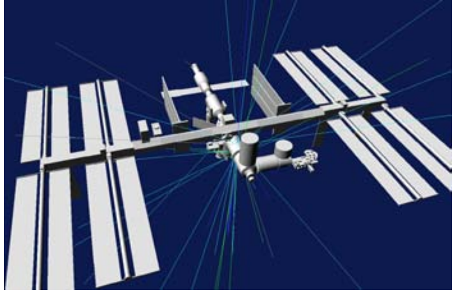
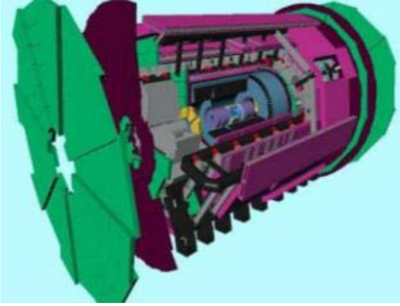
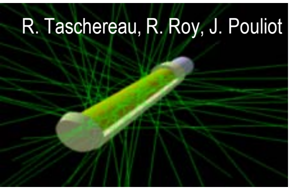


*Courtesy T. Ersmark, KTH Stockholm*

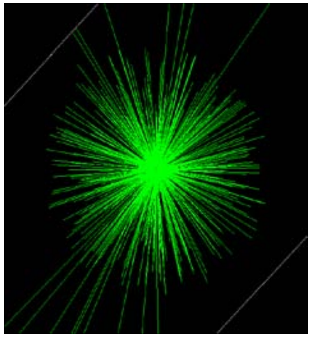
# Geant 4

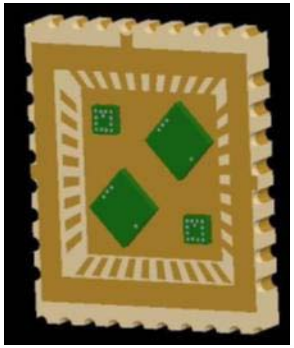


*Courtesy of ATLAS Collaboration*




## Simulation for multi-disciplinary applications

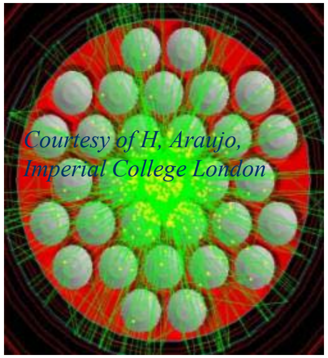


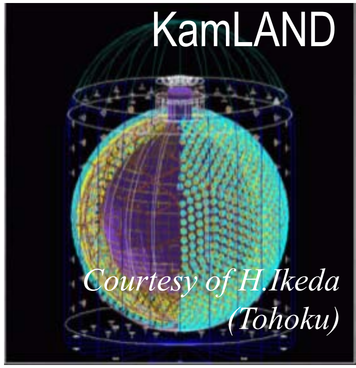


Maria Grazia Pia

*INFN Genova, Italy*

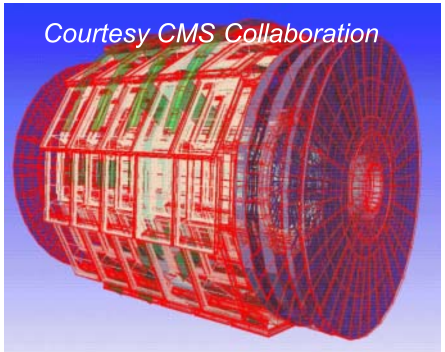
DESY - XFEL
Hamburg, 4 February 2011

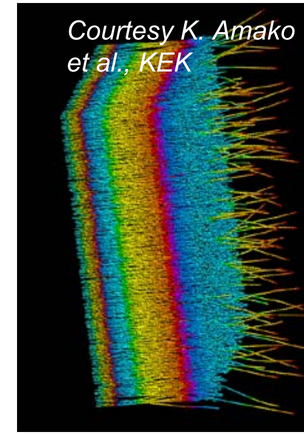



http://cern.ch/geant4

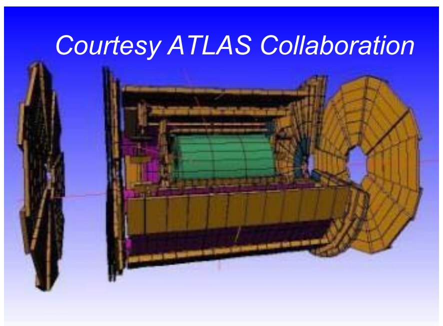
# Geant 4



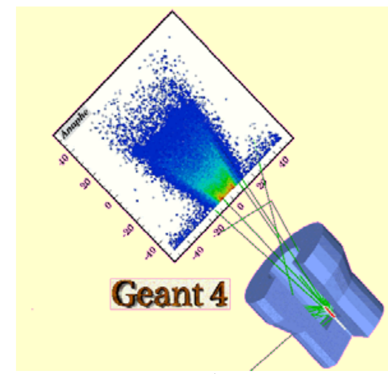

Object oriented toolkit for the simulation of particle interactions with matter

**Born from the requirements of large scale HEP experiments**

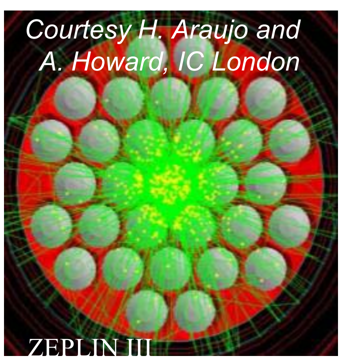


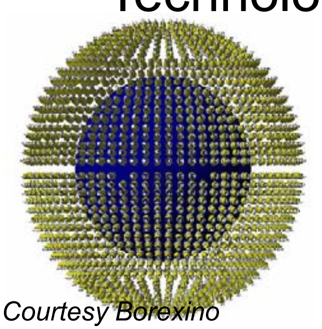

Widely used in:

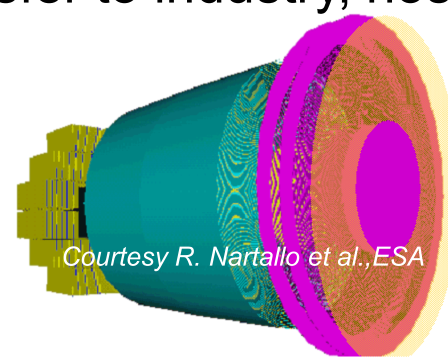
- Space science and astrophysics
- Medical physics, nuclear medicine
- Radiation protection
- Accelerator physics
- Pest control, food irradiation
- Humanitarian projects, security
- etc.
- Technology transfer to industry, hospitals

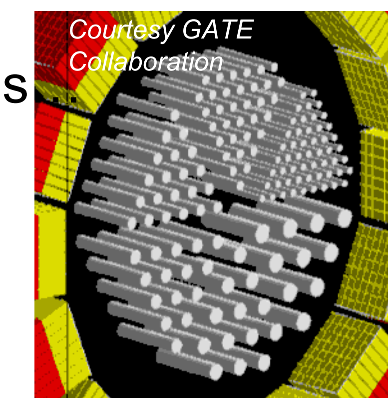



IST and INFN Genova



S. Agostinelli et al.,
**Geant4—a simulation toolkit**
NIM A 506 (2003) 250–303

**Most cited**
**“Nuclear Science and Technology” publication**
Thomson-Reuters,
ISI Web of Science
Database since 1970

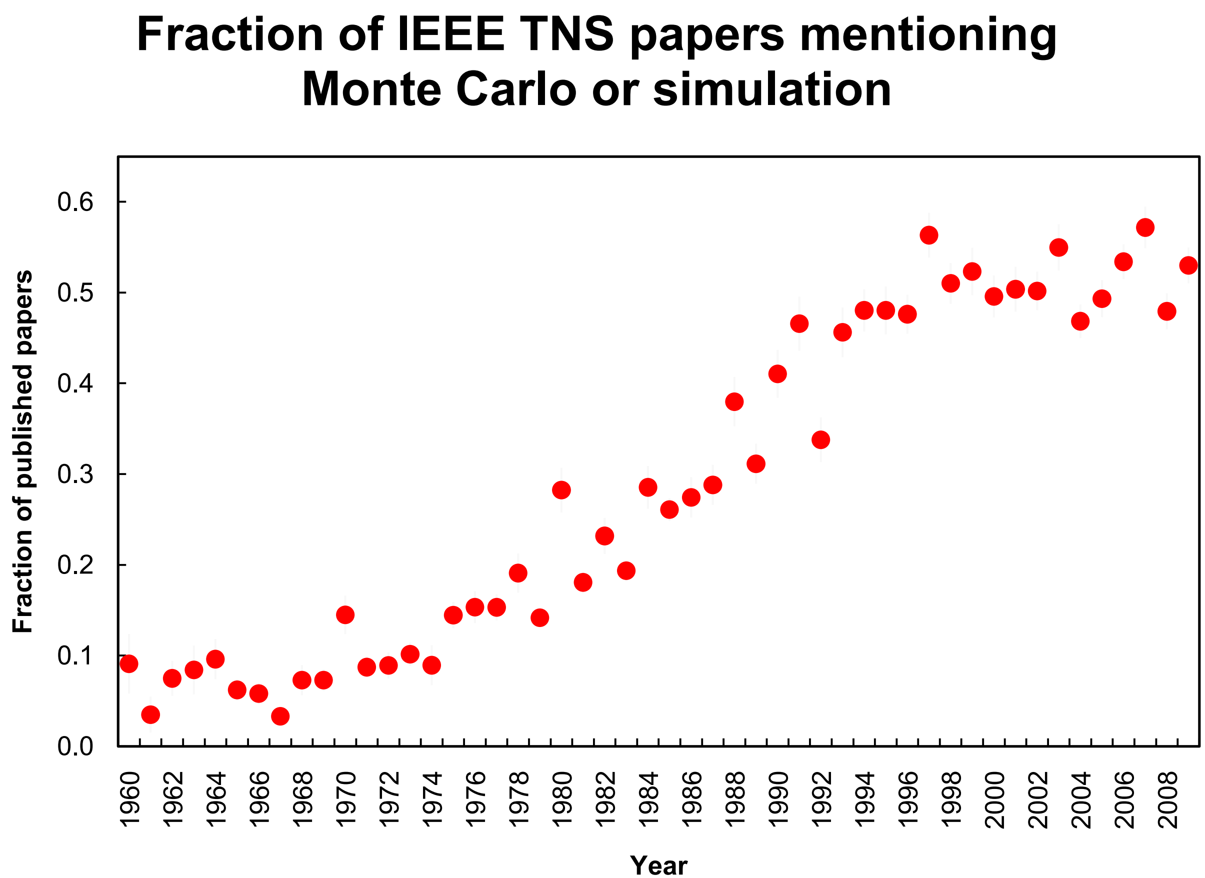

Available online at www.sciencedirect.com
SCIENCE DIRECT
ELSEVIER
Nuclear Instruments and Methods in Physics Research A 506 (2003) 250–303
NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH Section A
www.elsevier.com/locate/nima


## GEANT4—a simulation toolkit


S. Agostinelli[ae], J. Allison[as,*], K. Amako[e], J. Apostolakis[a], H. Araujo[aj], P. Arce[l,m,x,a], M. Asai[g,ai], D. Axen[i,t], S. Banerjee[bi,l], G. Barrand[an], F. Behner[l], L. Bellagamba[c], J. Boudreau[bd], L. Broglia[ar], A. Brunengo[c], H. Burkhardt[a], S. Chauvie[bj,bl], J. Chuma[h], R. Chytracek[a], G. Cooperman[az], G. Cosmo[a], P. Degtyarenko[d], A. Dell'Acqua[a,j], G. Depaola[y], D. Dietrich[af], R. Enami[ab], A. Feliciello[bj], C. Ferguson[bh], H. Fesefeldt[l,o], G. Folger[a], F. Foppiano[ac], A. Forti[as], S. Garelli[ac], S. Giani[a], R. Giannitrapani[bo], D. Gibin[m,bc], J.J. Gómez Cadenas[m,bp], I. González[q], G. Gracia Abril[n], G. Greeniaus[p,h,ag], W. Greiner[af], V. Grichine[f], A. Grossheim[m,z], S. Guatelli[ad], P. Gumplinger[h], R. Hamatsu[bk], K. Hashimoto[ab], H. Hasui[ab], A. Heikkinen[ah], A. Howard[aj], V. Ivanchenko[a,ba], A. Johnson[g], F.W. Jones[h], J. Kallenbach[aa], N. Kanaya[i,h], M. Kawabata[ab], Y. Kawabata[ab], M. Kawaguti[ab], S. Kelner[at], P. Kent[r], A. Kimura[ay,bb], T. Kodama[aw], R. Kokoulin[at], M. Kossov[d], H. Kurashige[am], E. Lamanna[w], T. Lampén[ah], V. Lara[a,l,bq], V. Lefebure[l], F. Lei[bh,be], M. Liendl[l,a,br], W. Lockman[j,bn], F. Longo[bm], S. Magni[k,au], M. Maire[ao], E. Medernach[a], K. Minamimoto[aw,al], P. Mora de Freitas[ap], Y. Morita[e], K. Murakami[e], M. Nagamatu[aw], R. Nartallo[b], P. Nieminen[b], T. Nishimura[ab], K. Ohtsubo[ab], M. Okamura[ab], S. O'Neale[s], Y. Oohata[bk], K. Paech[af], J. Perl[g], A. Pfeiffer[a], M.G. Pia[ad], F. Ranjard[n], A. Rybin[ak], S. Sadilov[a,ak], E. Di Salvo[c], G. Santin[bm], T. Sasaki[e], N. Savvas[as], Y. Sawada[ab], S. Scherer[af], S. Sei[aw], V. Sirotenko[i,al], D. Smith[g], N. Starkov[f], H. Stoecker[af], J. Sulkimo[ah], M. Takahata[ay], S. Tanaka[bg], E. Tcherniaev[a], E. Safai Tehrani[g], M. Tropeano[ae], P. Truscott[be], H. Uno[aw], L. Urban[v], P. Urban[aq], M. Verderi[ap], A. Walkden[as], W. Wander[av], H. Weber[af], J.P. Wellisch[a,l], T. Wenaus[u], D.C. Williams[j,bf], D. Wright[g,h], T. Yamada[aw], H. Yoshida[aw], D. Zschiesche[af]

