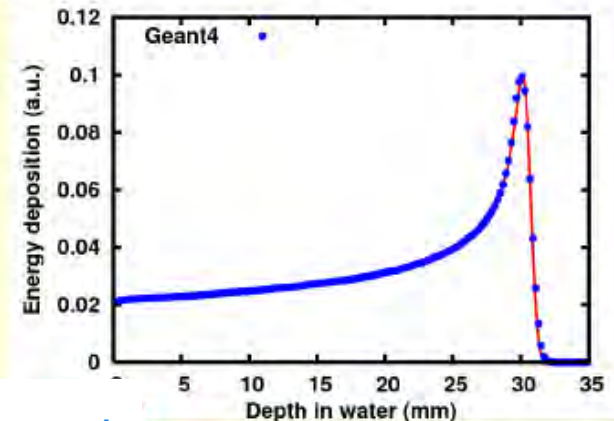
# Processes: hadrons

Particle	Processes
<b>Hadrons, Ions</b>	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)



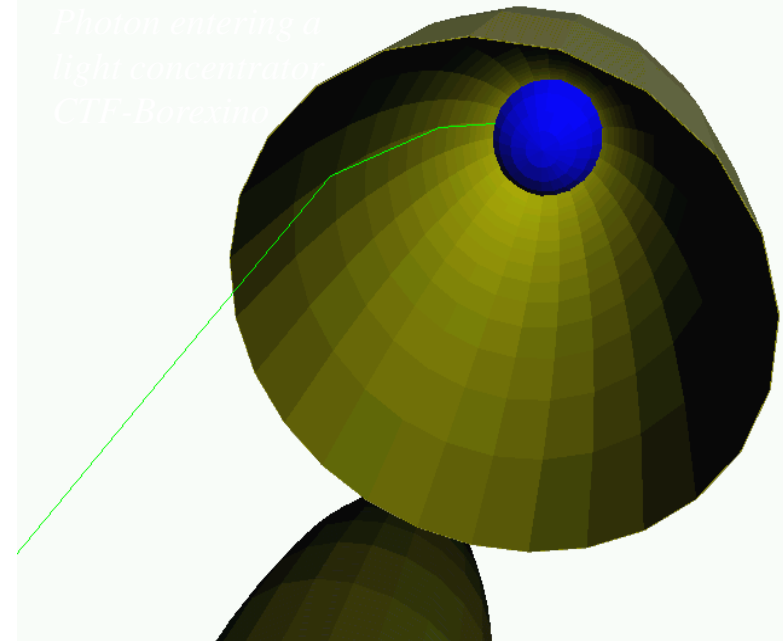
Example: proton Bragg peak

# 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)



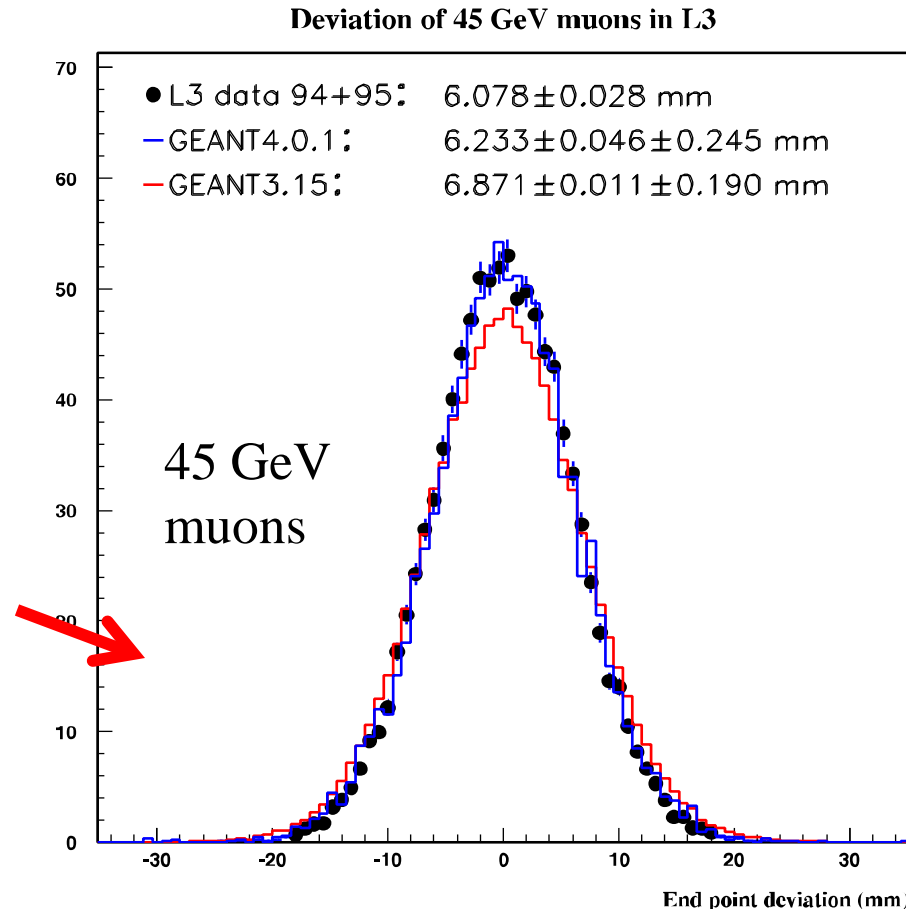
# Muons

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

Limited documentation of **validation** in the literature of the high energy end

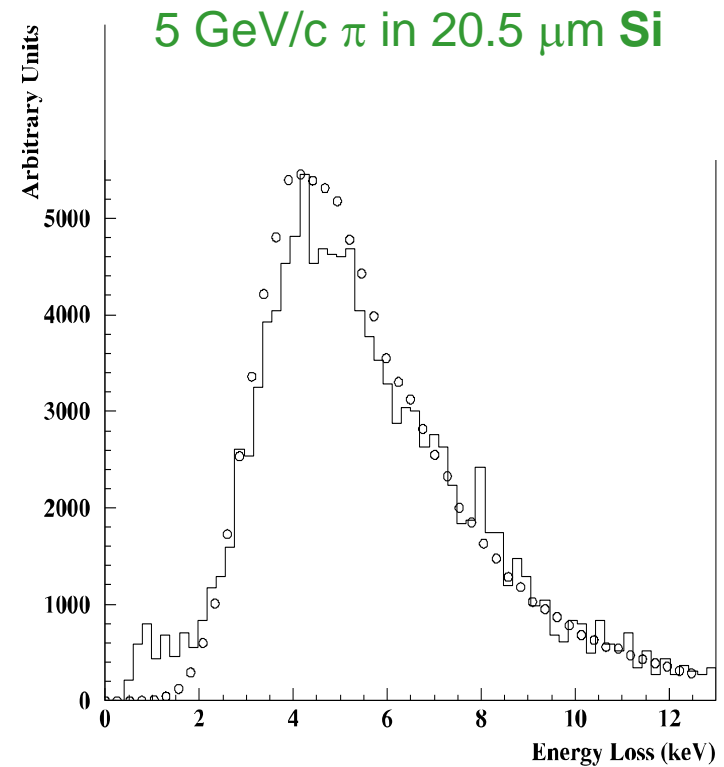
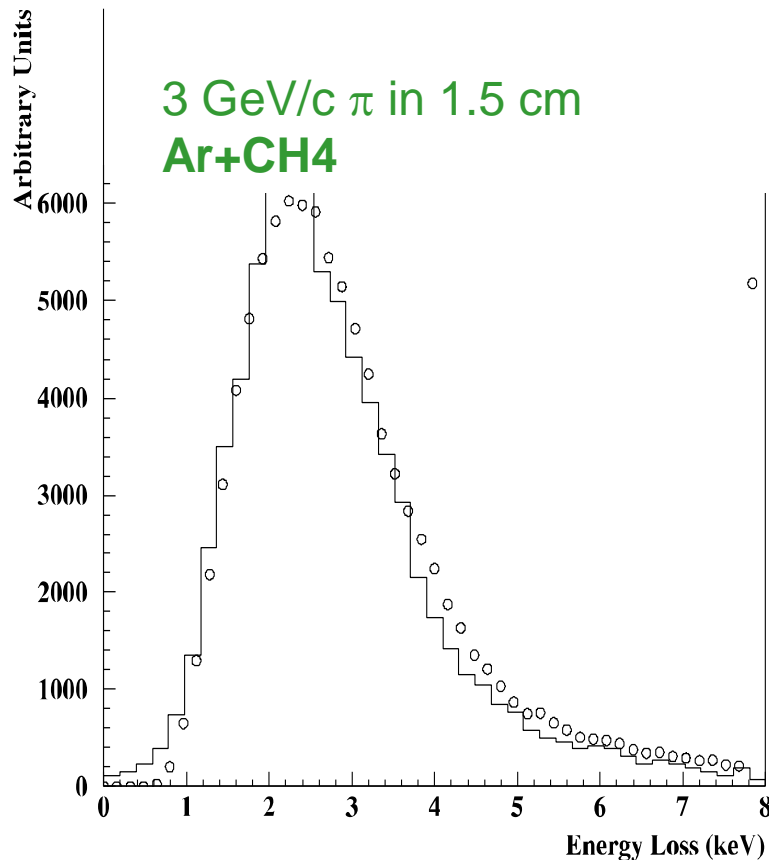
Data at 1 PeV?

Test of multiple scattering modeling (2000) by P. Arce, documented in CMS note



# 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*

# Multiple scattering

- Original Geant4 (Urban) model based on Lewis theory
  - Uses phenomenological functions to sample angular and spatial distributions after a step in particle transport
  - The function parameters are chosen, in order that the moments of the distribution are the same as given by the Lewis theory
- Recent development of other models
  - Goudsmit-Sanderson
  - WentzelVI
  - Single scattering
  - Urban in various flavours (Urban90, Urban92, Urban93...)
  - Specialized by particle type (beware of design tricks!)
  - etc.
- See Geant4 *Physics Reference Manual* and various conference proceedings for details



# Low energy electrons and photons

- Two “flavours” of models:
  - based on the **Livermore Library**
  - **à la Penelope**
- Nominally down
  - to 250 eV
    - based on the Livermore library
  - to a few hundreds eV
    - Penelope-like
- Compton scattering
- Rayleigh scattering
- Photoelectric effect
- Pair production
- Bremsstrahlung
- Ionisation
- Polarised Compton

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)

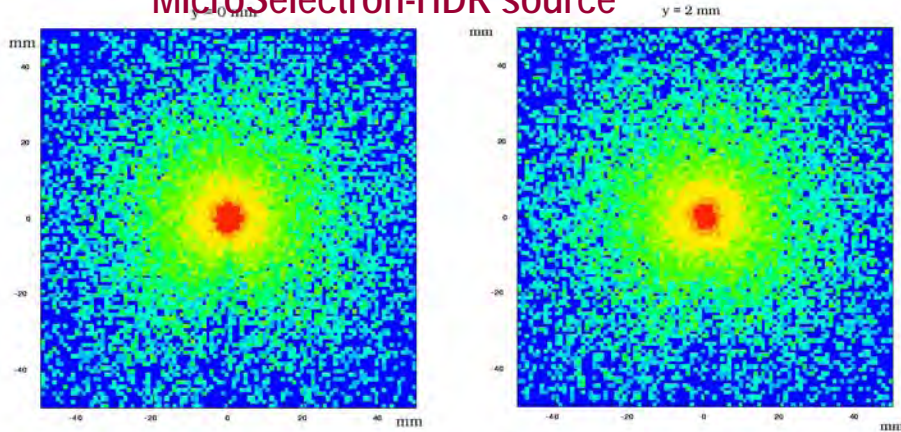
- + atomic relaxation
  - fluorescence
  - Auger effect

*following processes leaving a vacancy in an atom*

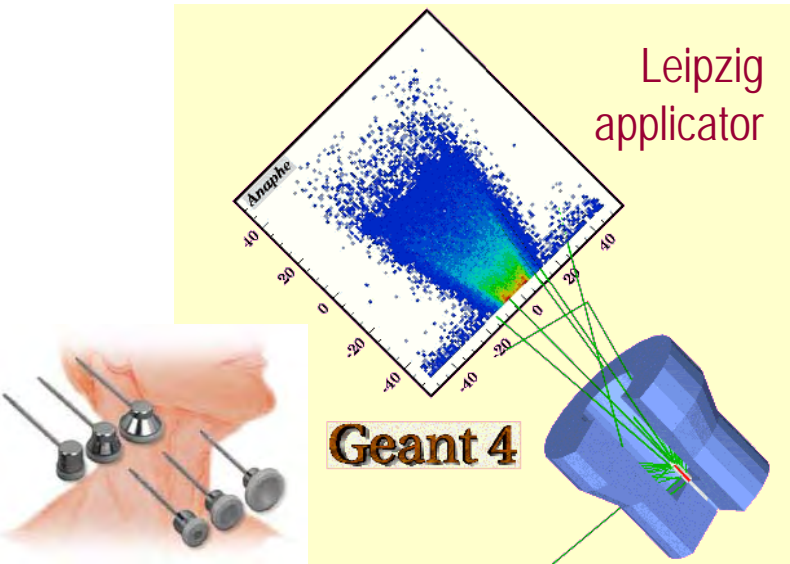
# Dosimetry Endocavitary brachytherapy



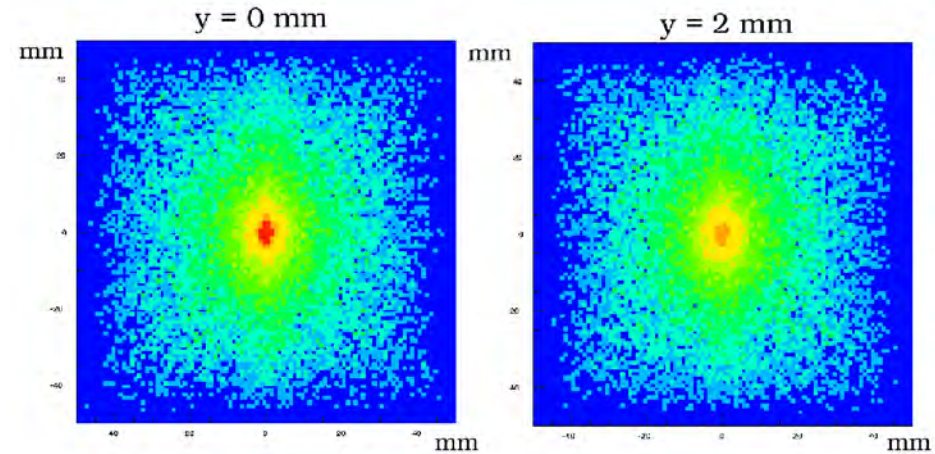
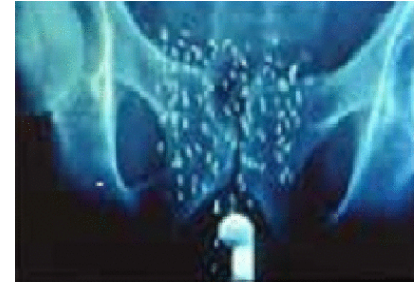
## MicroSelectron-HDR source