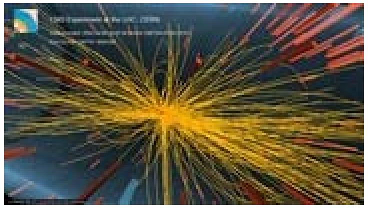
[a] *European Organization for Nuclear Research (CERN) Switzerland*
[b] *European Space Agency (ESA), ESTEC, The Netherlands*
[c] *Istituto Nazionale di Fisica Nucleare (INFN), Italy*
[d] *Jefferson Lab, USA*
[e] *KEK, Japan*

# Monte Carlo simulation in literature

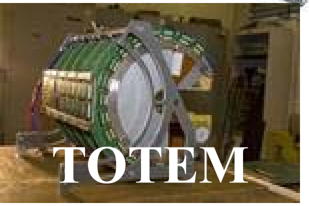


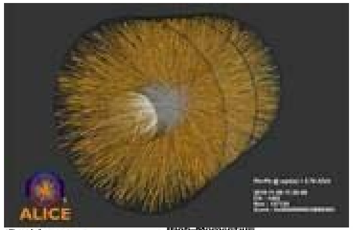

Same trend in NIM

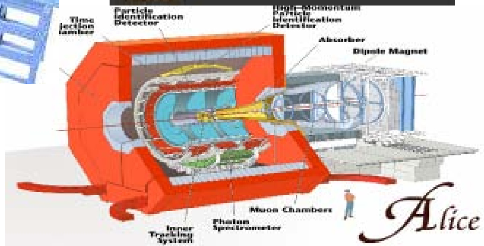
MGP, T. Basaglia, Z.W. Bell, P.V. Dressendorfer
The butterfly effect: correlations between modeling in nuclear-particle physics and socioeconomic factors
NSS 2010 Conf. Rec.

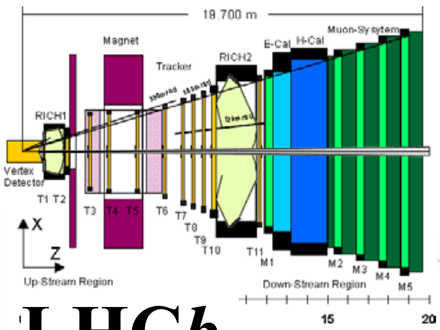



**Complex physics**
**Complex detectors**
**~20 years software life-span**

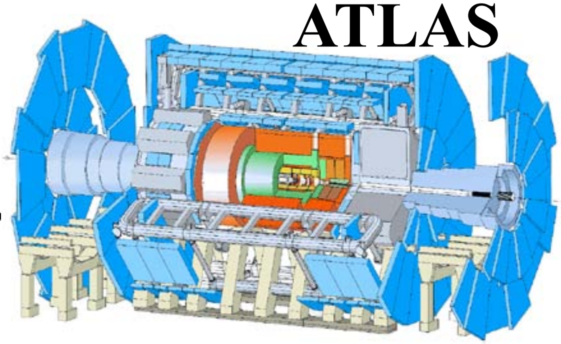




LHCb



# Three years ago…

**Subject:** range cuts, step sizes, and thresholds in G4 low energy extension
**From:** Georg Weidenspointner <Georg.Weidenspointner@hll.mpg.de>
**Date:** Wed, 27 Feb 2008 09:43:27 +0100
**To:** MariaGrazia.Pia@ge.infn.it, "Georg Weidenspointner (HLL)" <Georg.Weidenspointner@hll.mpg.de>

Dear Dr. Pia,

I am sorry to bother you, but I would really appreciate some authoritative advice on various aspects on the G4 low energy extension from you or one of your co-workers. Until a few months ago I was using GEANT3, but recently I had to extend the energy range of my work below 10 keV, and I very much appreciate the effort that has been invested in creating the G4 low energy extension. It addresses many fundamental needs in my area of interest, namely the study of X-ray and gamma-ray detectors on the ground and in space.

Basically, I would like to understand how to best "tune" G4 for simulations of
photons, electrons, protons and neutrons in the context of my work on X-ray and gamma-ray detectors on the ground and in space.

# Two weeks later…

**Subject:** Re: range cuts, step sizes, and thresholds in G4 low energy extension
**From:** Georg Weidenspointner <Georg.Weidenspointner@hll.mpg.de>
**Date:** Tue, 11 Mar 2008 14:02:41 +0100
**To:** Maria Grazia Pia <MariaGrazia.Pia@ge.infn.it>, "Georg Weidenspointner (HLL)" <Georg.Weidenspointner@hll.mpg.de>

Dear Dr. Pia,

this morning we had a short meeting on PIXE in our local group. As I pointed out aready, PIXE is a very important aspect for the design of X-ray detectors,
therefore we have a vested interest in having PIXE improved in Geant4.

If possible, I would like to be involved in your PIXE work. In particular, I might be able to run tests of beta-versions of code upgrades, based on the applications of the local group.
We might even consider doing some experimental work - if necessary - to obtain actual data for testing a new version of a PIXE implemenation in Geant4. You are surely aware of the fact that PIXE is a widely used

October 2008

IEEE Nucl. Sci. Symp., Dresden

Application of the Geant4 PIXE implementation for space missions

New models for PIXE simulation with Geant4

Georg Weidenspointner, Maria Grazia Pia, and Andreas Zoglauer

The "beast"

36 page paper

PIXE simulation software released in Geant4 9.4, 17 December 2010



# PIXE Simulation With Geant4

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

***Abstract*—Particle induced X-ray emission (PIXE) is an important physical effect that is not yet adequately modelled in Geant4. This paper provides a critical analysis of the problem domain associated with PIXE simulation; it evaluates the conceptual approach, design and implementations of PIXE modelling so far available in Geant4, and describes a set of software developments to improve PIXE simulation with Geant4. The capabilities of the developed software prototype are illustrated and applied to a study of the passive shielding of the X-ray detectors of the German eROSITA telescope on the upcoming Russian *Spectrum-X-Gamma* space mission.**

***Index Terms*—Geant4, ionization, Monte Carlo, PIXE.**

## I. Introduction

THE use of charged particle beams like protons, $\alpha$ particles and other heavy ions as a means of characteristic X-ray production has received considerable attention in recent years. The origin of the emission lies in the ionization of target material atoms by incident energetic charged particles: some atoms are ionized by removing an electron from an inner electronic shell; this inner shell vacancy is subsequently filled by an electron from an outer shell. Such an electron transition may give rise to the emission of characteristic X-rays at energies corresponding to the difference in the binding energies of the involved atomic shells.

The application of particle induced X-ray emission (PIXE) to non-destructive trace element analysis of materials has first been proposed by Johansson and co-workers in 1970 [1]. Today, this experimental technique is widely exploited in diverse fields, from industrial applications to biological, environmental, geological and forensic sciences, as well as in archeometry and studies of the cultural heritage. An overview of PIXE experimental methods and scope of application is documented in [2].

Manuscript received April 03, 2009; revised September 06, 2009. Current version published December 09, 2009.

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G. Weidenspointner is with the Max-Planck-Institut für extraterrestrische Physik, 85740 Garching, Germany, and also with MPI Halbleiterlabor, 81739 München, Germany (e-mail: Georg.Weidenspointner@hll.mpg.de).

M. Augelli is with the Centre d'Etudes Spatiales (CNES), 31401 Toulouse, France (e-mail: mauroaugelli@mac.com).

L. Quintieri is with INFN Laboratori Nazionali di Frascati, I-00044 Frascati, Italy (e-mail: Lina.Quintieri@lnf.infn.it).

M. Sudhakar is with INFN Sezione di Genova, 16146 Genova, Italy and also with the Department of Physics, University of Calicut, India. She is on leave from ISRO, Bangalore, India (e-mail: Manju.Sudhakar@ge.infn.it).

A. Zoglauer is with the Space Sciences Laboratory, University of California, Berkeley, Berkeley, CA 94720 USA (e-mail: zog@ssl.berkeley.edu).

Color versions of one or more of the figures in this paper are available online at http://ieeexplore.ieee.org.

Digital Object Identifier 10.1109/TNS.2009.2033993

The physical process of PIXE may also give rise to unwanted instrumental background X-ray lines, as is the case for space missions and for some laboratory environments. It also affects the spatial distribution of the energy deposit associated with the passage of charged particles in matter: in this respect, its effects may become significant in the domain of microdosimetry.

The wide application of this experimental technique has motivated the development of several dedicated software systems; nevertheless, despite its large experimental interest, limited functionality for PIXE simulation is available in general-purpose Monte Carlo codes.

This paper discusses the problem of simulating PIXE in the context of a general-purpose Monte Carlo system; it analyzes the current status of PIXE simulation with Geant4 [3], [4] and describes a set of developments to improve it. Finally, it illustrates an application of the developed PIXE simulation prototype to a concrete experimental problem: the study of the passive shield of the X-ray detectors of the German eROSITA [5] (extended Roentgen Survey with an Imaging Telescope Array) telescope on the upcoming Russian *Spectrum-X-Gamma* [6] space mission.

## II. Software for PIXE: An Overview

Software tools are available in support of PIXE experimental applications as specialized codes or included in general-purpose simulation systems. Their main characteristics are briefly summarized below with emphasis on modelling the physics interactions underlying PIXE.

### A. Specialized PIXE Codes

Dedicated PIXE codes are focussed on the application of this technique to elemental analysis. They are concerned with the calculation of experimentally relevant X-ray yields resulting from the irradiation of a material sample by an ion beam: primarily transitions concerning the K shell, and in second instance transitions originating from vacancies in the L shell.

For this purpose various analysis programs have been developed, which are able to solve the inverse problem of determining the composition of the sample from an iterative fitting of a PIXE spectrum; some among them are GeoPIXE [7], GUPIX [8]–[10], PIXAN [11], PixeKLM [12], Sapix [13], WinAxil [14] and Wits-HEX [15]. A few codes concern PIXE simulation [16]–[18] specifically.

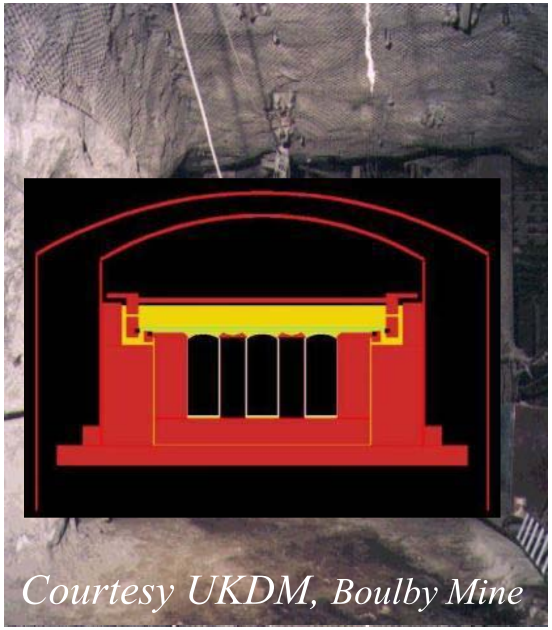
Physics modelling issues are considered in specialized codes insofar as they can affect the measurable X-ray spectrum; other physics effects are often subject to simplification or neglected.

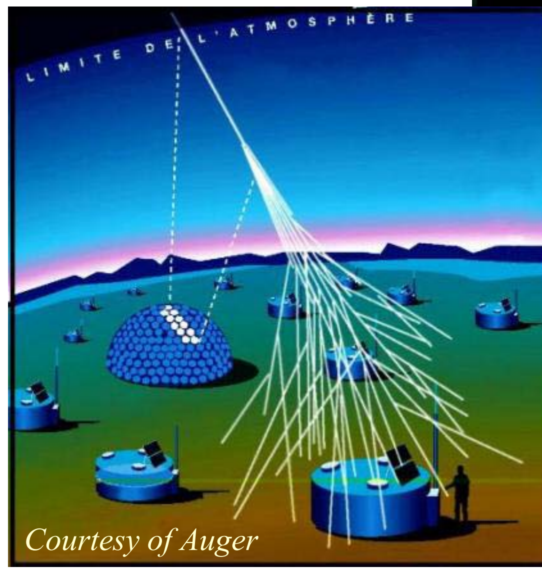
These codes adopt similar strategies to address the problem domain: they share basic physics modelling options, like the

# From deep underground…

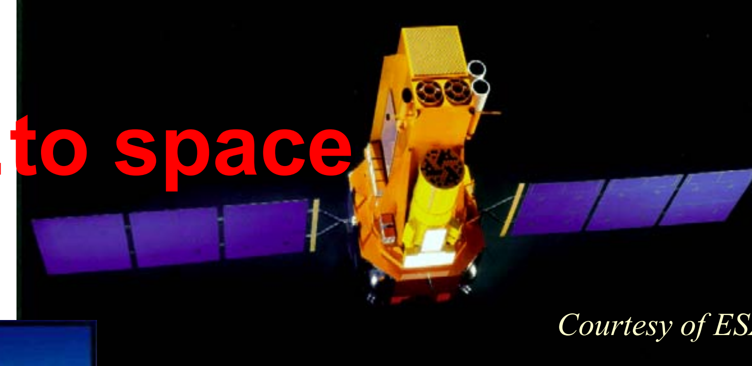
# …to space

**Dark matter and ν experiments**




**Cosmic ray experiments**




**X and γ astronomy, gravitational waves, radiation damage to components etc.**

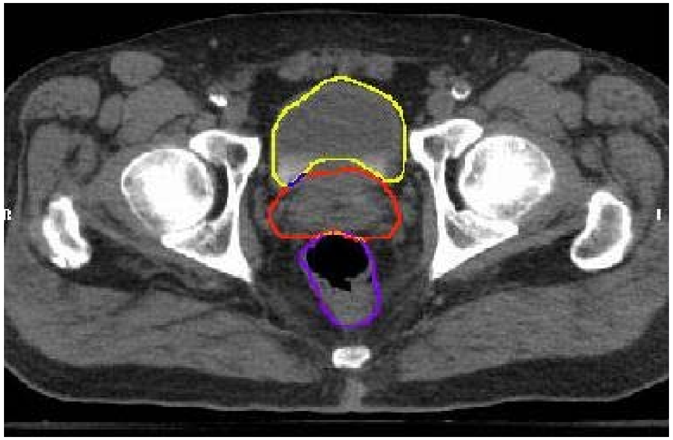
Variety of requirements from diverse experiments

**Physics**
from the **eV** to the **PeV** scale

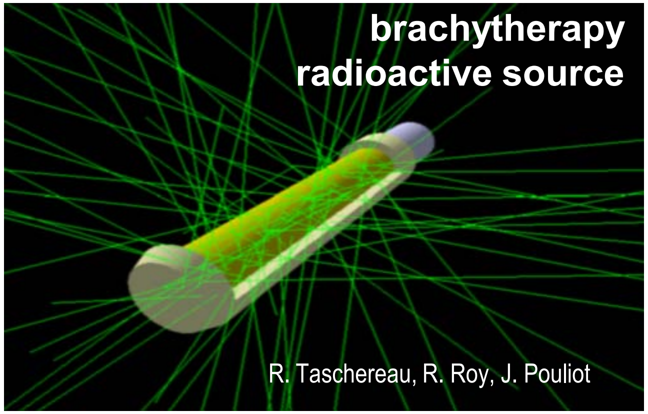
**Detectors**,
spacecrafts and **environment**

For such experiments **simulation software** is often **mission critical**

Require **reliability**, rigorous **software engineering standards**



# Medical Physics

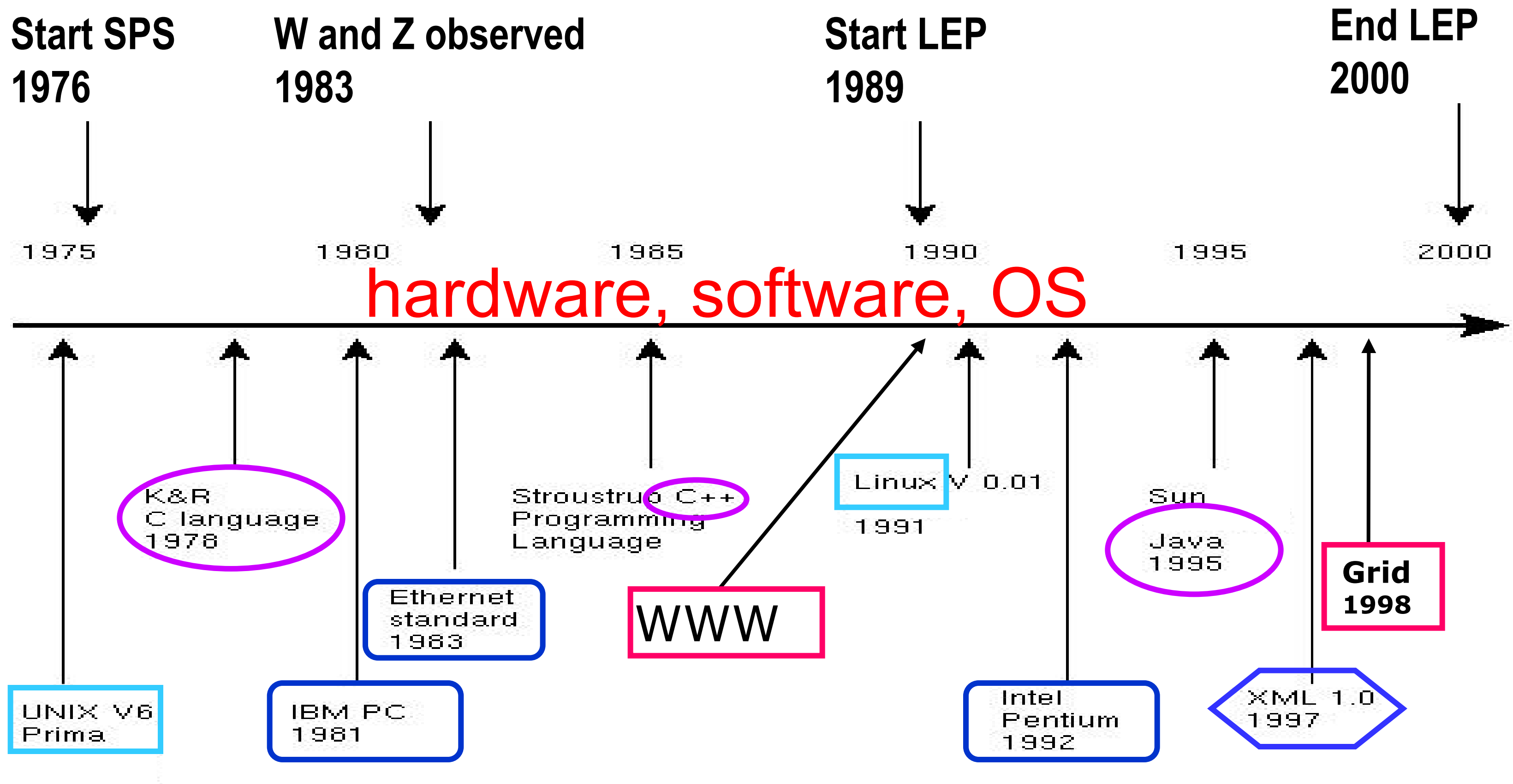



Radiotherapy Simulator

# Radiation protection


- Modeling radiation sources, devices and human body
- Precision of physics
- Reliability
- Easy configuration and friendly interface
- Speed

# …in a fast changing computing environment




…and don't forget changes of requirements!

Evolution towards greater diversity → we must **anticipate changes**

## OO technology

- Open to **extension** and **evolution**

new implementations can be added w/o changing existing code

- **Robustness** and ease of **maintenance**

**protocols** and well defined **dependencies** minimize coupling

# Strategic vision

## Toolkit

A set of **compatible components**

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

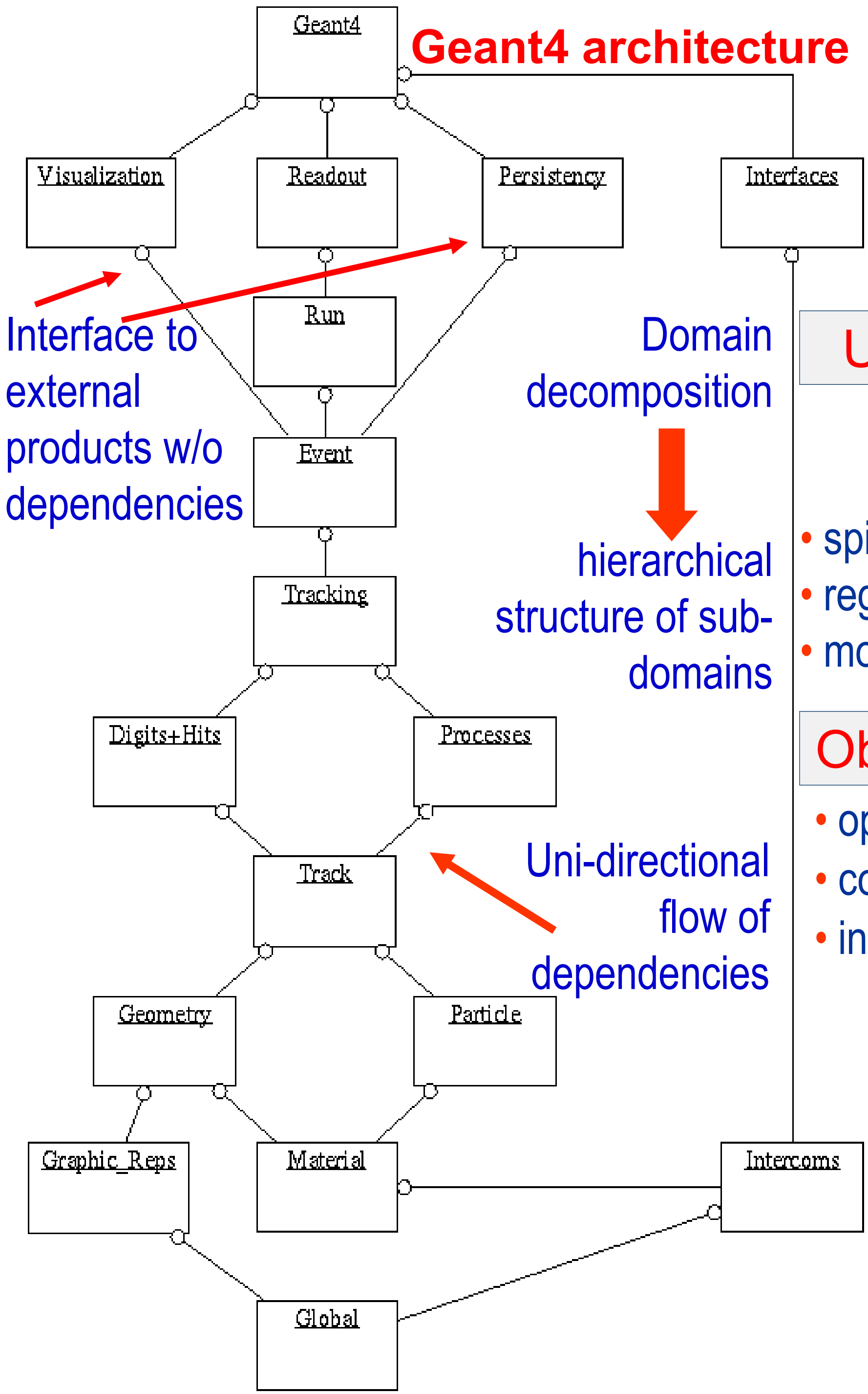
# The foundation

**RD44**
**CERN R&D project**
**1994-1998**

# 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




# Software Engineering

plays a fundamental role in Geant4

## User Requirements

- formally collected
- systematically updated
- PSS-05 standard

## Software Process

- spiral iterative approach
- regular assessments and improvements (SPI process)
- monitored following the ISO 15504 model

## Object Oriented methods

- OOAD
- use of CASE tools
- openness to extension and evolution
- contribute to the transparency of physics
- interface to external software without dependencies

## Quality Assurance

- commercial tools
- code inspections
- automatic checks of coding guidelines
- testing procedures at unit and integration level
- dedicated testing team

## Use of Standards

- de jure and de facto

# Functionality

What Geant4 can do
How well it does it

# Geant4 kernel: **Run** and **Event**

- Conceptually, a **run** is a collection of **events** that share the *same detector conditions*
  - Detector and physics settings are frozen in a run
- An event initially contains the primary particles; they are pushed into a stack and further processed
  - When the stack becomes empty, processing of an event is over
- **Multiple events**
  - possibility to handle pile-up
- **Multiple runs** in the same job
  - with different geometries, materials etc.
- Powerful stacking mechanism
  - three levels by default: handle trigger studies, loopers etc.