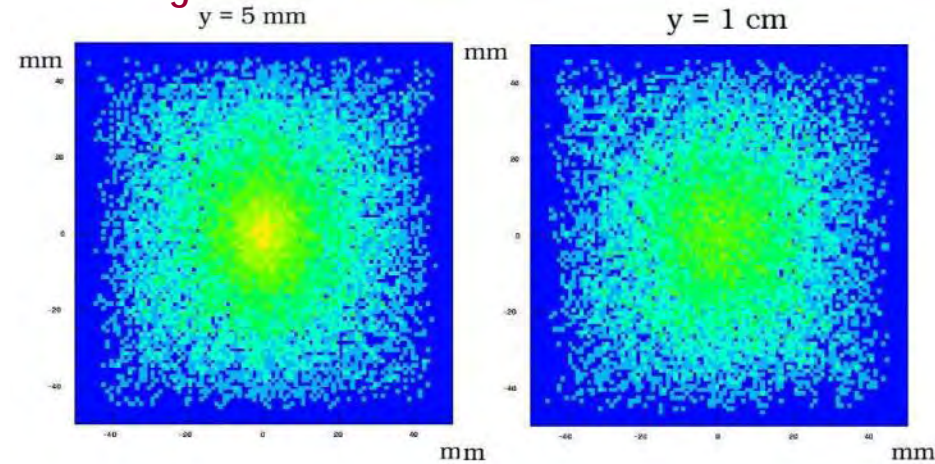
# Dosimetry Superficial brachytherapy



# Dosimetry Interstitial brachytherapy



## Bebig Isoseed I-125 source



# Polarisation

Cross section:

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

Low Energy  
Polarised Compton

250 eV - 100 GeV

Sample Methods:

Integrating over  $\phi$

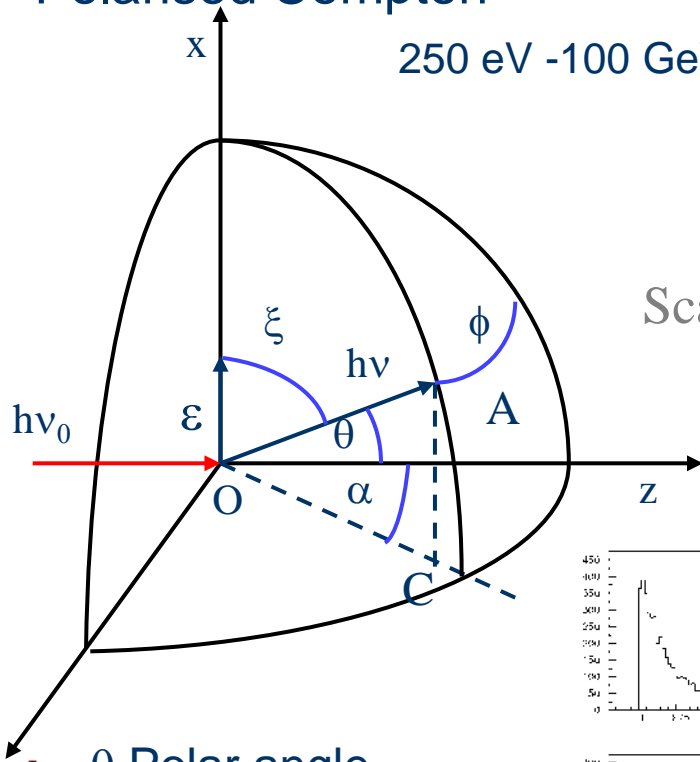
- Sample  $\theta$
- $\theta$  - Energy Relation  $\Rightarrow$  Energy
- Sample of  $\phi$  from  $P(\phi) = a(b - c \cos^2 \phi)$  distribution

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

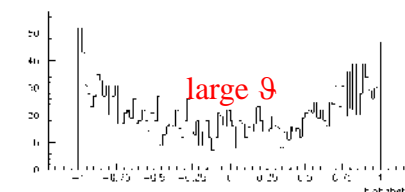
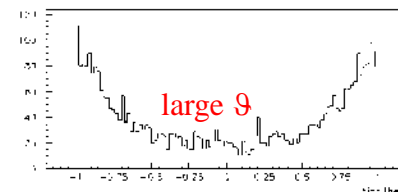
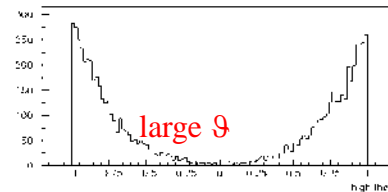
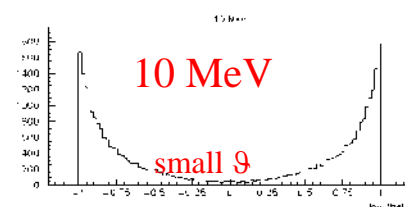
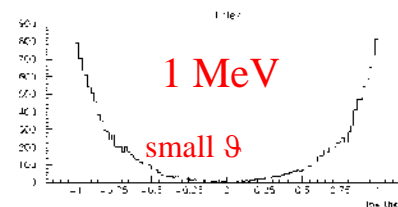
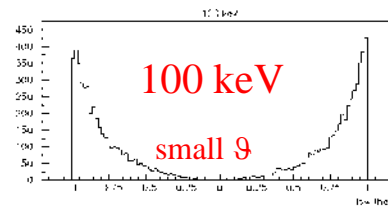
Scattered Photon Polarization

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

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



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



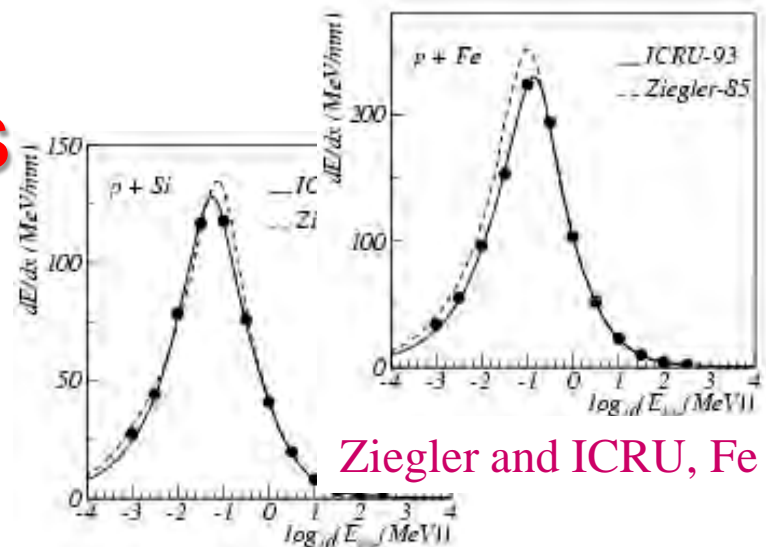


# Positive charged hadrons

- 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

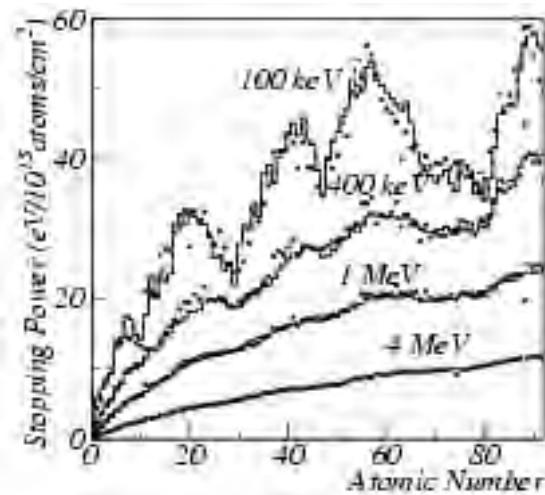
- Chemical effect for compounds
- Nuclear stopping power
- PIXE included



Ziegler and ICRU, Fe

Ziegler and ICRU, Si

- Spin dependent term
- Barkas and Bloch terms

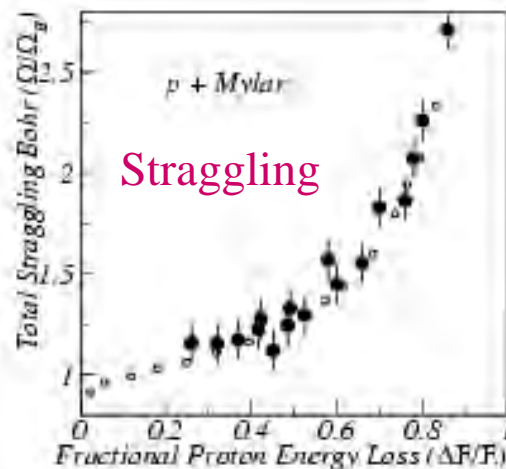


Stopping power

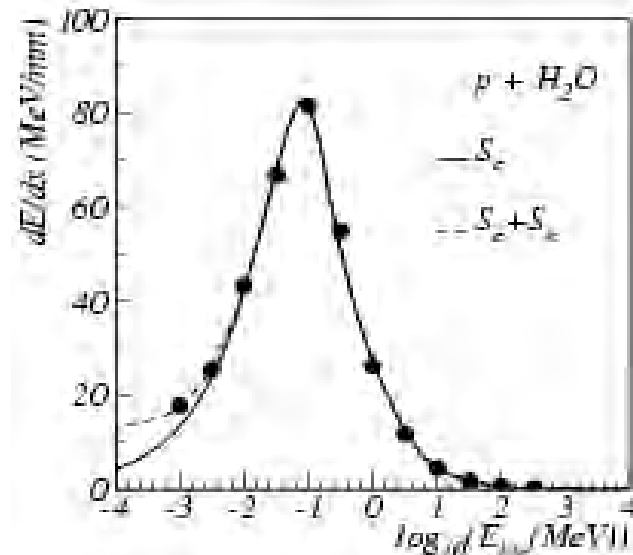
Z dependence for various energies

Maria Grazia Pia, INFN Genova

Ziegler and ICRU models



Straggling

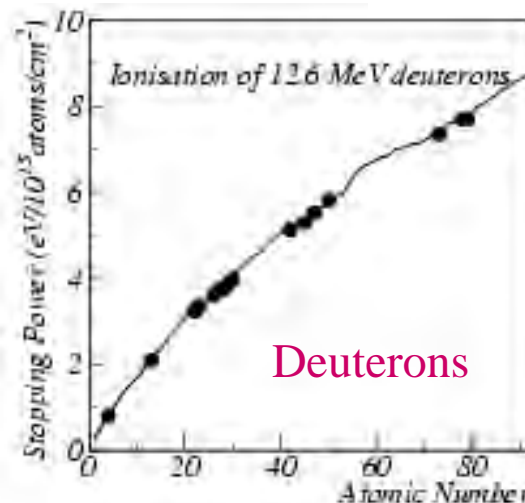
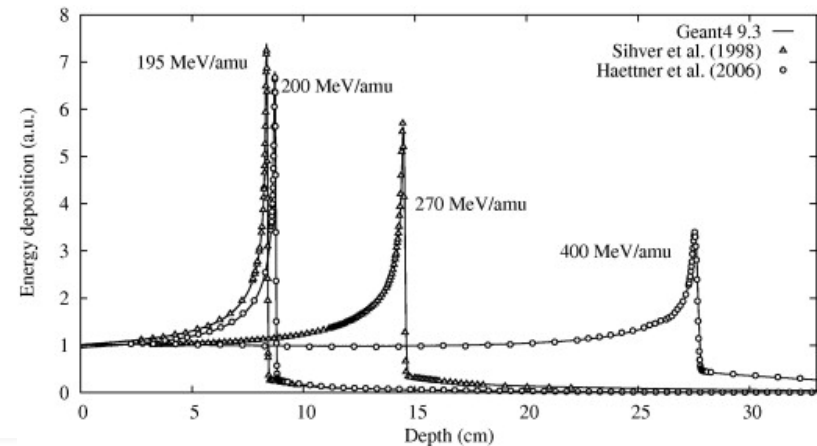


Nuclear stopping power

# Positive charged ions

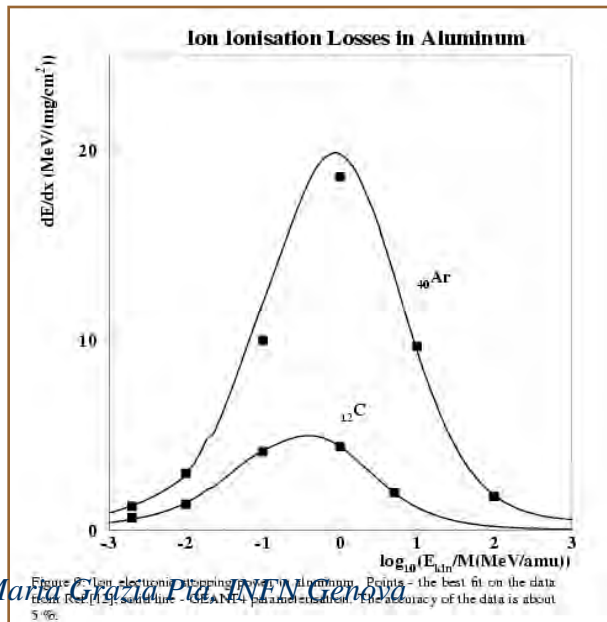
Recent implementation of ICRU73-based model and comparison with experimental data (A. Lechner et al.)

- 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



Comparison of simulated and measured  $^{12}\text{C}$  depth-dose profiles in water ( $0.997 \text{ g/cm}^3$ ). Simulations were performed with Geant4 9.3, using revised ICRU 73 stopping power tables and the QMD nuclear reaction model. Experimental data derive from Sihver et al. (triangles) and Haettner et al. (circles), where profiles of Haettner et al. were shifted to match more precise measurements of the peak position by D. Schardt et al. All experimental data by courtesy of D. Schardt.