# Geant4 kernel: **Tracking**

- Decoupled from physics
  - all processes handled through the same abstract interface
- Independent from particle type
- New physics processes can be added to the toolkit without affecting tracking

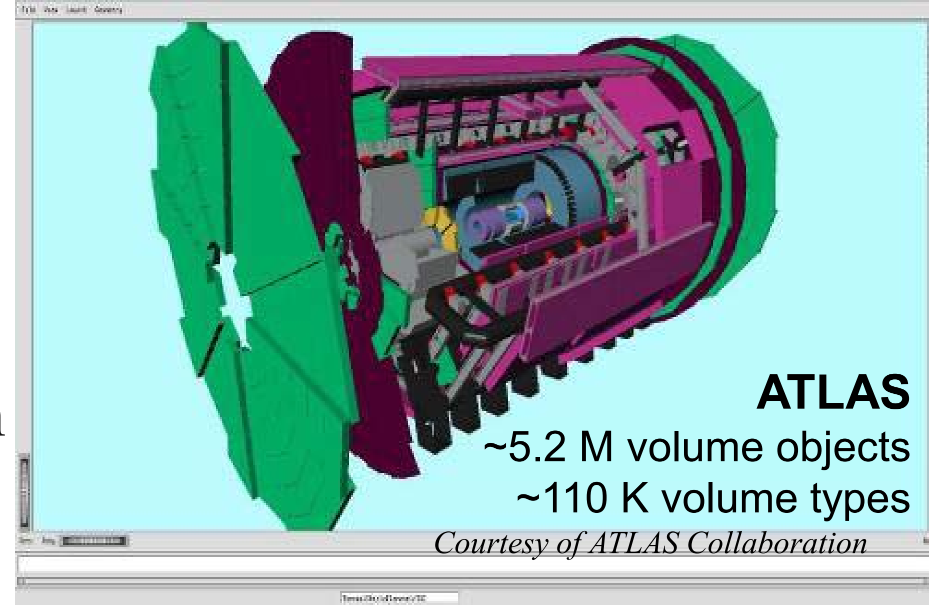
- Geant4 has only **secondary production thresholds**, **no tracking cuts**
  - all particles are tracked down to zero range
  - energy, TOF ... cuts can be defined by the user

# Materials

- Different kinds of materials can be defined
  - **isotopes** ⟺ G4Isotope
  - **elements** ⟺ G4Element
  - **molecules** ⟺ G4Material
  - **compounds** and **mixtures** ⟺ G4Material
- Associated attributes:
  - temperature
  - pressure
  - state
  - density

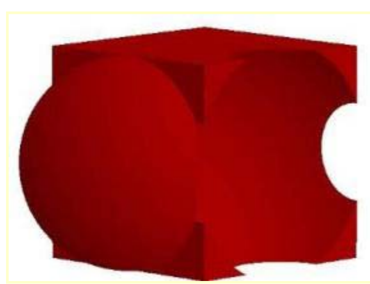
# Geometry

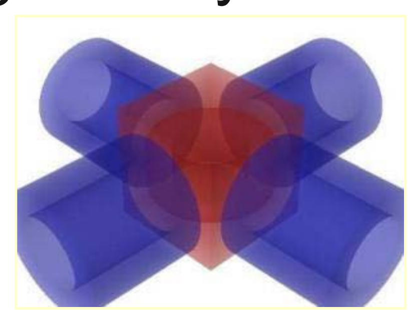
- Role
  - detailed detector description
  - efficient navigation



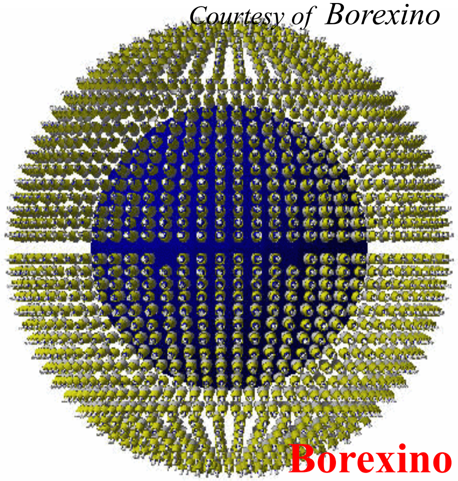

- Three conceptual layers
  - **Solid**: shape, size
  - **LogicalVolume**: material, sensitivity, daughter volumes, etc.
  - **PhysicalVolume**: position, rotation
- One can do fancy things with geometry…

Boolean operations

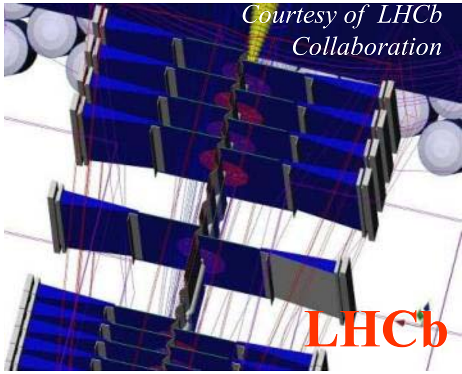




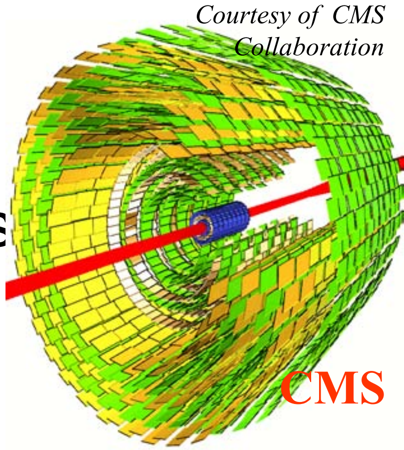
Transparent solids

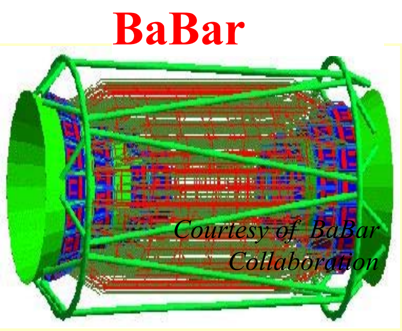


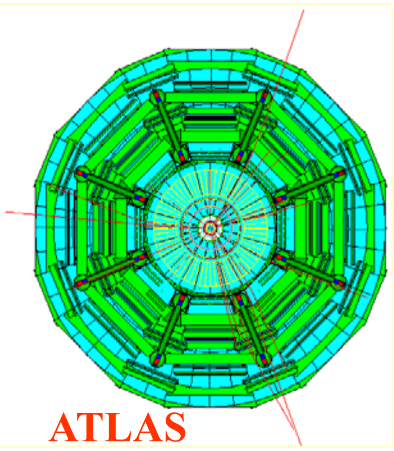

# Solids




**Multiple representations**
**Same abstract interface**

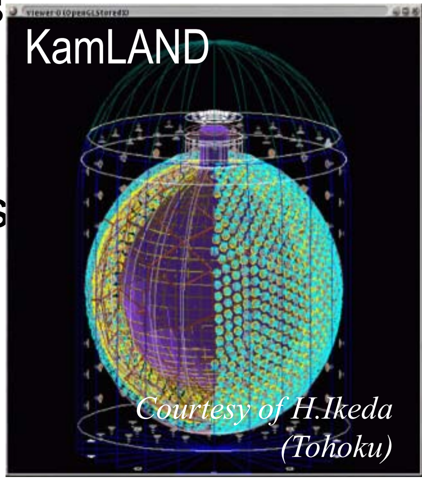


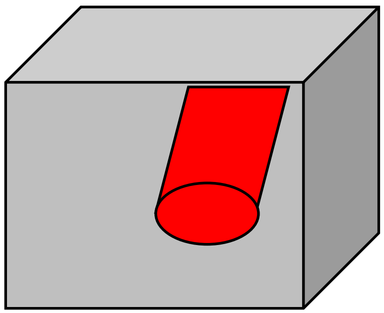




- **CSG** (**C**onstructed **S**olid **G**eometries)
  – simple solids
- **STEP extensions**
  – polyhedra, spheres, cylinders, cones, toroids, etc.
- **BREPS** (**B**oundary **REP**resented **S**olids)
  – volumes defined by boundary surfaces