A. Lechner et al., NIM B 268-14 (2010) 2343-2354



# Models for antiprotons

## Geant4 Model for the Stopping Power of Low Energy Negatively Charged Hadrons

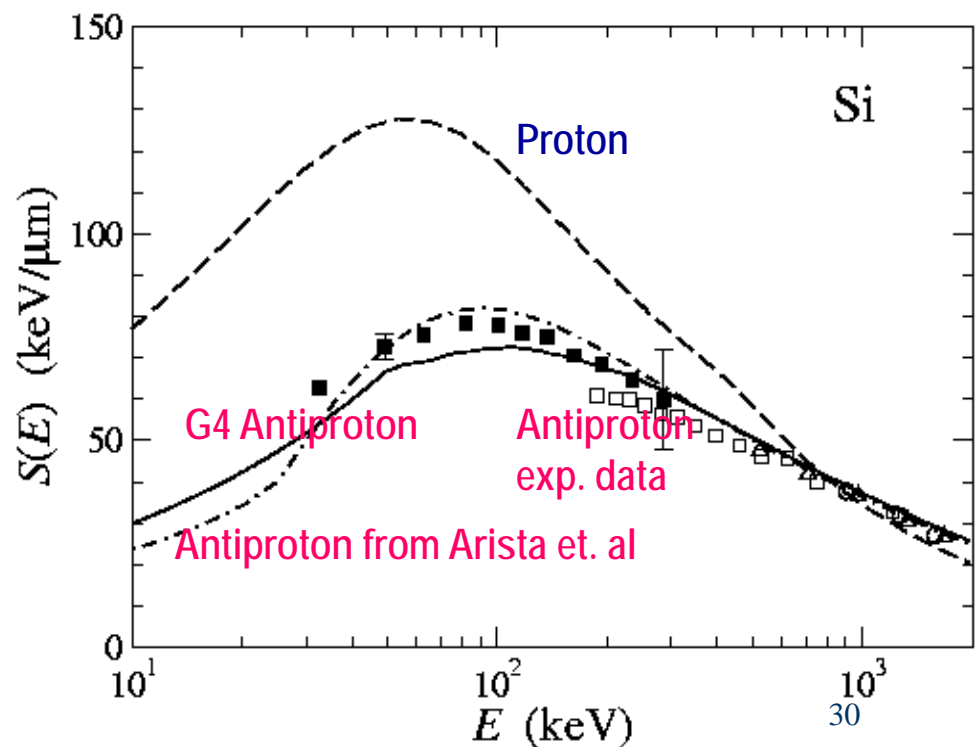
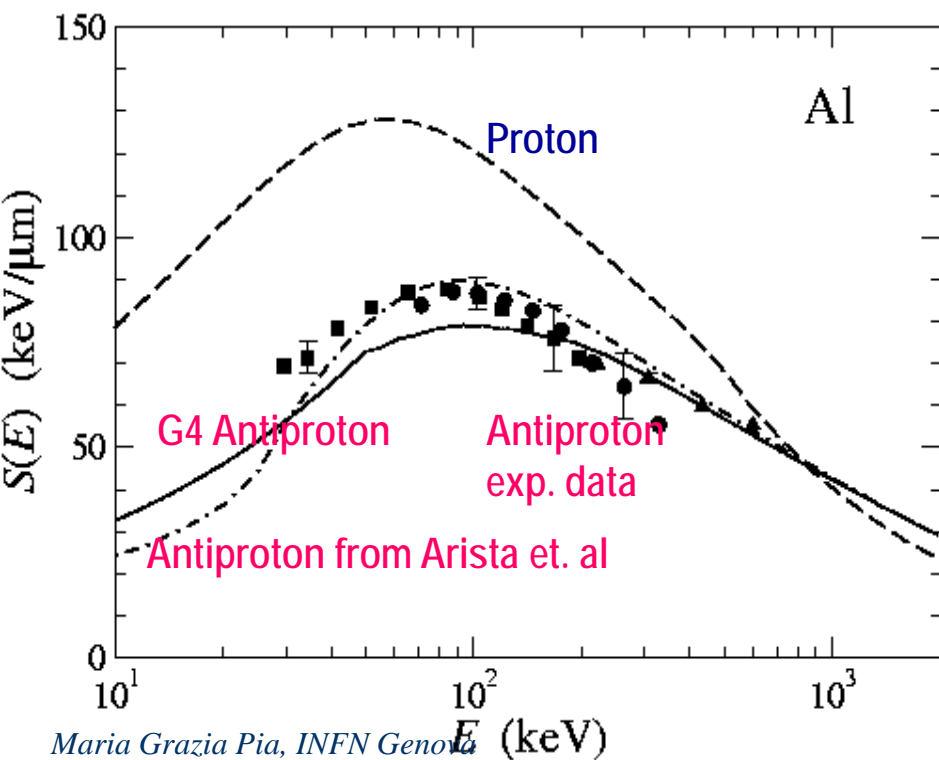
Stéphane Chauvie, Petteri Nieminen, and Maria Grazia Pia

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

Bethe-Bloch formula

Quantum harmonic oscillator model

Free electron gas model



## Geant4 Atomic Relaxation **9 pages**

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 **10 pages**

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

3650

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 56, NO. 6, DECEMBER 2009

## Validation of K and L Shell Radiative Transition Probability Calculations **12 pages**

Maria Grazia Pia, Paolo Saracco, and Manju Sudhakar

3614

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 56, NO. 6, DECEMBER 2009

## PIXE Simulation With Geant4 **36 pages**

Maria Grazia Pia, Georg Weidenspointner, Mauro Augelli, Lina Quintieri, Paolo Saracco, Manju Sudhakar, and Andreas Zoglauer

+ further ongoing activity and results

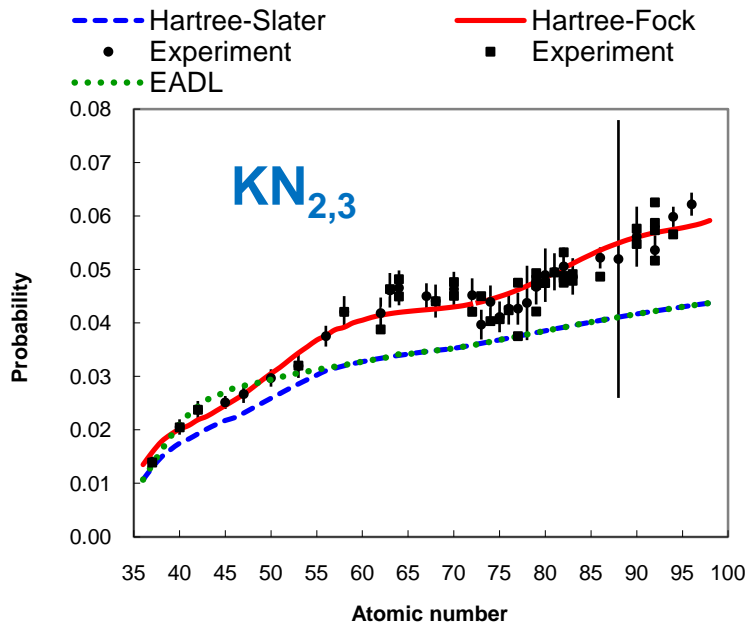
# Recent validation results

Geant4 Atomic Relaxation: X-ray fluorescence + Auger electron emission

**Data-driven** → Based on **EADL** (Evaluated Atomic Data Library)

Geant4 X-ray fluorescence simulation is as good as EADL

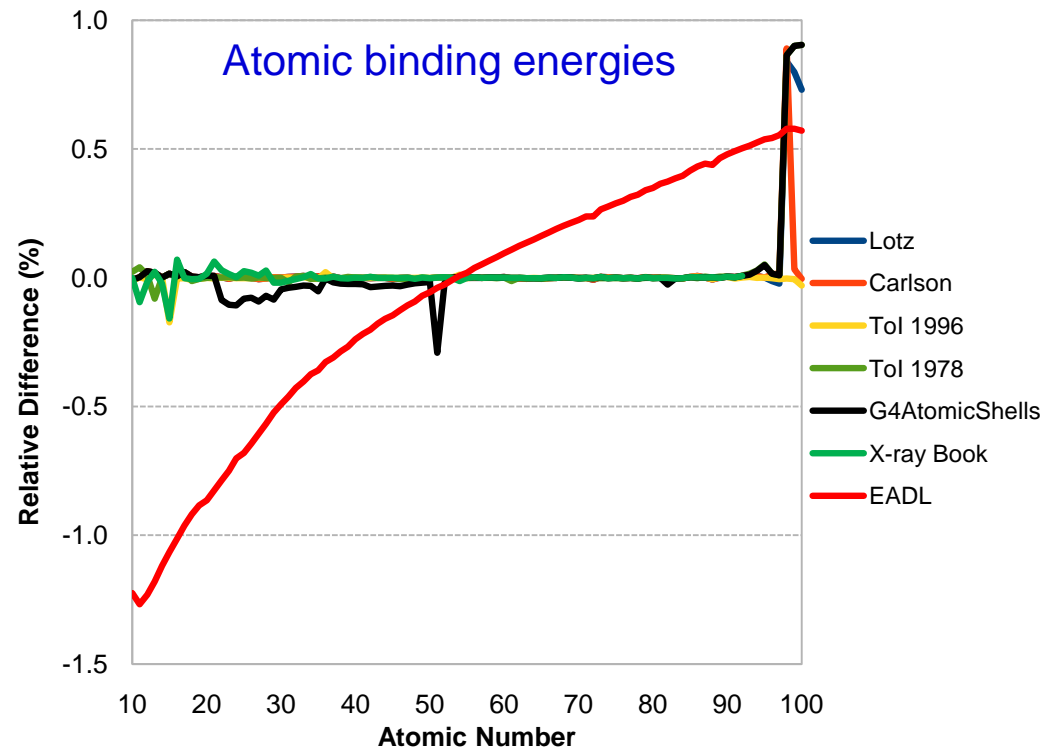
## Radiative transition probabilities



Hartree-Slater and Hartree-Fock calculations compared to experiments

*Maria Grazia Pia, INFN Genova*

## Atomic binding energies

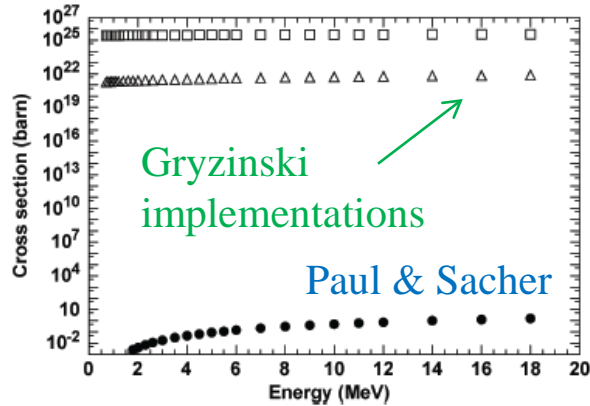


Difference w.r.t. DesLattes et al., experimental review

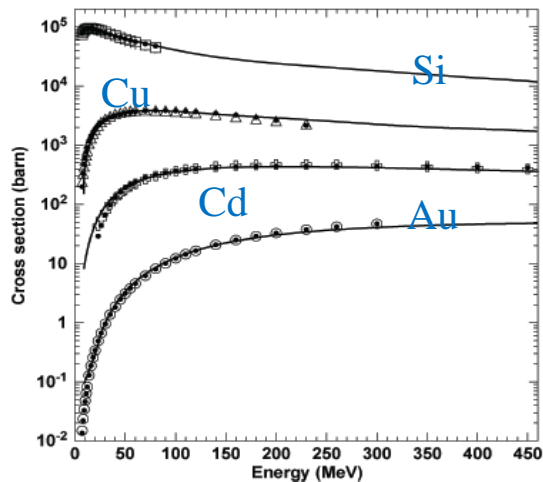


# Mishaps of Geant4 PIXE...

## 1<sup>st</sup> development cycle

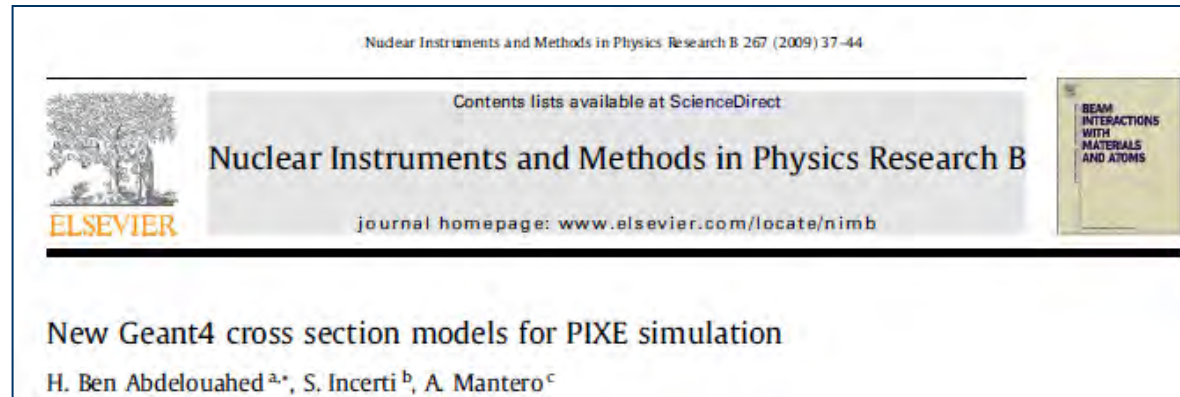


K shell ionisation, Au



Correctly implemented empirical  
(Paul&Bolik) cross sections for  $\alpha$   
particles incorrectly documented as  
Paul&Sacher cross sections for protons

## Current low energy group's development



Released in  
Geant4 9.2

Several flaws documented in  
*Pia et al., TNS 56(6), 3614-3649, 2003*

# Recent progress

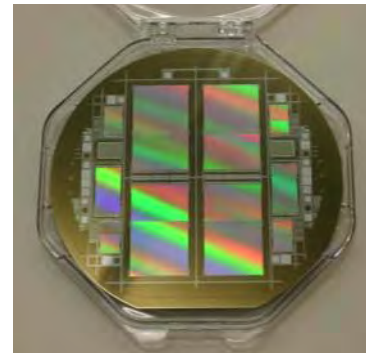
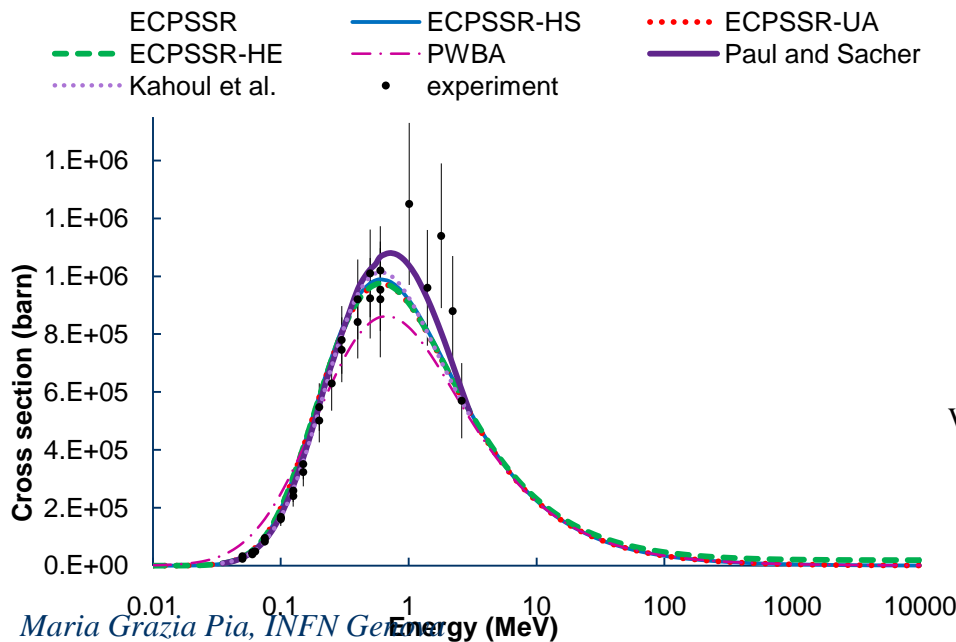
Hopefully, Geant4 collaboration will authorize the authors to release this code in Geant4, as requested by users, in December 2010

3614 IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 56, NO. 6, DECEMBER 2009

## PIXE Simulation With Geant4

Maria Grazia Pia, Georg Weidenspointner, Mauro Augelli, Lina Quintieri, Paolo Saracco, Manju Sudhakar, and Andreas Zoglauer

- Critical evaluation of **conceptual challenges**
- Wide collection of ionisation **cross section** models
- **Validation** and **comparative evaluation** of theoretical and empirical cross sections



Wafer including 4 eROSITA PNCCDs  
Courtesy R. Andritschke,  
MPI-MPE Halbleiterlabor

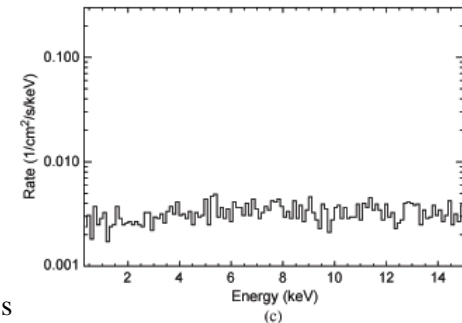
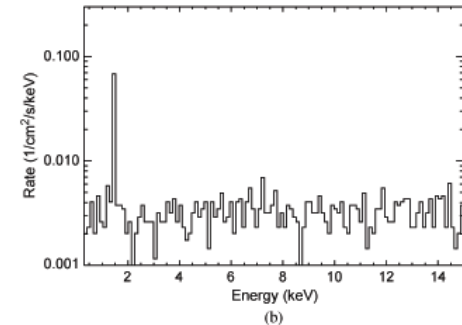
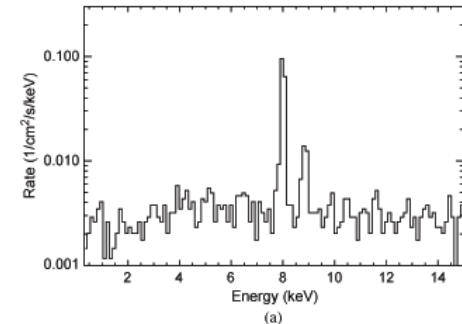
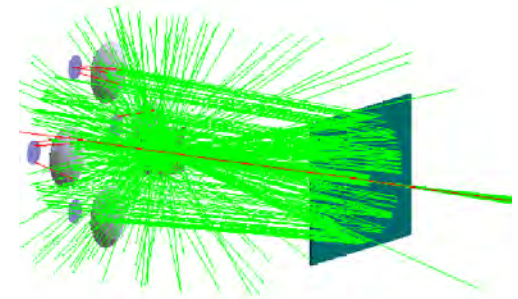
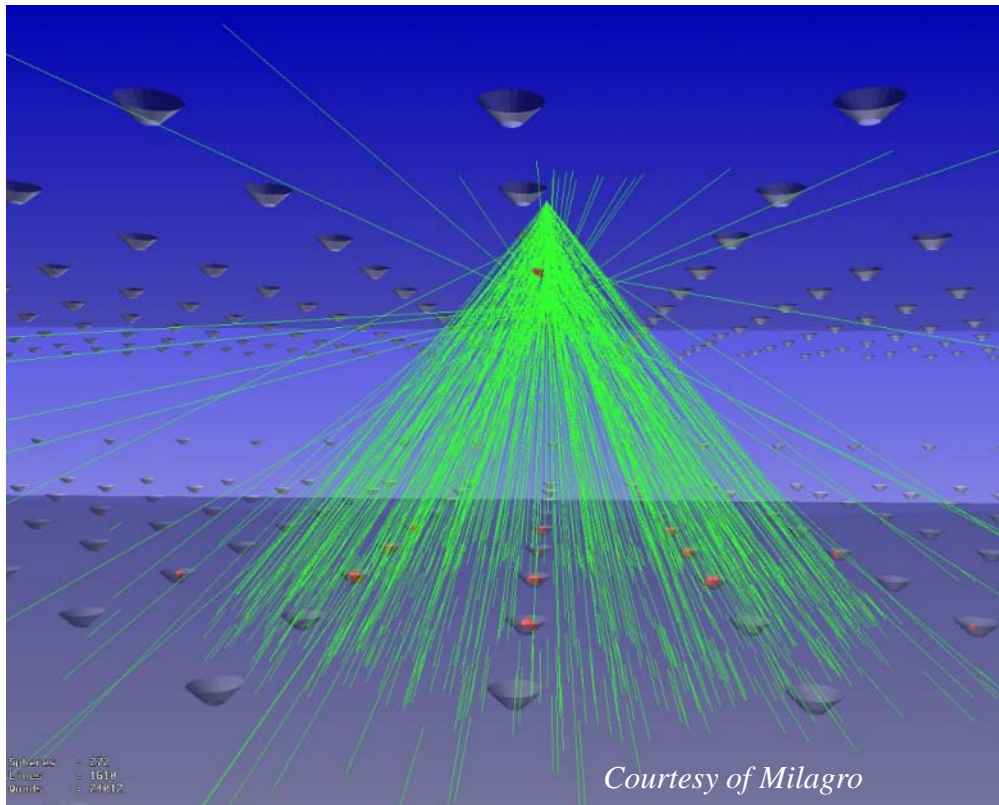


Fig. 12. A comparison of the fluorescence background due to ionization by cosmic-ray protons in an L2 orbit for three different graded Z shield designs for the eROSITA X-ray detectors. (a) Cu shield; (b) Cu-Al shield; (c) Cu - Al - B<sub>4</sub>C shield.

Software applied to a real-life problem:  
X-ray full-sky survey mission eROSITA

# Cherenkov

Milagro is a Water-Cherenkov detector located in a 60m x 80m x 8m covered pond near Los Alamos, NM

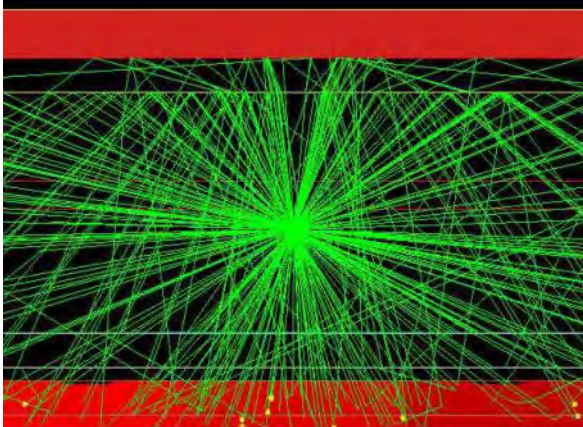


LHCb

Aerogel Thickness	Yield Per Event	Cherenkov Angle mrad
4 cm DATA	$6.3 \pm 0.7$	$247.1 \pm 5.0$
MC	$7.4 \pm 0.8$	$246.8 \pm 3.1$
8 cm DATA	$9.4 \pm 1.0$	$245.4 \pm 4.8$
MC	$10.1 \pm 1.1$	$243.7 \pm 3.0$

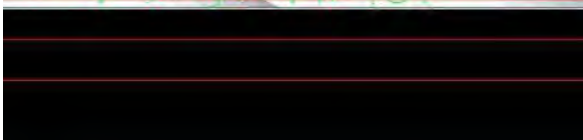


prompt scintillation

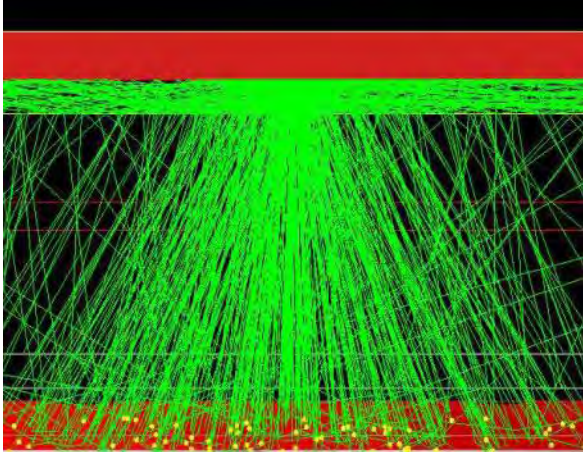


ZEPLIN III  
Dark Matter Detector

signal in PMT



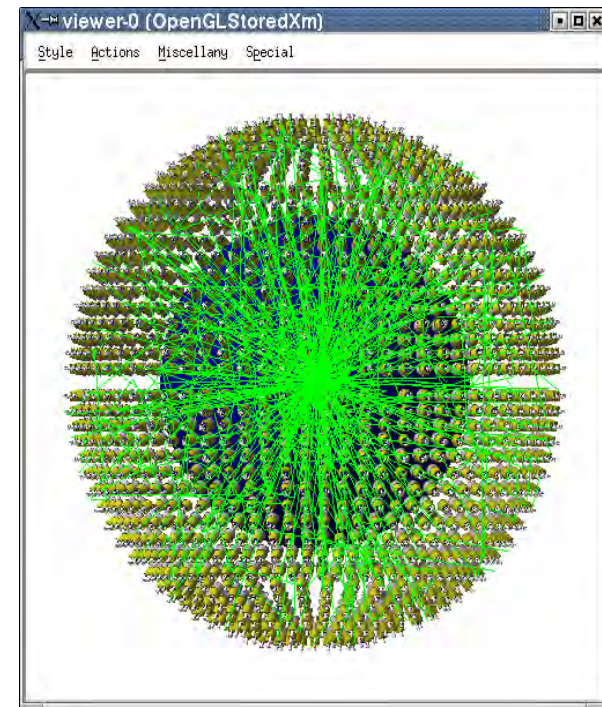
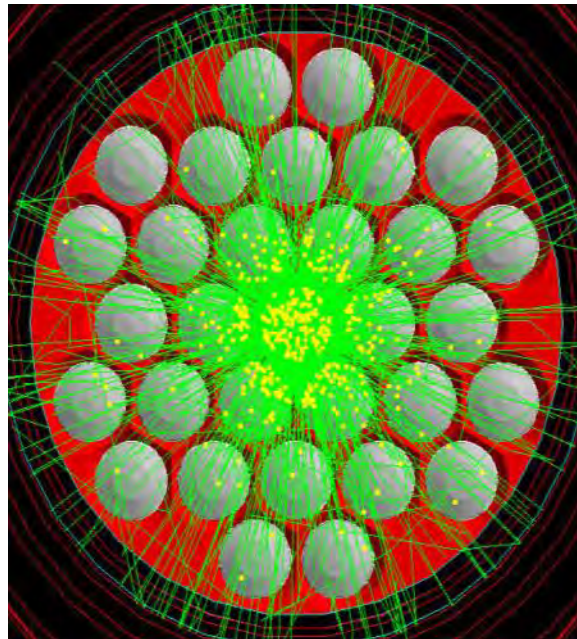
termoluminescence



*Courtesy of H, Araujo,  
Imperial College London*

# Scintillation

GEANT4 Scintillation Event in  
**BOREXINO**,  
INFN Gran Sasso  
National Laboratory



*Courtesy of Borexino*

# Very low energy extensions

1<sup>st</sup> development cycle:  
**Physics of interactions in water down to the eV scale**

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 54, NO. 6, DECEMBER 2007

2619

## Geant4 Physics Processes for Microdosimetry Simulation: Design Foundation and Implementation of the First Set of Models

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

## Further developments

*Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2010 (SNA + MC2010)*  
Hitotsubashi Memorial Hall, Tokyo, Japan, October 17-21, 2010

### Modeling Radiation Chemistry and Biology in the Geant4 Toolkit

M. Karamitros<sup>1</sup>, A. Mantero<sup>2</sup>, S. Incerti<sup>1\*</sup>, G. Baldacchino<sup>3</sup>, P. Barberet<sup>1</sup>, M. Bernal<sup>4,5</sup>, R. Capra<sup>6</sup>, C. Champion<sup>7</sup>, Z. El Bitar<sup>8</sup>,  
Z. Francis<sup>9</sup>, W. Friedland<sup>10</sup>, P. Guèye<sup>11</sup>, A. Ivanchenko<sup>1</sup>, V. Ivanchenko<sup>7,12</sup>, H. Kurashige<sup>13</sup>, B. Mascialino<sup>14</sup>, P. Moretto<sup>1</sup>,  
P. Nieminen<sup>15</sup>, G. Santin<sup>15</sup>, H. Seznec<sup>1</sup>, H. N. Tran<sup>1</sup>, C. Villagrasa<sup>9</sup> and C. Zacharatou<sup>16</sup>

***Still consistent with transport assumptions?***



# Ionisation models for nano-scale simulation

Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2010 (SNA + MC2010)

Hitotsubashi Memorial Hall, Tokyo, Japan, October 17-21, 2010

## Design, development and validation of electron ionisation models for nano-scale simulation

Hee SEO<sup>1</sup>, Maria Grazia PIA<sup>2\*</sup>, Paolo SARACCO<sup>2</sup>, Chan-Hyeung KIM<sup>1</sup>