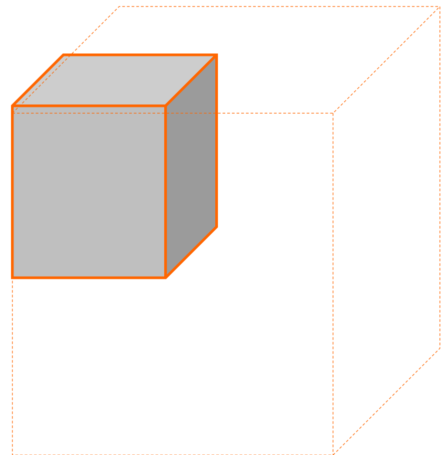
*CAD exchange*

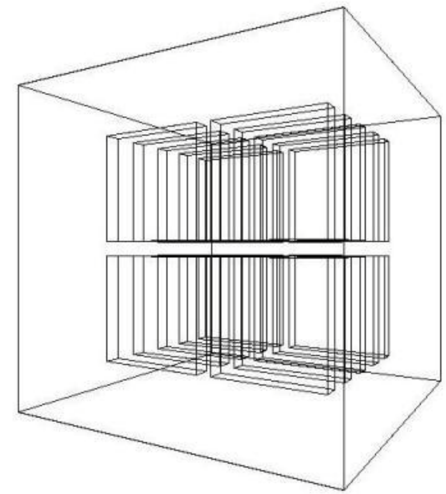


# Physical Volumes

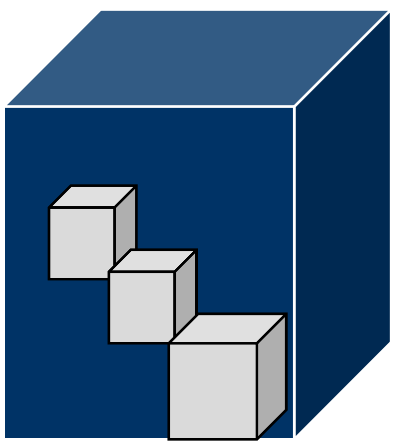


placement

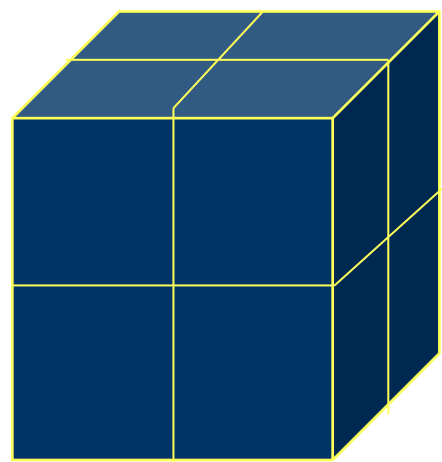




assembled



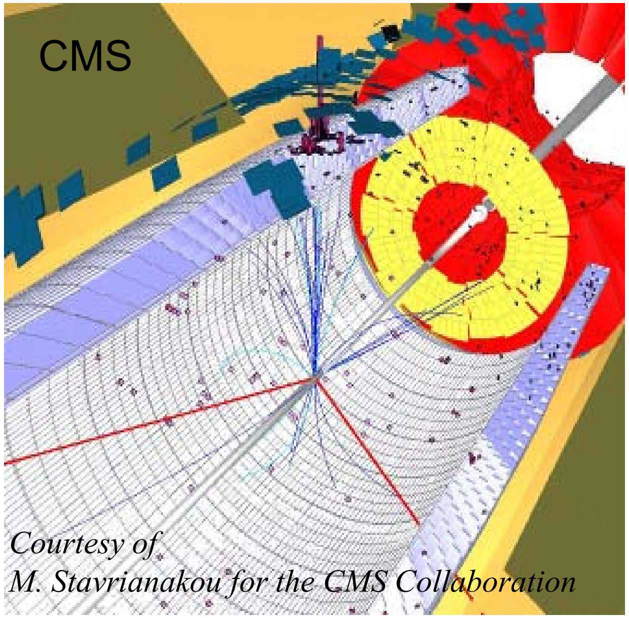
parameterised



replica

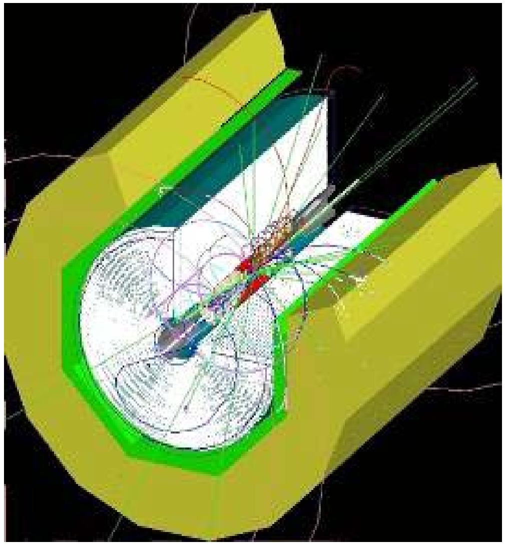
# Electric and magnetic fields

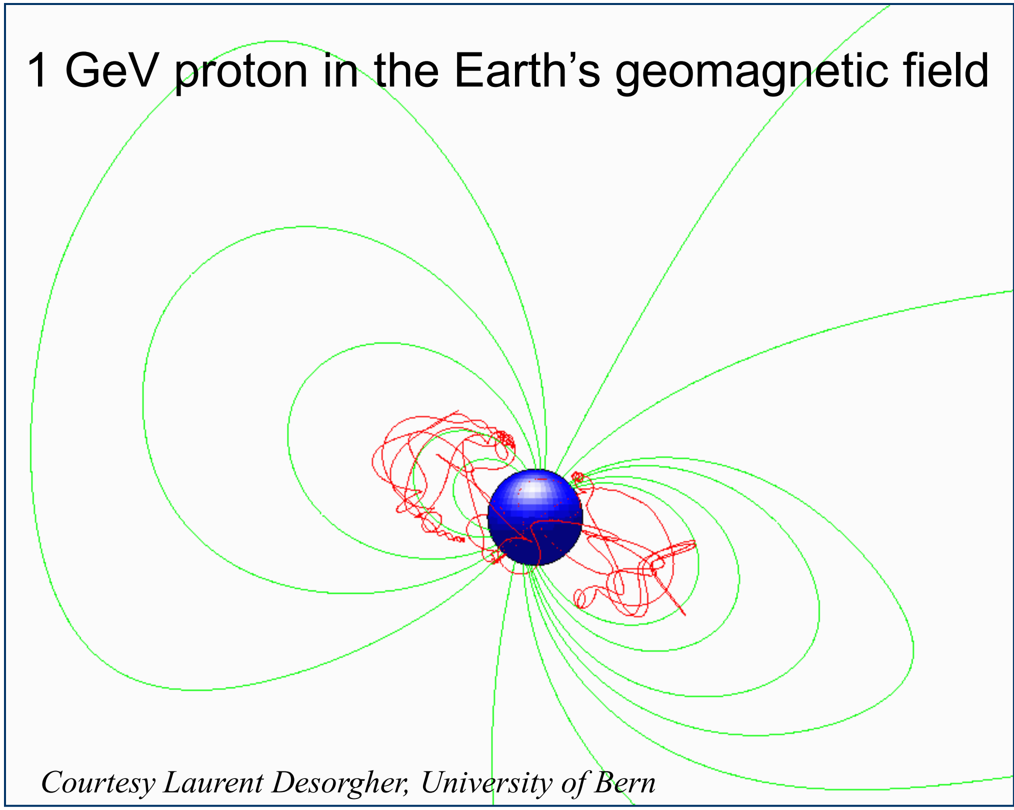
of variable non-uniformity
and differentiability

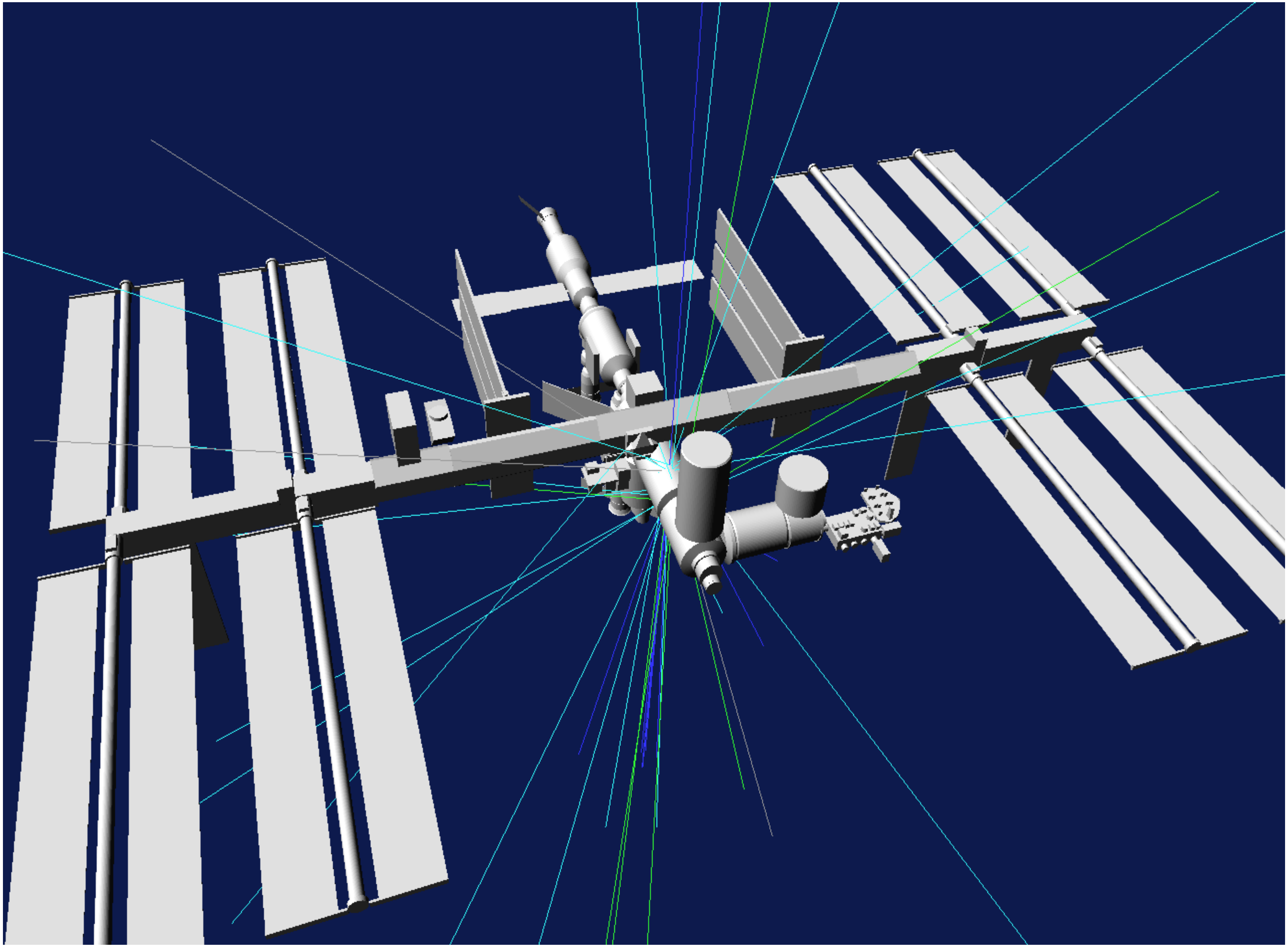



MOKKA

Linear Collider Detector

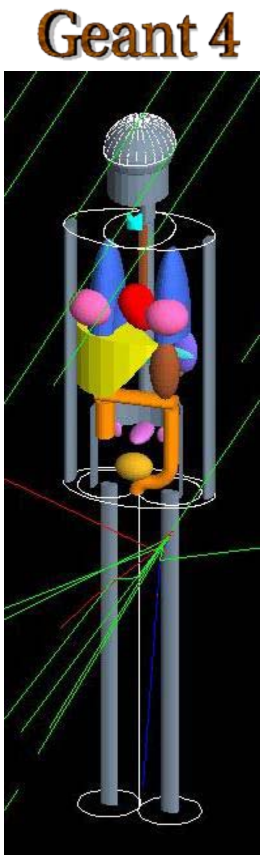




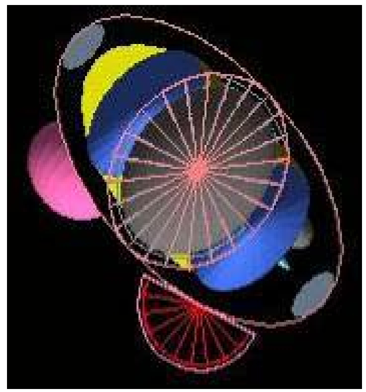


Courtesy T. Ersmark, KTH Stockholm

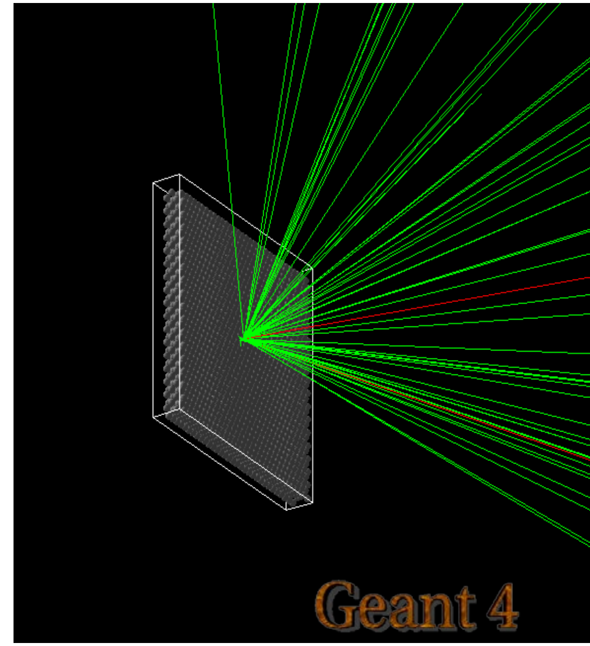
# Not only large scale, complex detectors…




Analytical breast

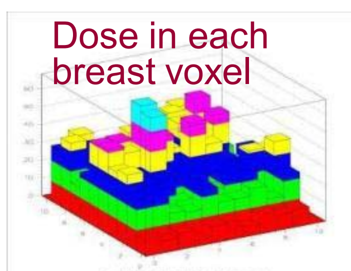


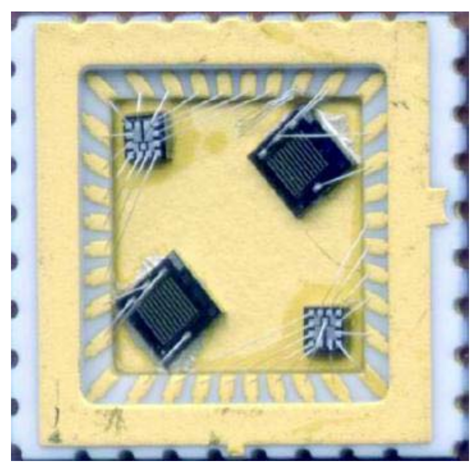
Voxel breast




simple geometries

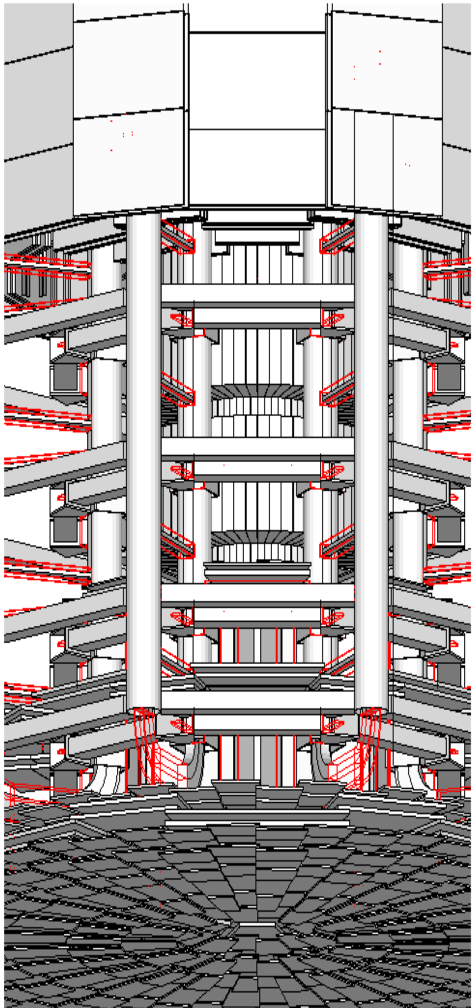
small scale components



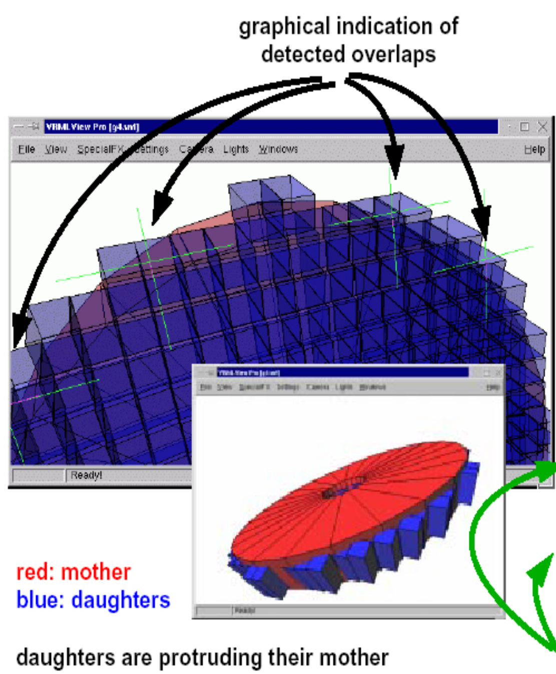

Geant4 anthropomorphic phantoms

# One may also do it wrong…



DAVID

Tools to detect badly defined geometries




Geant4 Macro:

```
/vis/scene/create
/vis/sceneHandler/create VRML2FILE
/vis/viewer/create
/olap/goto ECalEnd
/olap/grid 7 7 7
/olap/trigger
/vis/viewer/update
```