**Student Paper Award  
Monte Carlo 2010**

<sup>1</sup> Hanyang University, 133-791 Seoul, Korea

<sup>2</sup> INFN Sezione di Genova, 16146 Genova, Italy

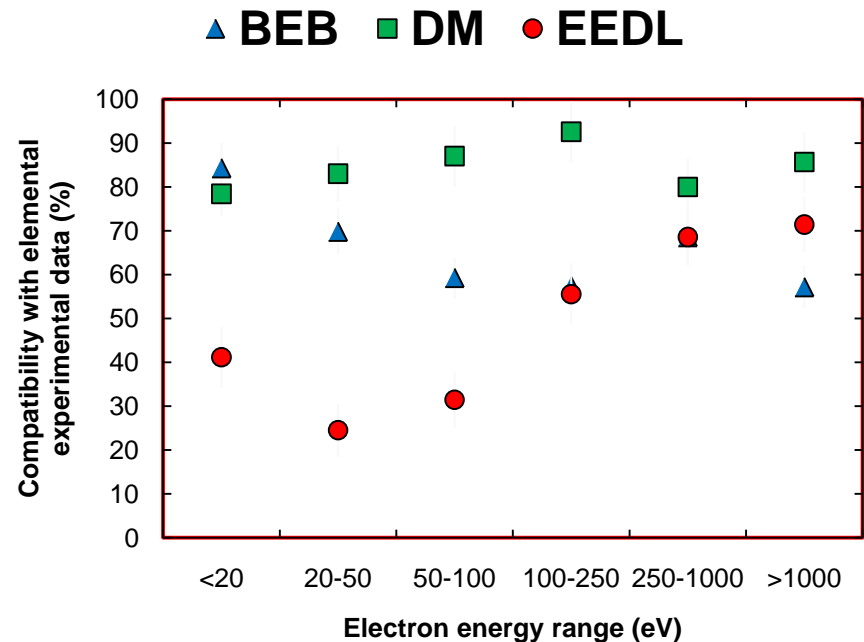
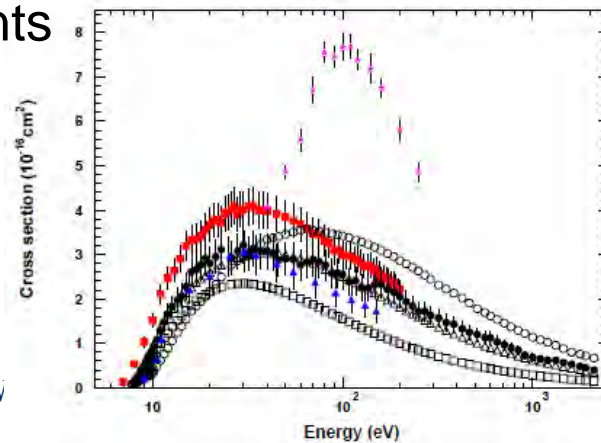
### Cross section models:

- Binary-Encounter-Bethe (**BEB**)
- Deutsch-Märk (**DM**)
- **EEDL**

**Validation**

181 experimental data sets

57 elements



Percentage of elements for which a model is compatible with experimental data at **95% CL**

# Hadronic physics challenge

- Even though there is an underlying theory (QCD), applying it is much more difficult than applying QED for simulating electromagnetic interactions
- Energy régimes:
  - Chiral perturbation theory ( $< 100$  MeV)
  - Resonance and cascade region (100 MeV – a few GeV)
  - QCD strings ( $> 20$  GeV)
- Within each régime several models are available
  - Many of these are phenomenological

# Hadronic framework



Computer Physics Communications 140 (2001) 65–75

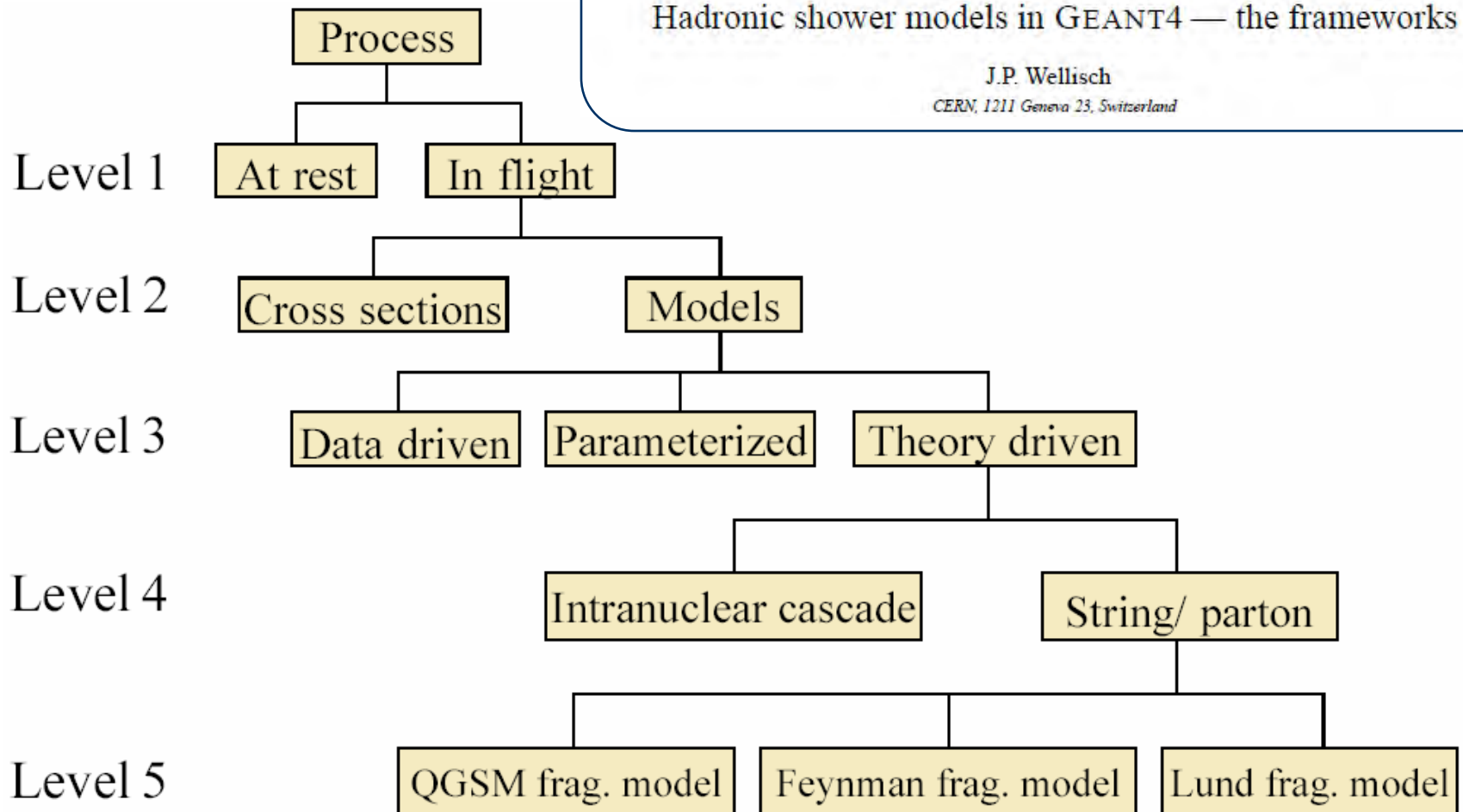
Computer Physics  
Communications

[www.elsevier.com/locate/cpc](http://www.elsevier.com/locate/cpc)

## Hadronic shower models in GEANT4 — the frameworks

J.P. Wellisch

CERN, 1211 Geneva 23, Switzerland





# Hadronic process

- **At rest**

- Stopped muon, pion, kaon, anti-proton
- Radioactive decay
- Particle decay (decay-in-flight is PostStep)

- **Elastic**

- Multiple models available

- **Inelastic**

- Different processes for each hadron (with multiple models)
- Photo-nuclear, electro-nuclear,  $\mu$ -nuclear

- **Capture**

- Pion- and kaon- in flight, neutron

- **Fission**

# Cross sections

- Default cross section data sets are provided for each type of hadronic process:
  - Fission, capture, elastic, inelastic
- Can be overridden
- Cross section data sets
  - Some contain only a few numbers
  - Some represent large databases

## Alternative cross sections

- To be used for specific applications, or for a given particle in a given energy range
- **Low energy neutrons**
  - elastic, inelastic, fission and capture ( $< 20$  MeV)
- **n and p inelastic** cross sections
  - $20 \text{ MeV} < E < 20 \text{ GeV}$
- **Ion-nucleus reaction** cross sections (several models)
  - Good for  $E/A < 1 \text{ GeV}$
- **Isotope production** data
  - $E < 100 \text{ MeV}$
- **Photo-nuclear** cross sections

# Parameterised and data-driven hadronic models

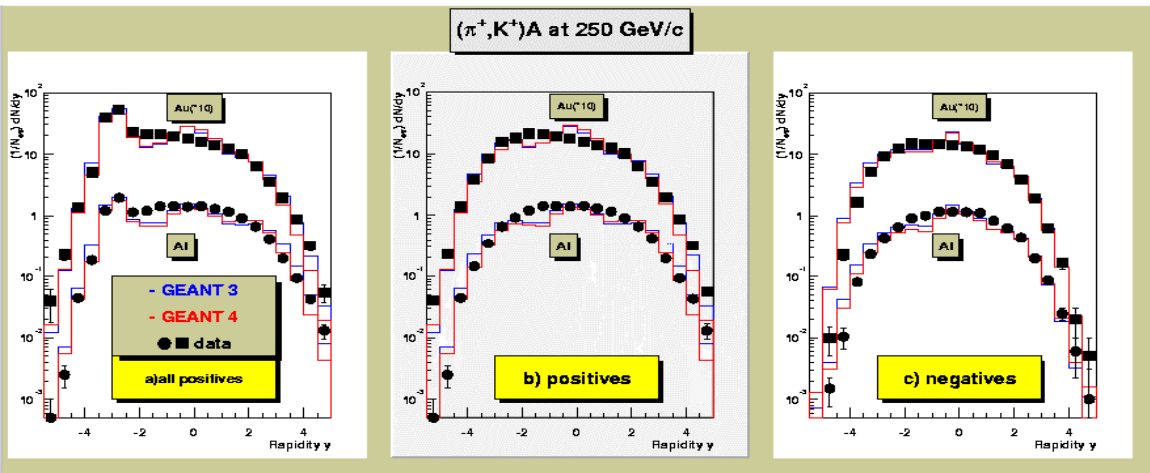
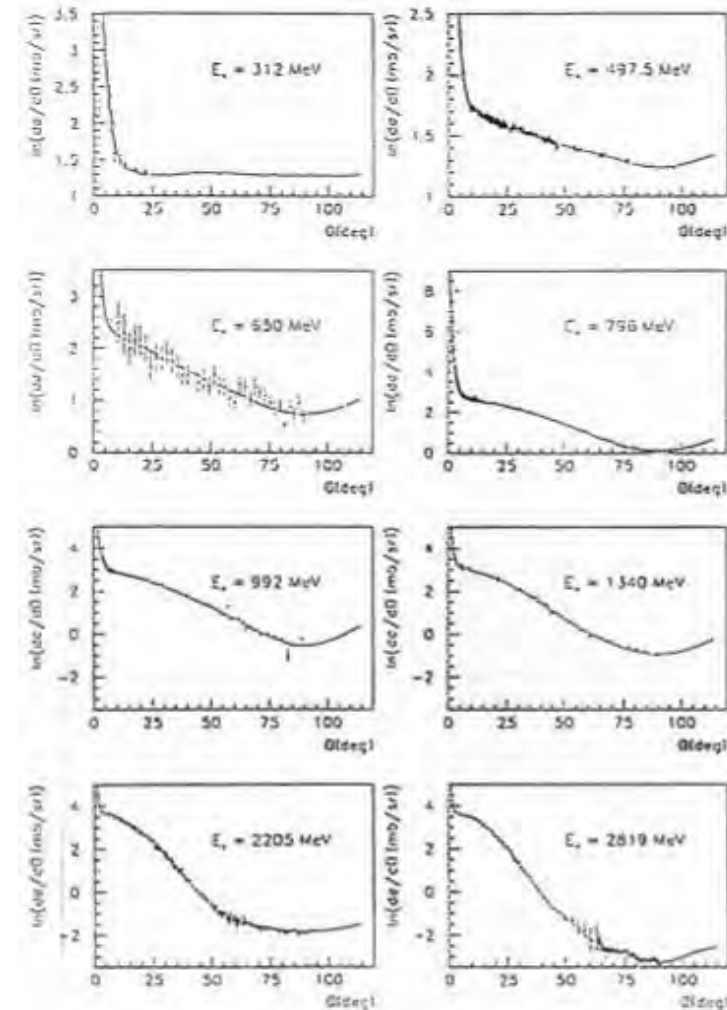
Based on experimental data

- Some models originally from **GHEISHA**

- reengineered into OO design
- refined physics parameterisations

- New parameterisations

- pp, elastic differential cross section
- nN, total cross section
- pN, total cross section
- np, elastic differential cross section
- $\pi$ N, total cross section
- $\pi$ N, coherent elastic scattering



# Transport of low-energy neutrons

- The energy coverage is from **thermal energies** to **20 MeV**
- Geant4 database deriving from evaluation of other databases
  - ENDFB/VI, JEFF, JENDL, CENDL...
  - Includes cross sections and final state information for **elastic** and **inelastic scattering**, **capture**, **fission** and **isotope production**
- The file system is used in order to allow granular access to, and flexibility in, the use of the cross-sections for different isotopes, and channels

# Nuclear elastic scattering

G4HadronElasticProcess

G4HadronElasticDataSet

G4LElastic

G4ElasticCascadeInterface

*Not to be confused with  
G4CascadeElasticInterface*

G4UHadronElasticProcess

G4HadronElastic

G4WHadronElasticProcess

*Meant to treat elastic models similarly to  
inelastic ones*

G4DiffuseElastic

V. Grichine, “GEANT4 hadron elastic diffuse model,”  
*Comp. Phys. Comm.*, vol. 181, pp. 921–927, 2010

G4QElasticProcess  
*AKA “CHIPS elastic”*

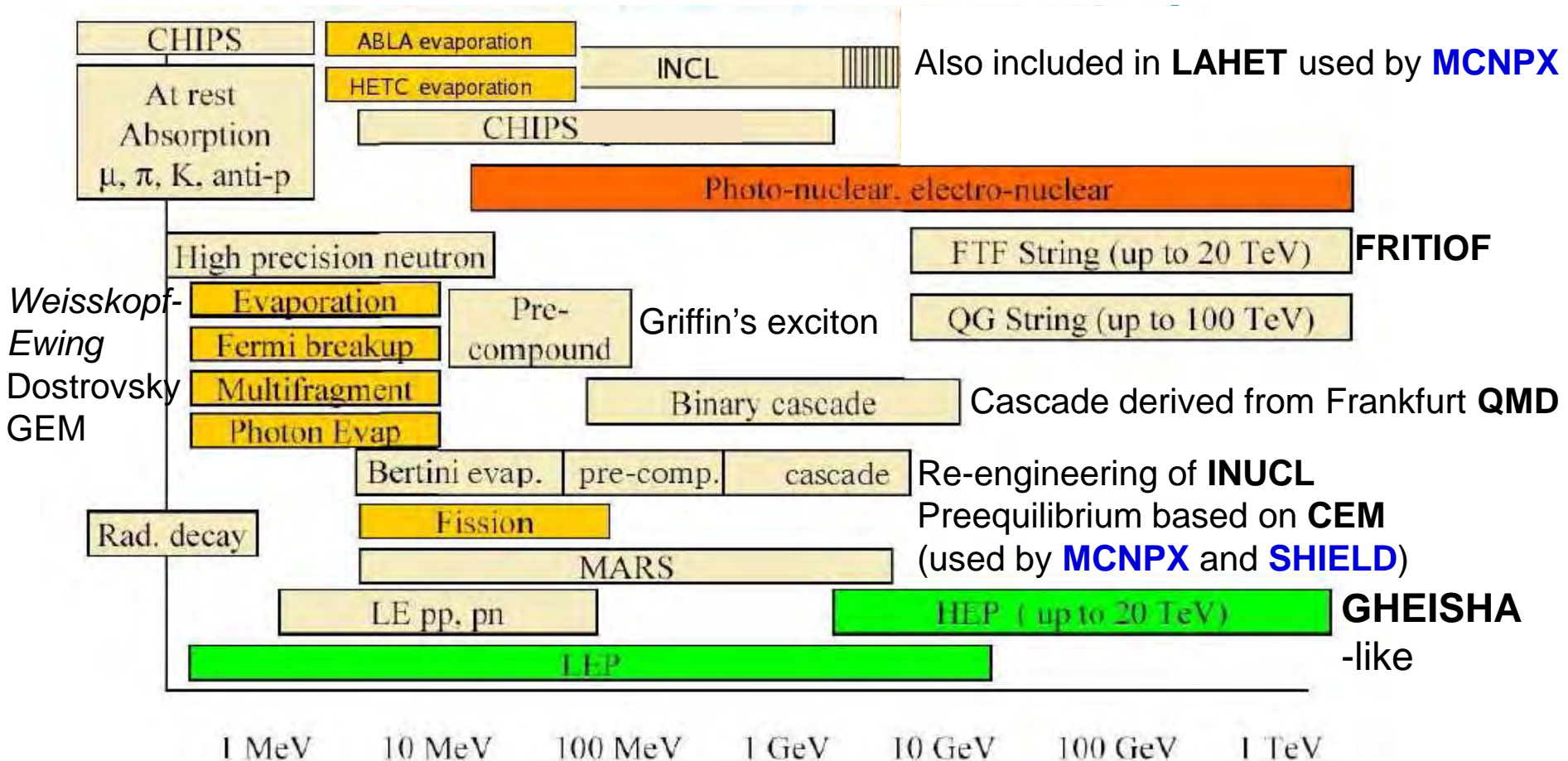
G4QElasticCrossSection

# Theory-driven hadronic non-elastic models

- Complementary and alternative models
  - **Evaporation** phase
  - Low energy range,  $O(100 \text{ MeV})$ : **pre-equilibrium**
  - Intermediate energy,  $O(100 \text{ MeV} - 5 \text{ GeV})$ : **intranuclear transport**
  - High energy range: **hadronic generator** régime
- **Deexcitation**
  - Dostrovsky, GEM, Fermi break-up, ABLA, multifragmentation...
- **Preequilibrium**
  - Precompound, Bertini-embedded
- **Cascade**
  - Binary, Bertini-like, INCL (*Liège*)
- **High energy**
  - Quark-gluon-string, FTF (*FRITIOF*)
- **CHIPS** (Chiral Invariant Phase Space)

# Hadronic inelastic model inventory

■ Data-driven ■ Parameterised ■ Theory-driven models



# Ion inelastic interactions

- Several cross section formulations for N-N collisions are available in Geant4
  - Tripathi, Shen, Kox , Sihver
- Final state according to models:  
**G4BinaryLightIonCascade** (variant of Binary cascade),  
**G4WilsonAbrasion**, **G4EMDissociation**

# Radioactive decay

- To simulate the decay of radioactive nuclei
- $\alpha$ ,  $\beta^+$ ,  $\beta^-$  decay and electron capture are implemented
- Data derived from Evaluated Nuclear Structure Data File (ENSDF)

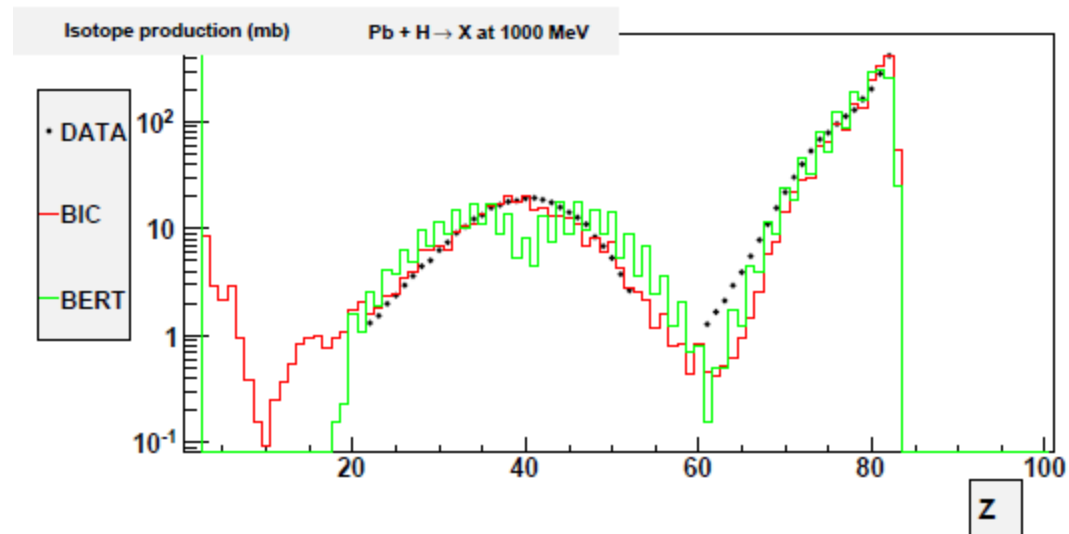


# Hadronic simulation validation

- Intensive activity since Geant4 early days
- Far from easy
  - Complex physics
  - Complex experimental data (e.g. LHC teast beam set-ups)
  - Lack of, or conflicting experimental data, large uncertainties etc.
- **Validation or calibration?**
  - Often not documented
  - “*Tuning*” (hand-made in most cases)

# Recent improvements

Low energy range:  
**Preequilibrium**  
and **deexcitation**



## Calibration or validation?


*Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2010 (SNA + MC2010)*  
Hitotsubashi Memorial Hall, Tokyo, Japan, October 17-21, 2010

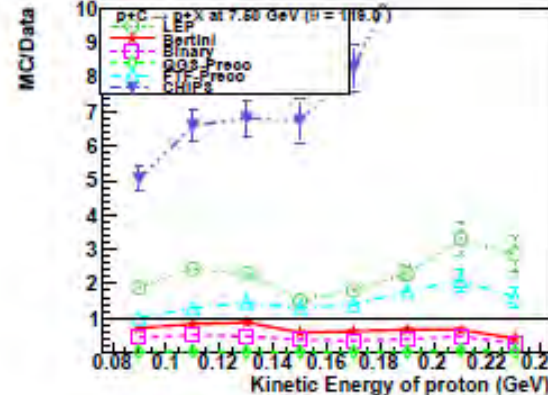
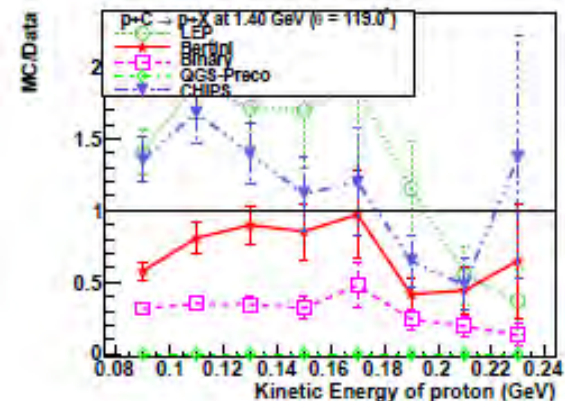
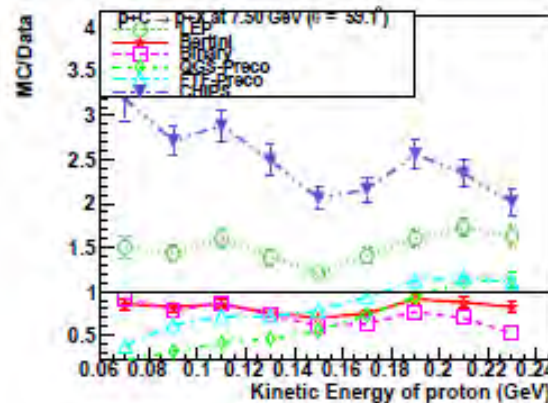
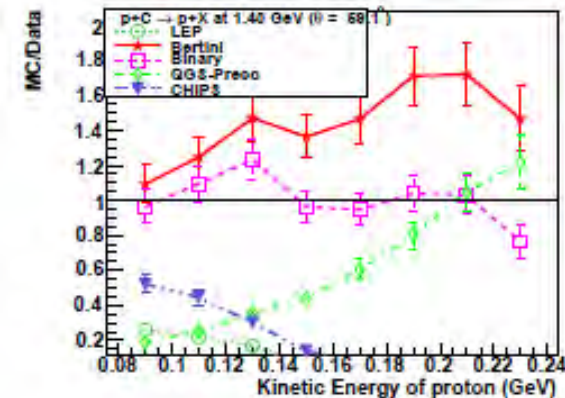
### Recent Developments In Pre-Equilibrium And De-Excitation Models In Geant4

José Manuel QUESADA<sup>1,\*</sup>, Vladimir IVANCHENKO<sup>2,3,4</sup>, Anton IVANCHENKO<sup>2,5</sup>,  
Miguel Antonio CORTÉS-GIRALDO<sup>1</sup>, Gunter FOLGER<sup>2</sup>, Alex HOWARD<sup>6</sup>, Dennis WRIGHT<sup>7</sup>  
on behalf of the Geant4 Hadronic Working Group

# Experimental comparisons

Lorentz invariant cross section for **inclusive proton production** at  $59^\circ$  (top row) and  $119^\circ$  (bottom row) in **p-Carbon** interactions at 1.4 GeV/c (left column) and 7.5 GeV/c (right column) as a function of proton kinetic energy, being compared with predictions of GEANT4 hadronic models

More in 



**Bertini** cascade  
**Binary** cascade  
**LEP**  
**QGS+Precompound**  
**CHIPS**

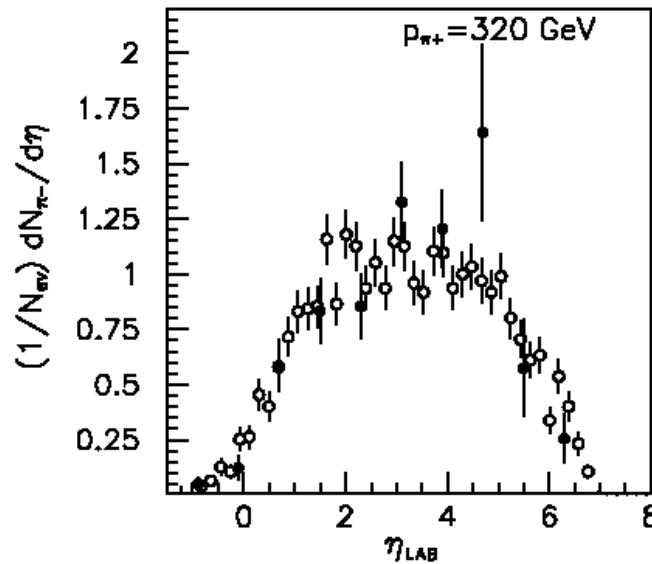
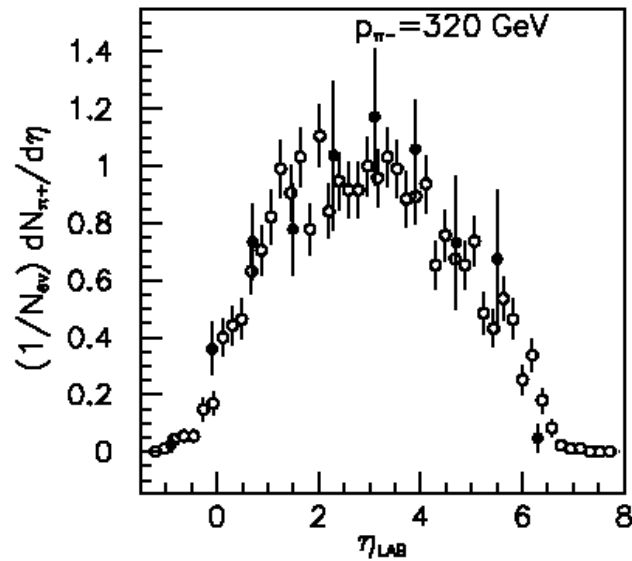
*Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2010 (SNA + MC2010)*  
 Hitotsubashi Memorial Hall, Tokyo, Japan, October 17-21, 2010