Output:

```
delta=59.3416
vol 1: point=(560.513,1503.21,-141.4)
vol 2: point=(560.513,1443.86,-141.4)
A -> B:
[0]:   ins=[2]   PVName=[NewWorld:0]  Type=[N]  ...
[1]:   ins=[0]   PVName=[ECalEndcap:0]  Type=[N]  ..
[2]:   ins=[1]   PVName=[ECalEndcap07:38]  Type=[N]

B -> A:
[0]:   ins=[2]   PVName=[NewWorld:0]  Type=[N]  ...
```

NavigationHistories of points of overlap
(including: info about translation, rotation, solid specs)

# 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

# Electromagnetic physics

- electrons and positrons
- photons (including optical photons)
- muons
- charged hadrons
- ions

- Multiple scattering
- Bremsstrahlung
- Ionisation
- Annihilation
- Photoelectric effect
- Compton scattering
- Rayleigh effect
- $\gamma$ conversion
- $e^+e^-$ pair production
- Synchrotron radiation
- Transition radiation
- Cherenkov
- Refraction
- Reflection
- Absorption
- Scintillation
- Fluorescence
- Auger emission

- Comparable to GEANT 3 already in $\alpha$ release1997
- Further extensions *(facilitated by OO technology)*

- High energy extensions
  - Motivated by LHC experiments, cosmic ray experiments…
- Low energy extensions
  - motivated by space and medical applications, dark matter and $\nu$ experiments, antimatter spectroscopy, radiation effects on components etc.
- Alternative models for the same process

# 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

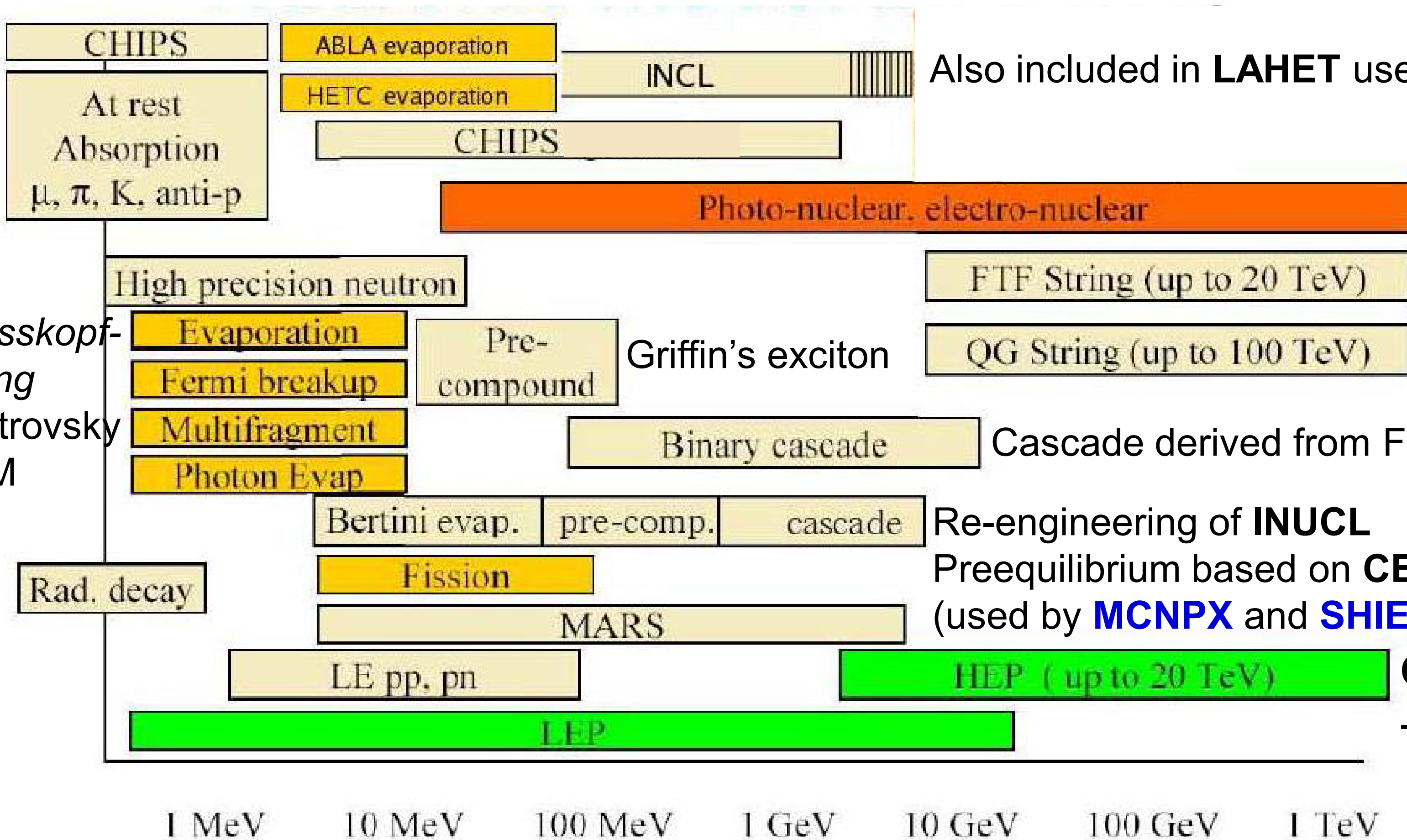
# Hadronic physics

- Completely different approach w.r.t. the past (GEANT 3)
  - native
  - transparent (in the original design)
  - **no longer interface to external packages**
  - clear separation between data and their use in algorithms
- **Cross section data sets**
  - Transparent and interchangeable
- **Final state calculation**
  - Models by particle, energy, material
- **Ample variety of models**
  - Alternative/complementary
  - It is possible to mix-and-match, with fine granularity
  - **Data-driven**, **parameterised** and **theory-driven** models

# Hadronic inelastic model inventory

- **Data-driven**
- **Parameterised**
- **Theory-driven**

**models**




*Weisskopf-Ewing*
Dostrovsky
GEM

Griffin's exciton

Also included in **LAHET** used by **MCNPX**

**FRITIOF**

Cascade derived from Frankfurt **QMD**

Re-engineering of **INUCL**
Preequilibrium based on **CEM**
(used by **MCNPX** and **SHIELD**)

**GHEISHA**
-like

# Other features

- **Particles**
  - all PDG data and more for specific Geant4 use, like ions
- **Hits & Digitization**
  - to describe detector response
- **Primary event generation**
  - some general purpose tools provided in the toolkit
- **Event biasing**
- **Fast simulation**
- **Persistency**
- **Parallelisation**

- No time to review them in detail
  - Geant4 user documentation

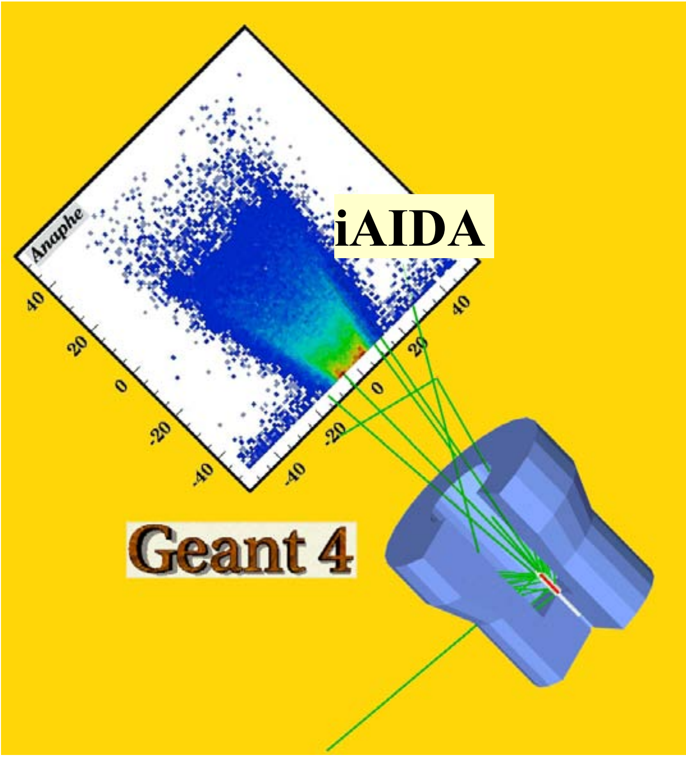
# Interface to external tools

through abstract interfaces

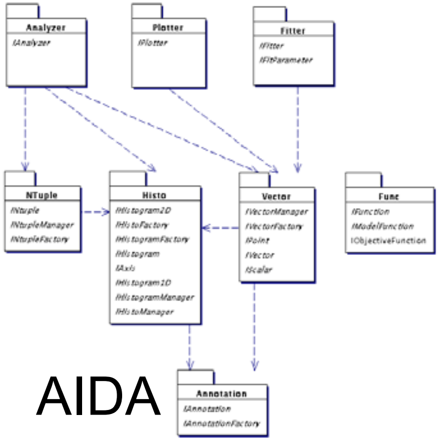
no dependency

minimize coupling of components

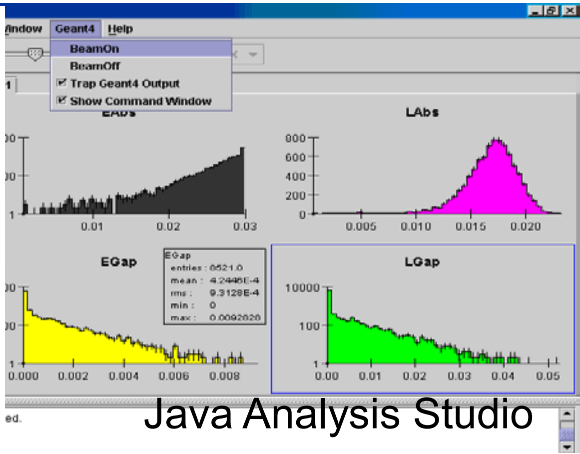
Similar approach
- **Visualisation**
- **(G)UI**
- **Persistency**
- **Analysis**