## Validation of GEANT4 Hadronic Generators versus Thin Target Data

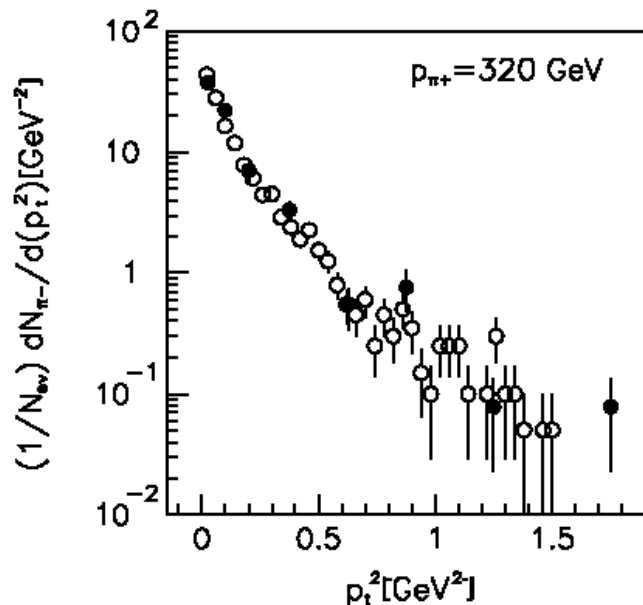
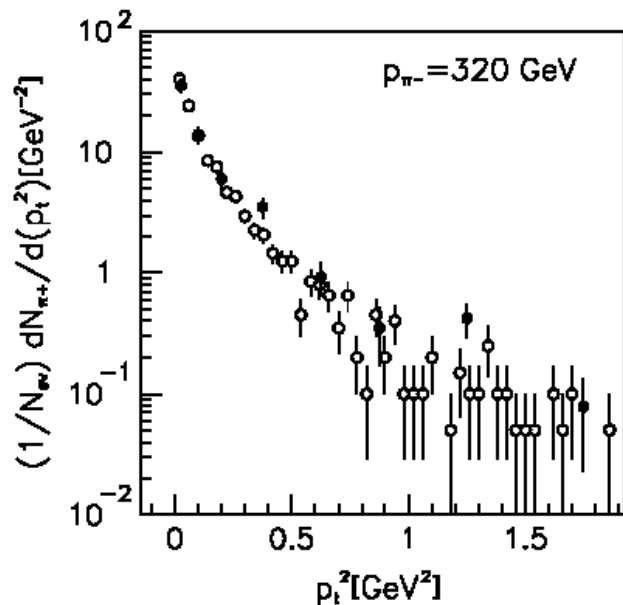
Banerjee<sup>1</sup>, G. Folger<sup>2</sup>, A. Ivanchenko<sup>2,3</sup>, V. N. Ivanchenko<sup>2,4,5</sup>, M. Kossov<sup>2</sup>, J. M. Quesada<sup>6</sup>, A. Schalelicke<sup>7</sup>,  
 V. Uzhinsky<sup>2</sup>, H. Wenzel<sup>1</sup>, D. H. Wright<sup>8</sup> and J. Yarba<sup>1</sup>

# Experimental comparisons: QGS

Scattering off Mg (Whitmore et al, Z.P. C62, p.199ff, 1994)

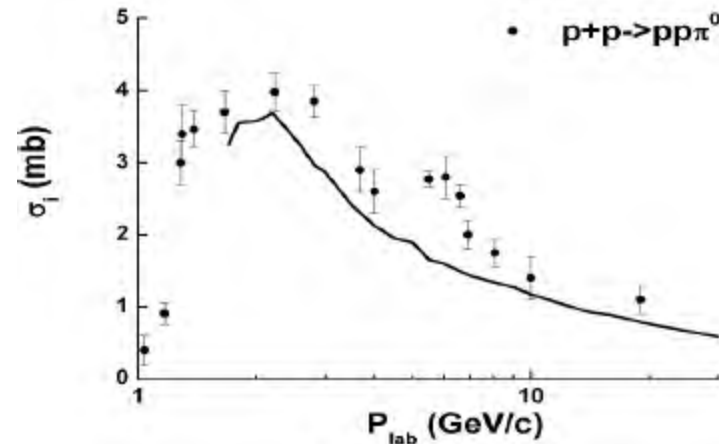
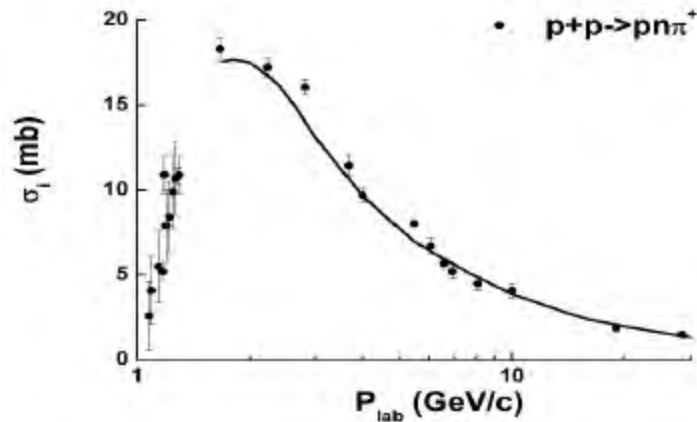


Comparison of differential pion yields for positive and negative pions in pion-Mg reactions at 320 GeV lab momentum




The dots are data and the open circles are Monte Carlo predictions by G4QGSMoDel

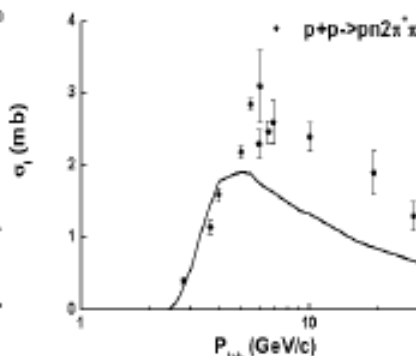
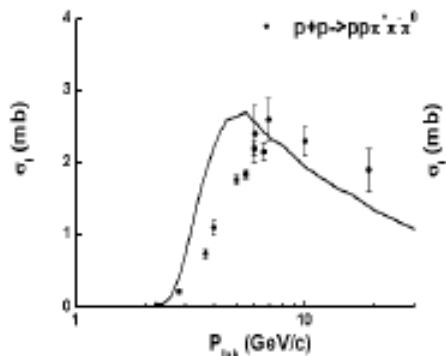
# Experimental comparisons - FRITIOF



Experimental data: E. Bracci et al., CERN/HERA 73-1 (1973)

More in 

Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2010 (SNA + MC2010)  
Hitotsubashi Memorial Hall, Tokyo, Japan, October 17-21, 2010



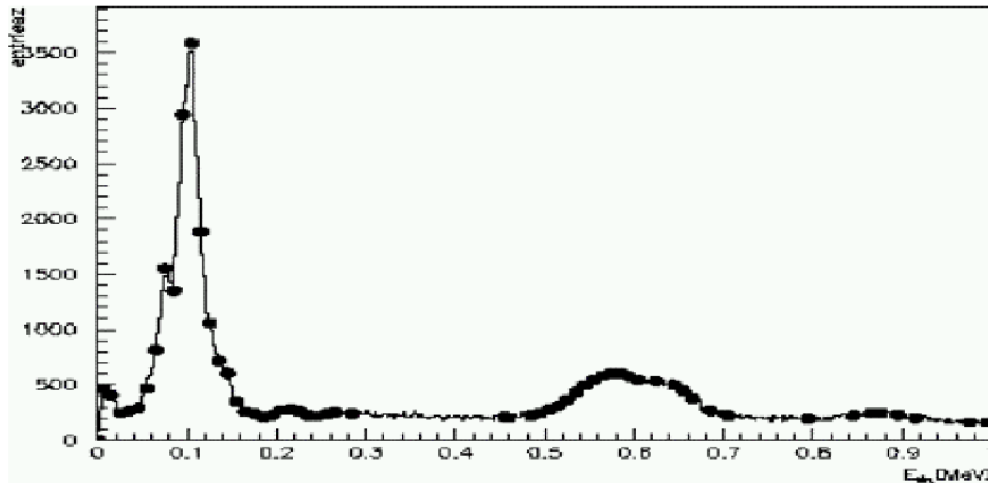
## Development of the Fritiof Model in Geant4

Vladimir UZHINSKY<sup>1,2\*</sup>  
On behalf of the Geant4 Hadronics Working Group

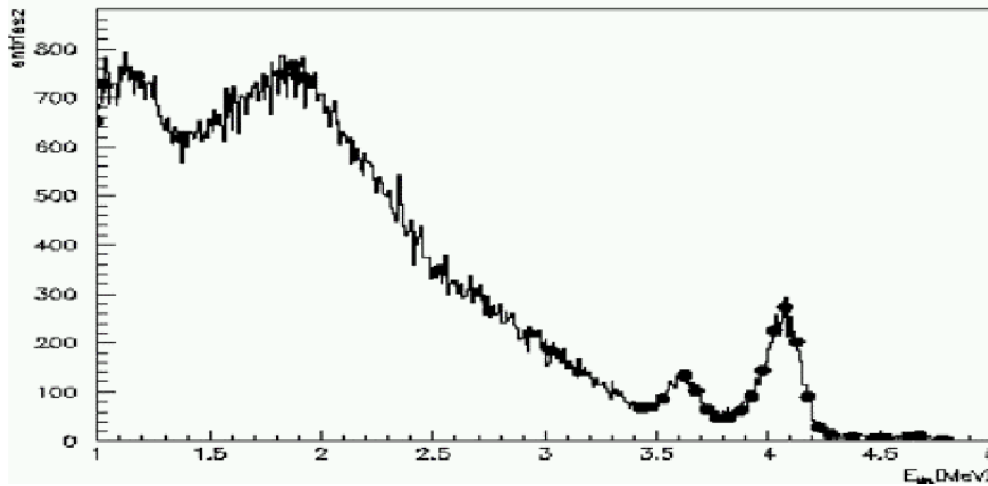
<sup>1</sup> CERN, CH-1211, Geneva 23, Switzerland

<sup>2</sup> LIT, JINR, 141980 Dubna, Russia

# HP neutron models



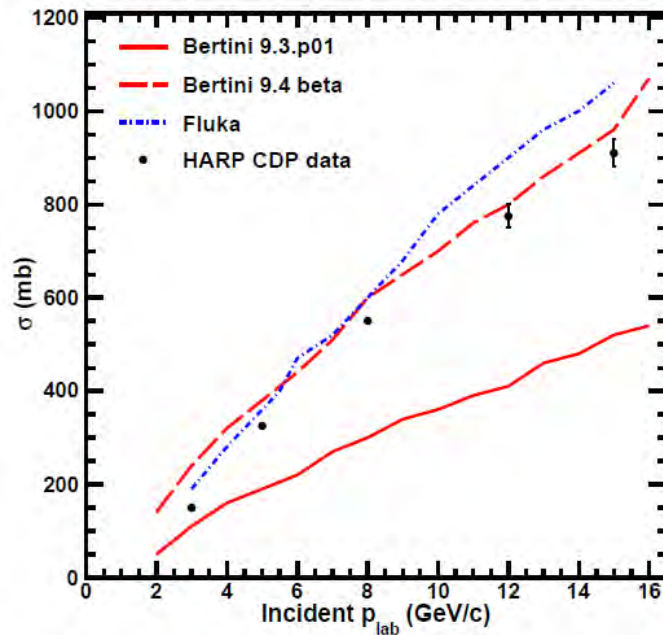
Geant4 simulation  
of  $\gamma$ -rays from  
14 MeV neutron  
capture on uranium



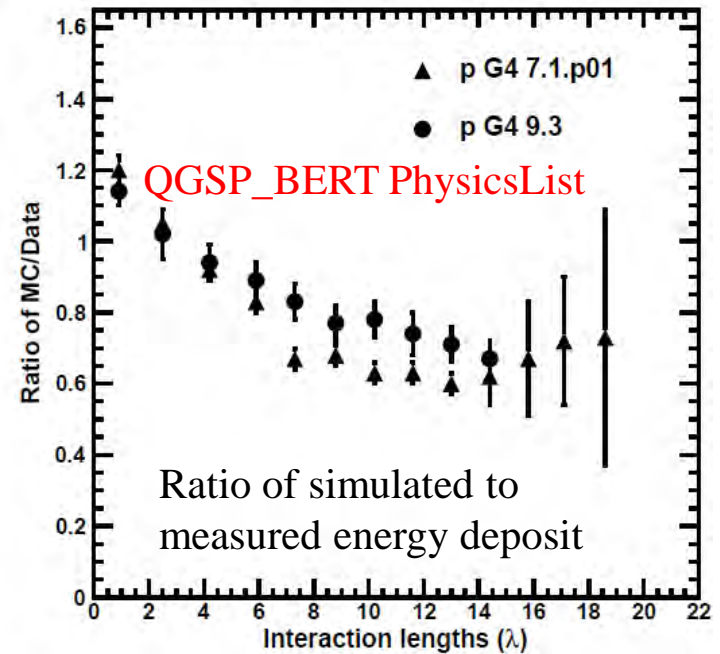


# Recent improvements

## Transition across models vs. energy



## Shower shapes



Longitudinal shower profile resulting from 180 GeV protons incident at 90° on the ATLAS TileCal wedge

More in



Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2010 (SNA + MC2010)  
Hitotsubashi Memorial Hall, Tokyo, Japan, October 17-21, 2010  
**An Overview of Geant4 Hadronic Physics Improvements**