The user is free to choose the concrete system he/she prefers for each component




AIDA

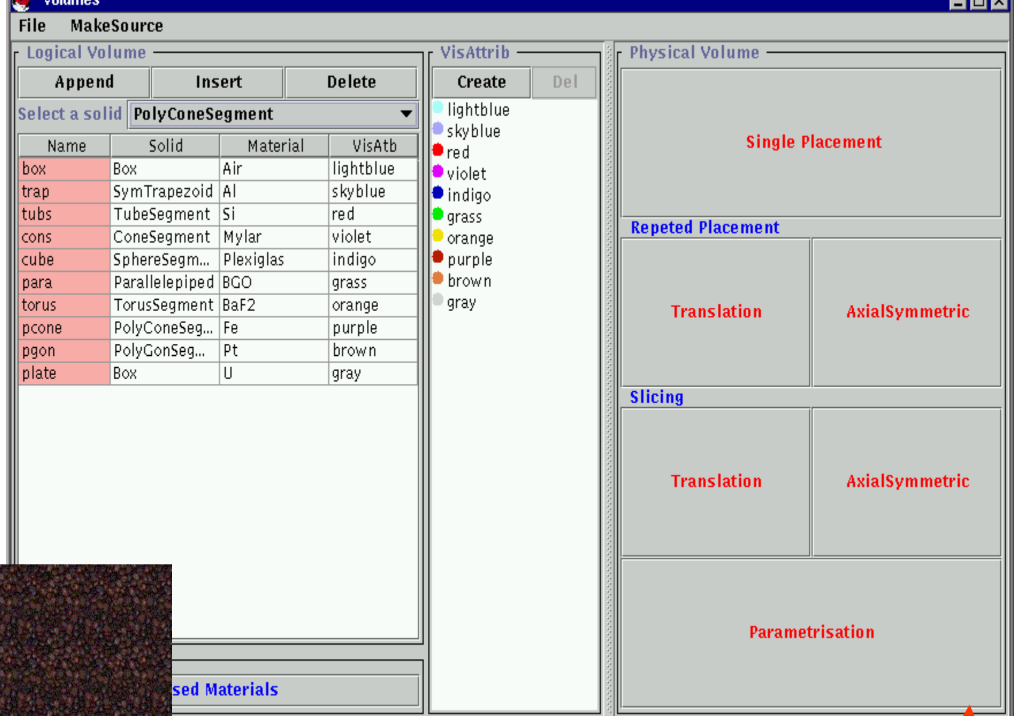


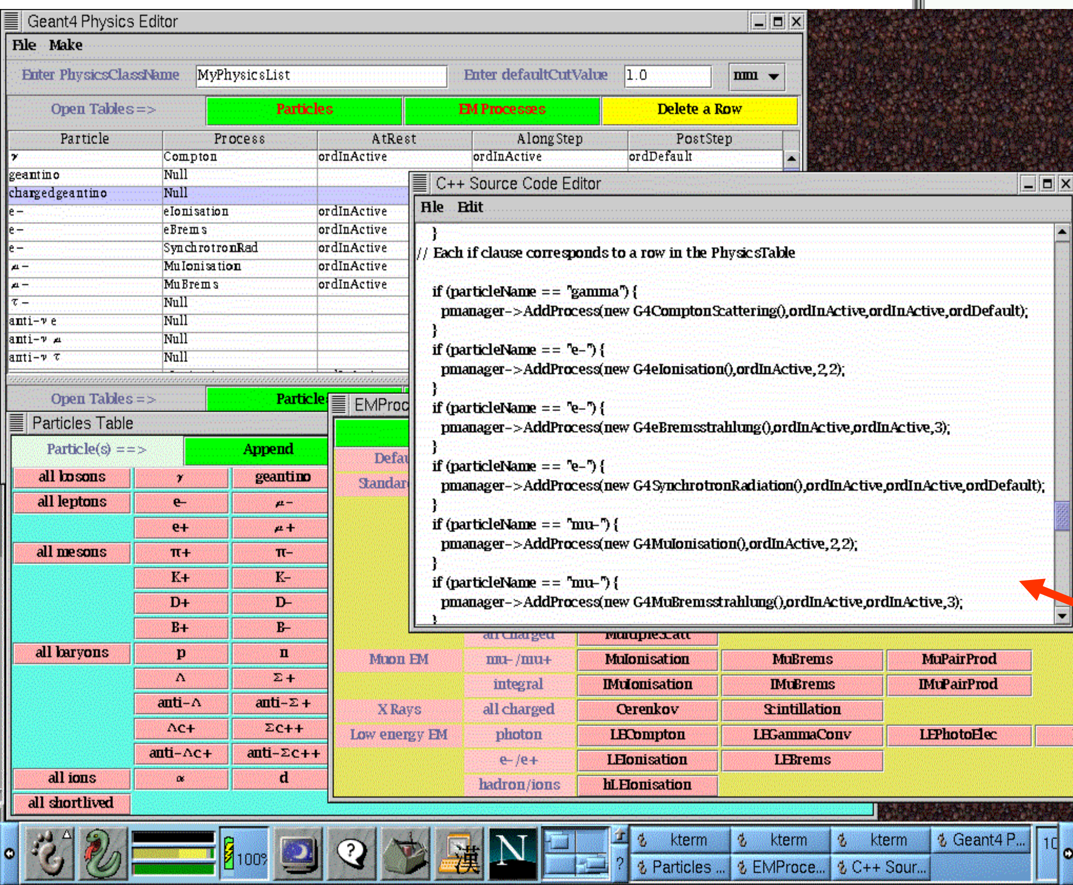

Java Analysis Studio

# User Interface

- Several implementations, all handled through abstract interfaces
- Command-line (batch and terminal)
- GUIs

  X11/Motif, GAG, MOMO, OPACS, Java



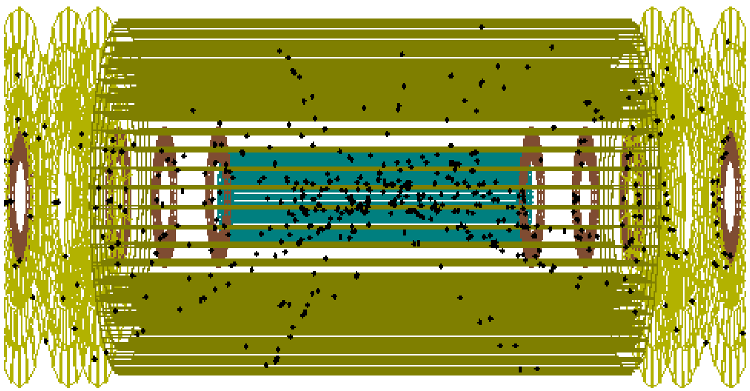

Automatic code generation for geometry and physics through a GUI

GGE (Geant4 Geometry Editor)

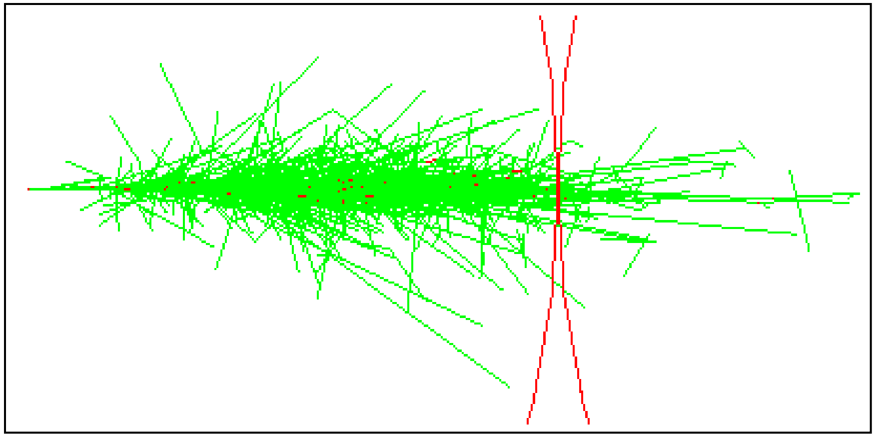
GPE (Geant4 Physics Editor)

# Visualisation

- Control of several kinds of visualisation
  - detector geometry
  - particle trajectories
  - hits in detectors



- Various **drivers**
  - OpenGL
  - OpenInventor
  - X11
  - Postscript
  - DAWN
  - OPACS
  - HepRep
  - VRML…



- all handled through abstract interfaces

# 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

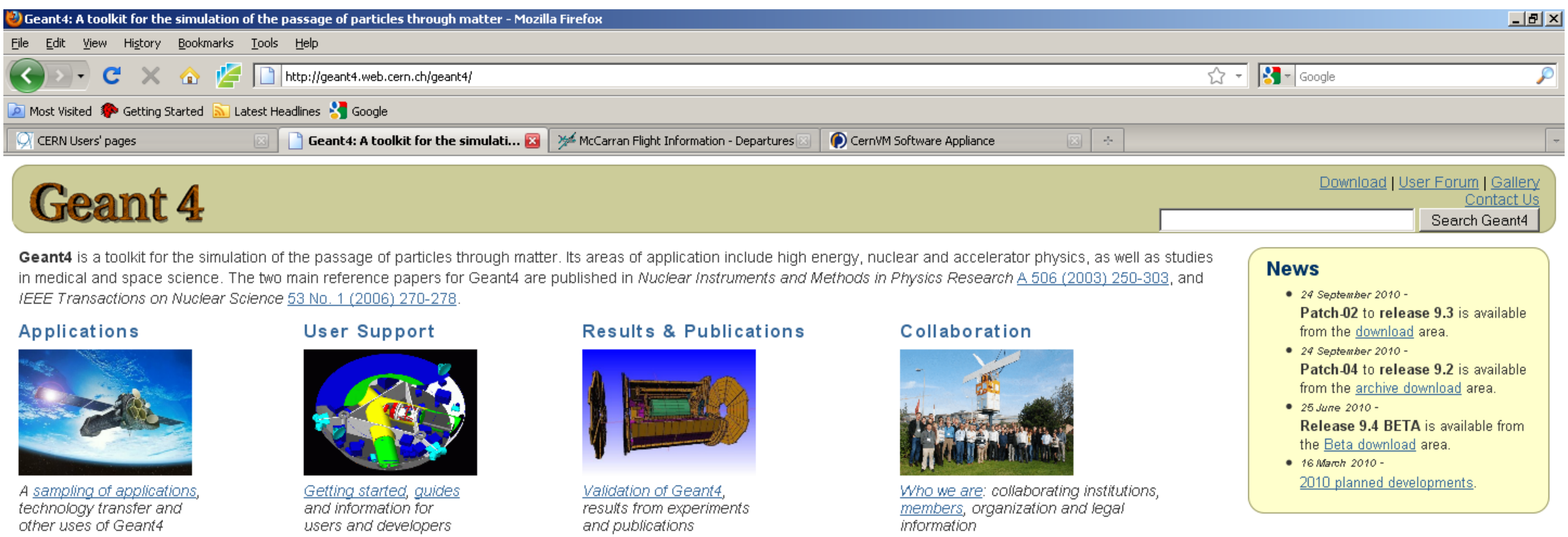
- Guidance: many **examples** are distributed with Geant4

# 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**

# Distribution

- Geant4 is **open-source**
- **Freely available**
  - Source code, libraries, associated data files and documentation can be downloaded from [http://cern.ch/geant4](http://cern.ch/geant4)
- User support provided by the Geant4 collaboration
  - On a best effort basis
  - User Forum: mutual support within the user community



# Geant4 physics and its validation

Further details in:

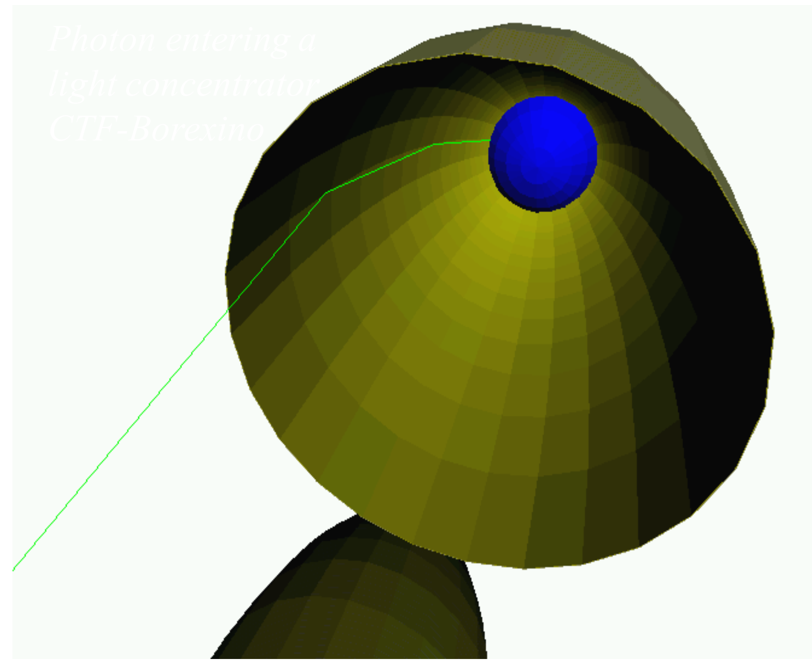
Geant4 Physics Reference Manual
Conference proceedings
Publications in refereed journals