# Validation

*Recognized as an  
American National Standard (ANSI)*

**IEEE Std 1012™-2004**  
(Revision of  
IEEE Std 1012-1998)

## IEEE Standard for Software Verification and Validation

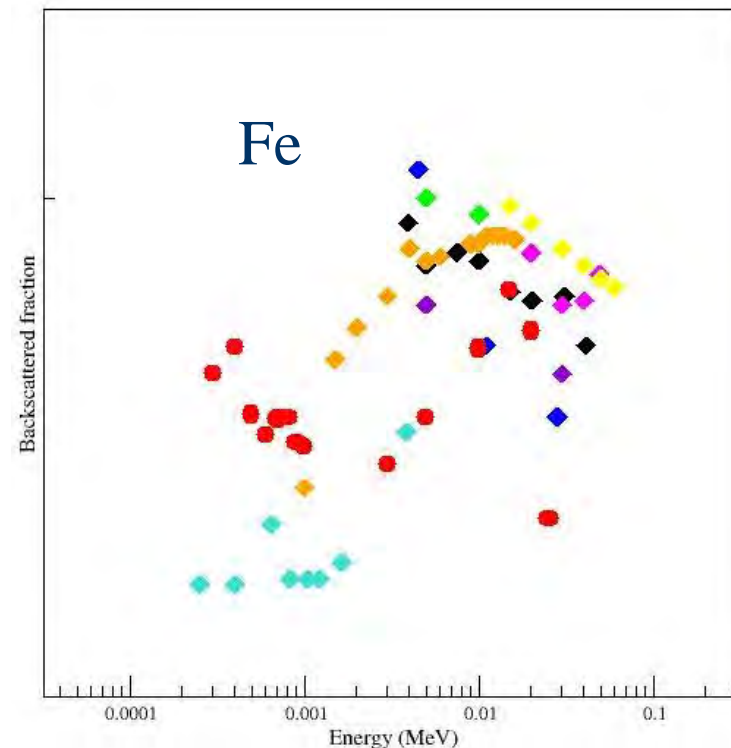
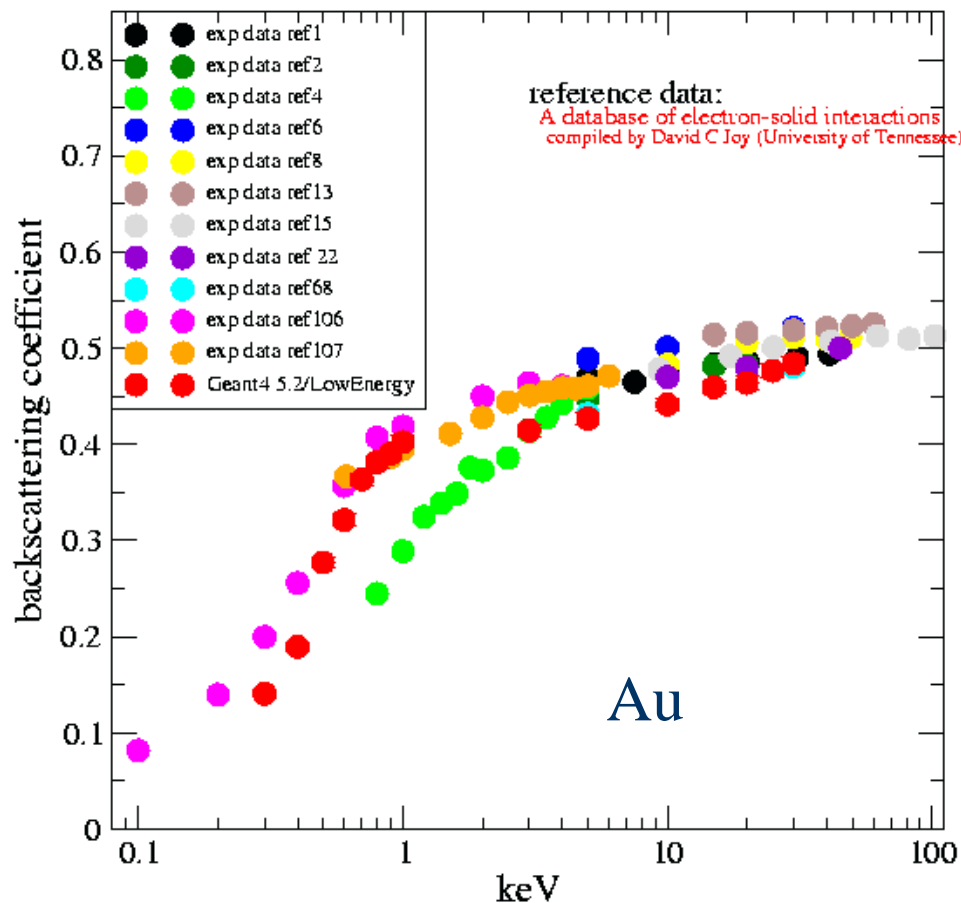
The **validation** process provides **evidence** whether the software and its associated products and processes

- 1) **Satisfy system requirements** allocated to software at the end of each life cycle activity
- 2) **Solve the right problem** (e.g., correctly model physical laws, implement business rules, use the proper system assumptions)
- 3) **Satisfy intended use and user needs**

# The main problem of validation: experimental data!

backscattering for e-

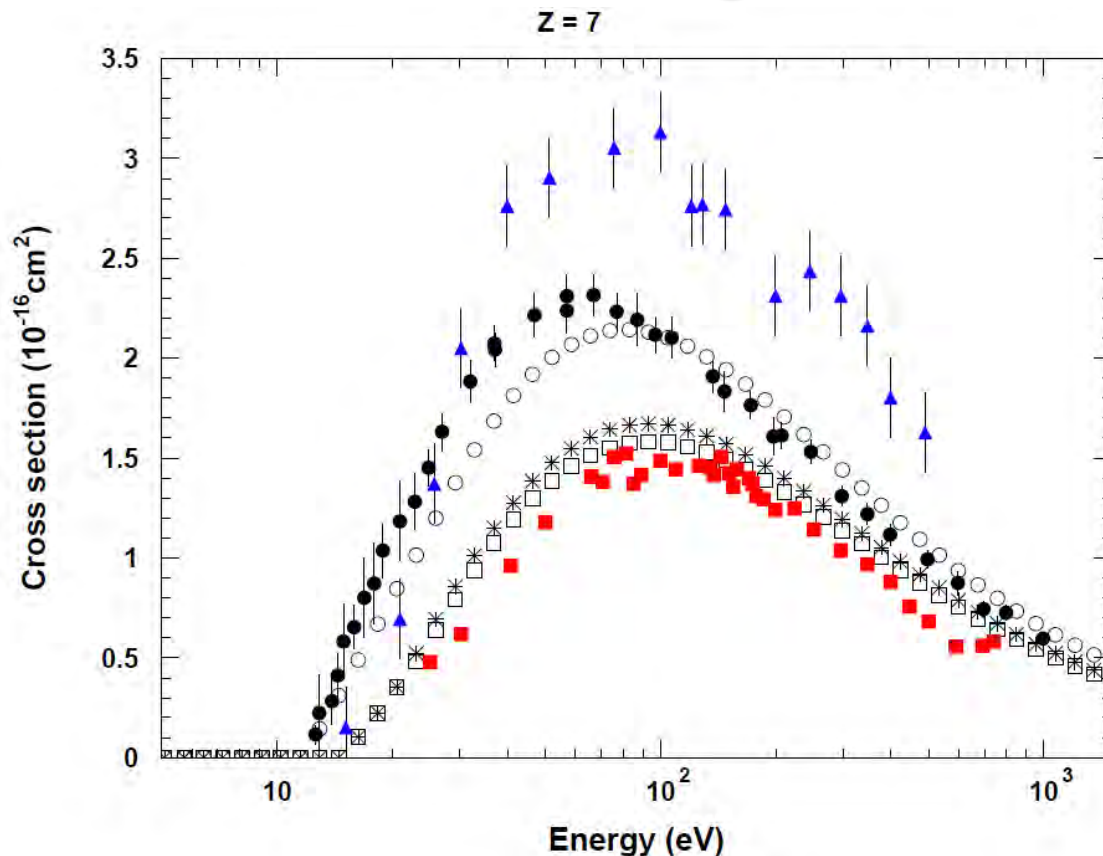
e- energy range: 0.1 keV -> 102. keV



Experimental data often  
exhibit large differences!

# Which one is right?

To be documented in  
a forthcoming paper



- Empty symbols: simulation models
- Filled symbols: experimental data

Often an answer  
can be found only  
through a  
**statistical analysis**  
over a large sample  
of simulated and  
experimental data  
(and would be a  
*result within a given  
CL, rather than  
black & white*)



Contents lists available at ScienceDirect

## Nuclear Instruments and Methods in Physics Research A

journal homepage: [www.elsevier.com/locate/nima](http://www.elsevier.com/locate/nima)



### Validation of the Geant4 electromagnetic photon cross-sections for elements and compounds

G.A.P. Cirrone<sup>a</sup>, G. Cuttone<sup>a</sup>, F. Di Rosa<sup>a</sup>, L. Pandola<sup>b,\*</sup>, F. Romano<sup>a</sup>, Q. Zhang<sup>a,c,\*\*</sup>

## Comparison to theoretical data libraries NOT validation!

*Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2010 (SNA + MC2010)*  
Hitotsubashi Memorial Hall, Tokyo, Japan, October 17-21, 2010

“After the migration to common design a new **validation** of photon cross sections versus various databases was published <sup>26)</sup> which demonstrated general good agreement with the data for both the Standard and Low-energy models.”

#### Recent Improvements in Geant4 Electromagnetic Physics Models and Interfaces

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# Validation or calibration?

**Calibration** is the process of improving the agreement of a code calculation with respect to a chosen set of benchmarks through the *adjustment of parameters* implemented in the code

**Validation** is the process of confirming that the predictions of a code adequately represent measured physical phenomena

T.G. Trucano et al., Calibration, validation, and sensitivity analysis: What's what, *Reliability Eng. & System Safety*, vol. 91, no. 10-11, pp. 1331-1357, 2006



# Validation is holistic

One must validate the entire calculation system

Including:

- User
- Computer system
- Problem setup
- Running
- Results analysis



An inexperienced user can easily get wrong answers out of a good code in a valid régime



Source: NASA

The launch of STS-107 on January 16, 2003

Columbia Space Shuttle accident, 2003



# Can we quantify our ignorance?

Simulation codes usually contain parameters or model assumptions, which are not validated (because of lack of experimental data, or conflicting data)

Or we may not have a complete understanding of some physics processes

Or we may use a simulation model outside the range where it has been validated (energy, material etc.)

These are sources of **epistemic uncertainties**, which in turn can be sources of **systematic effects**

## Can we quantify them?

No generally accepted method of measuring epistemic uncertainties

**Interval analysis**

**Dempster-Shafer theory of evidence**

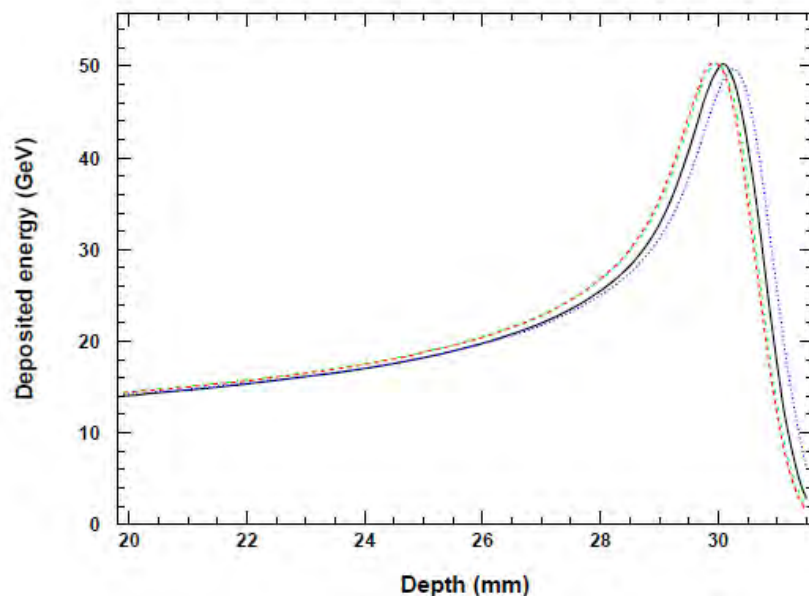


# Fresh from the oven...

IEEE Trans. Nucl. Sci., vol. 57, no. 5,  
pp. 2805-2830, October 2010

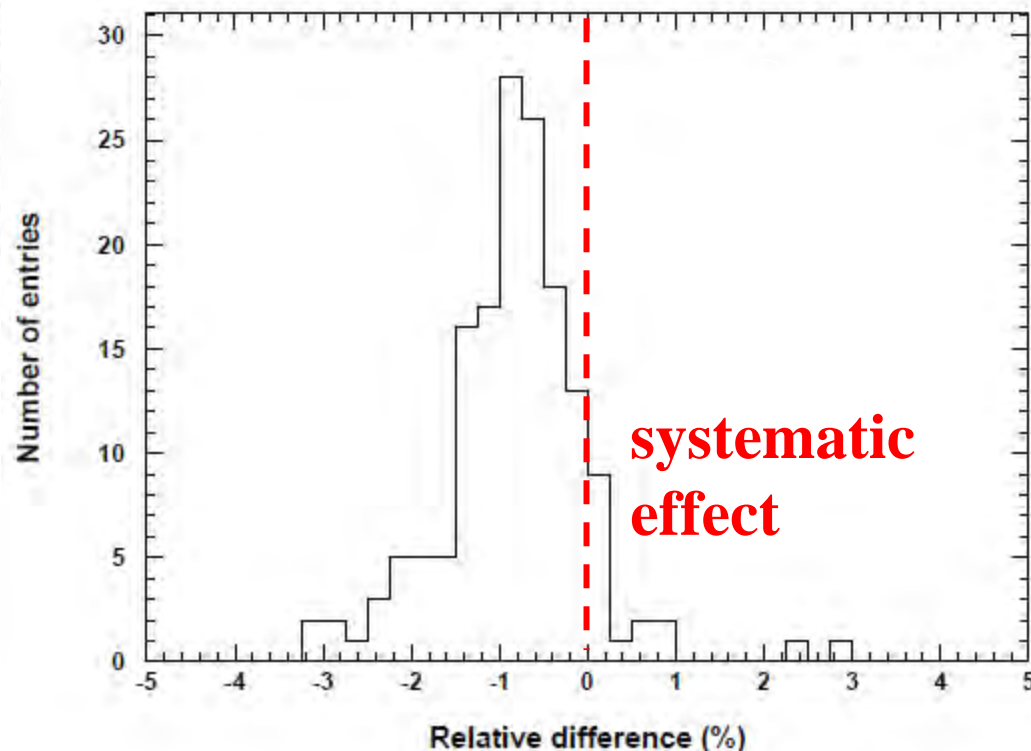
## Physics-Related Epistemic Uncertainties in Proton Depth Dose Simulation

Maria Grazia Pia, Marcia Begalli, Anton Lechner, Lina Quintieri, and Paolo Saracco



**Warm-up exercise:**  
epistemic uncertainties  
quantification in proton  
Bragg peak simulation

**Precompound** model activated  
through **Binary Cascade** w.r.t.  
standalone Precompound model



# Geant4 pre-assembled physics lists

- Initially a set of example PhysicsLists suitable to address specific **use cases**
  - “educated guess” in most cases
  - Not necessarily validated
- Now: **combinatorial assembly** of processes and models
  - Not necessarily validated
- Can be a starting point for a user application
- Not necessarily the end
- *Can you build your own PhysicsList from scratch?*

# Summary

- **Transparency** and **modularity** were key characteristics of Geant4 original physics design in its **RD44** phase
- Ample variety of processes and models
  - Open to extension and evolution thanks to the OO technology
- Geant4 design exposes, **deliberately**, the user to the **choice** of physics (*particles + processes*) relevant to his/her application
  - This is a critical task
  - Examples can be used as starting point
  - Not a “push the button” system, the user is invested of the **responsibility** of selecting the physics for his/her simulation
- Documentation in Geant4 Physics Reference Manual
- Growing set of Geant4 physics references in the literature
  - Conference proceedings and **refereed journals**
  - User application results

# Conclusion

- Geant4 is a rich and powerful tool for experimental research
- ...but it invests the user with responsibility of making **choices**
- **Validation** is ongoing
- Check what is documented in the literature, that may be relevant to your experimental problem
  - **Refereed journals** (conference papers )
  - *Beware of some slips even in refereed journals*
- Geant4 is **widely used** in a variety of environments
  - **Applications** and application **frameworks** on top of Geant4

Slides available at  
<http://www.ge.infn.it/geant4/training>

Collection of physics references  
<http://www.ge.infn.it/geant4/papers>

General information: <http://cern.ch/geant4>

Acknowledgment: **Geant4 developers** and **users**