# 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 |

# Optical photons

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

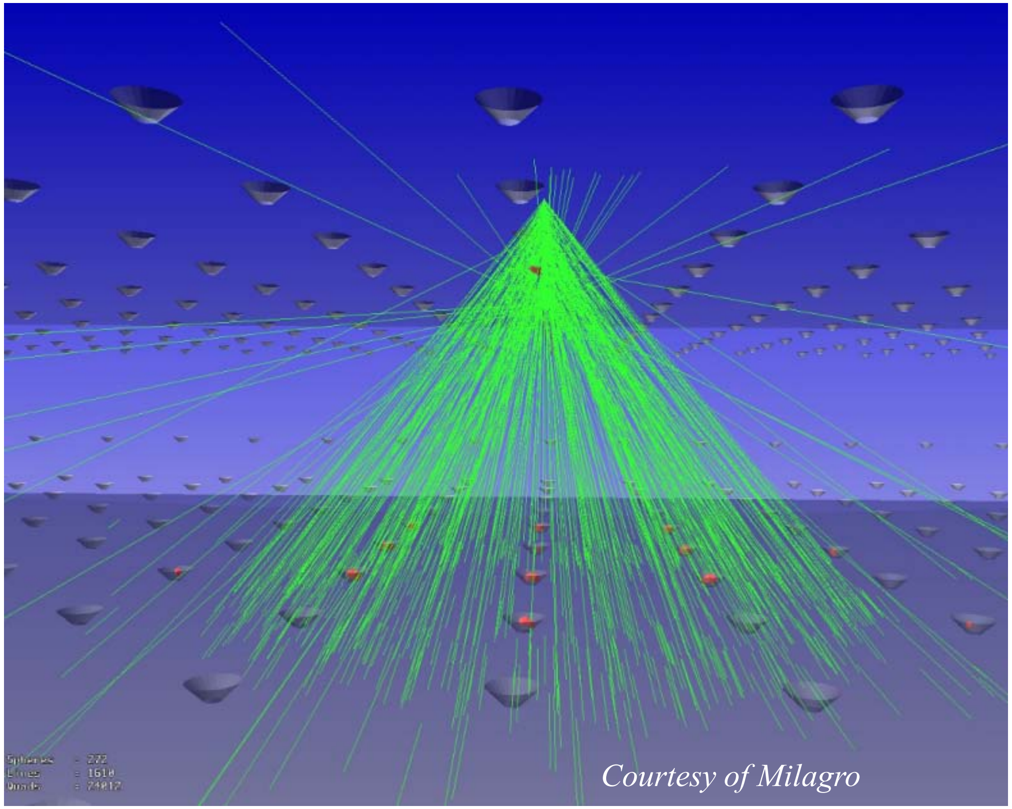


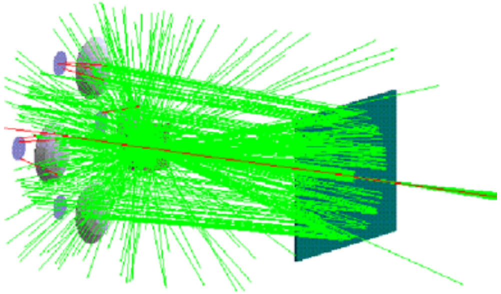

## Processes in Geant4:

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

# Cherenkov

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

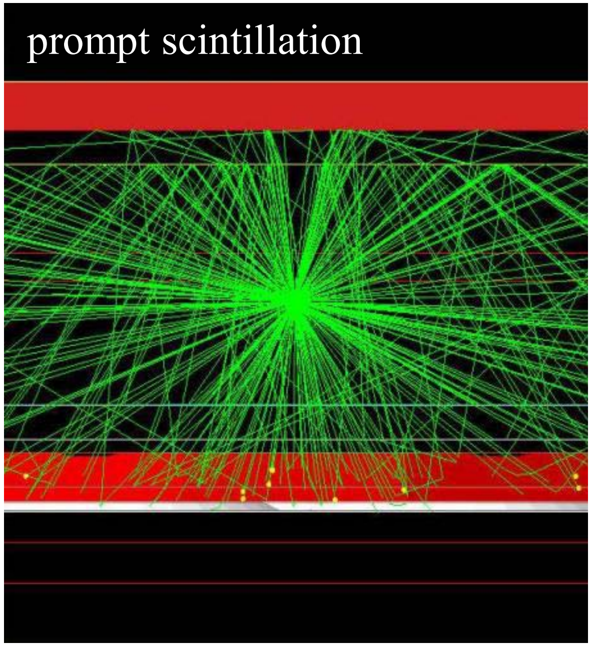


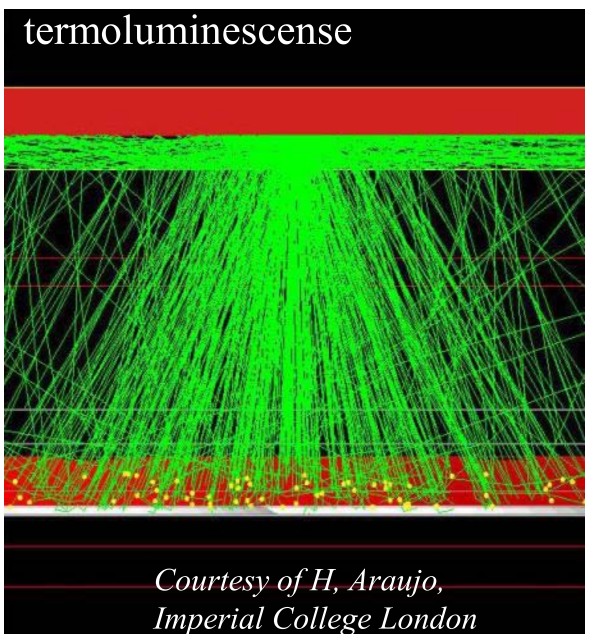



LHCb

| Aerogel Thickness | | Yield Per Event | Cherenkov Angle mrad |
|---|---|---|---|
| 4 cm | DATA | **6.3 ± 0.7** | 247.1+-5.0 |
| | MC | **7.4 ± 0.8** | 246.8+-3.1 |
| 8 cm | DATA | **9.4 ± 1.0** | 245.4+-4.8 |
| | MC | **10.1 ±1.1** | 243.7+-3.0 |

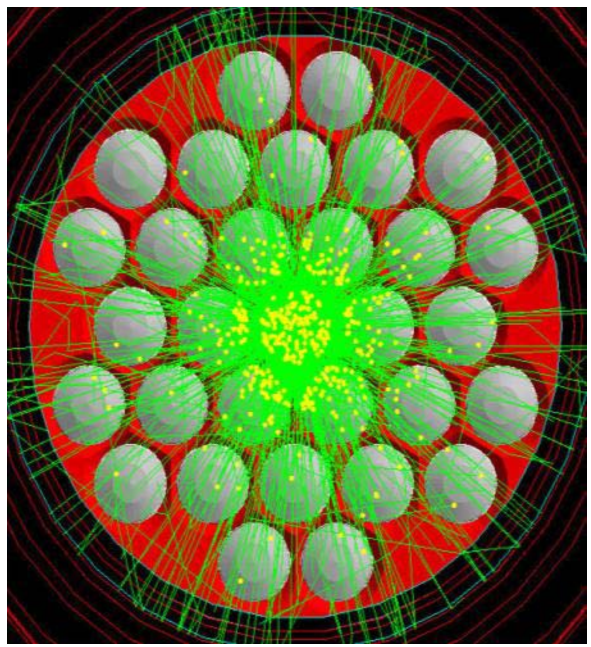
# Scintillation



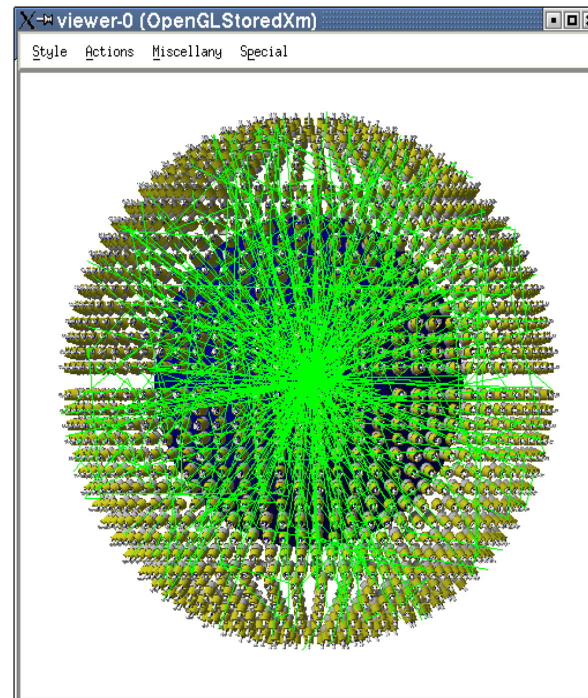




ZEPLIN III
Dark Matter Detector

signal in PMT



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




*Courtesy of Borexino*

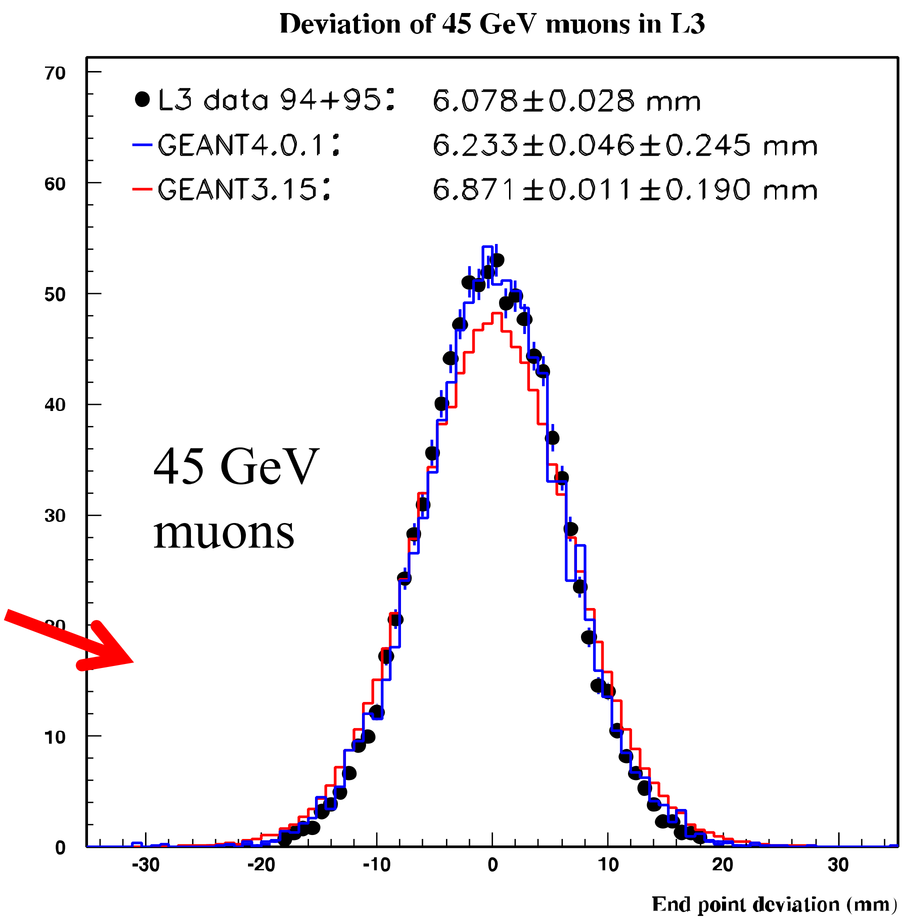
# Muons

- *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



# 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

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)*

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

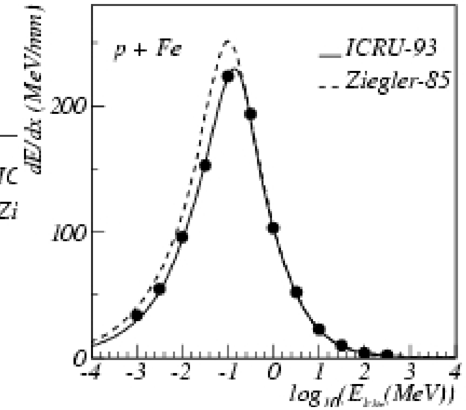
- Bremsstrahlung
- Ionisation

- Polarised Compton

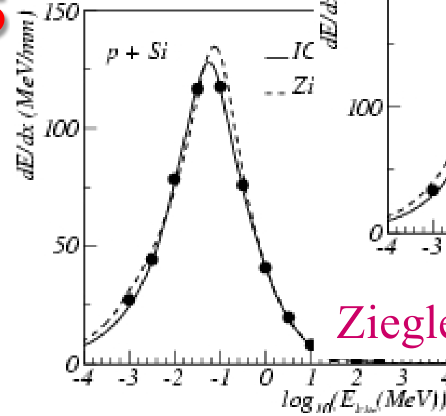
- + atomic relaxation
  - fluorescence
  - Auger effect

*following processes leaving a vacancy in an atom*

# Positive charged hadrons




Ziegler and ICRU, Fe



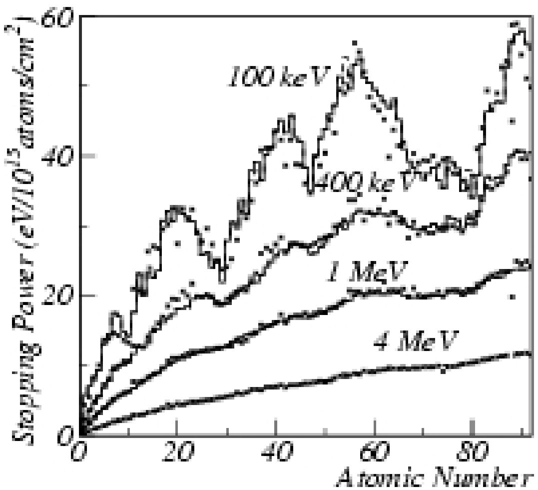

Ziegler and ICRU, Si

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

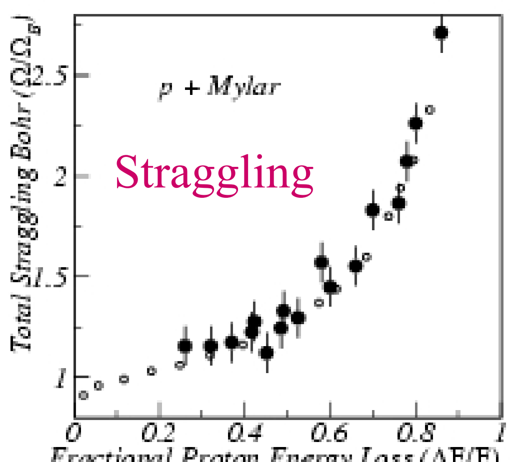
- Density correction for high energy
- Shell correction term for intermediate energy

**-Spin dependent term**
**- Barkas and Bloch terms**

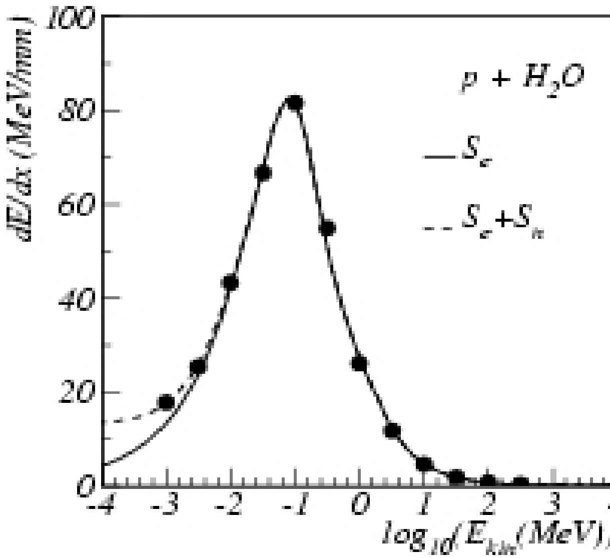
**-Chemical effect for compounds**
**- Nuclear stopping power**
**- PIXE included**




Stopping power
Z dependence for various energies
Ziegler and ICRU models




Straggling



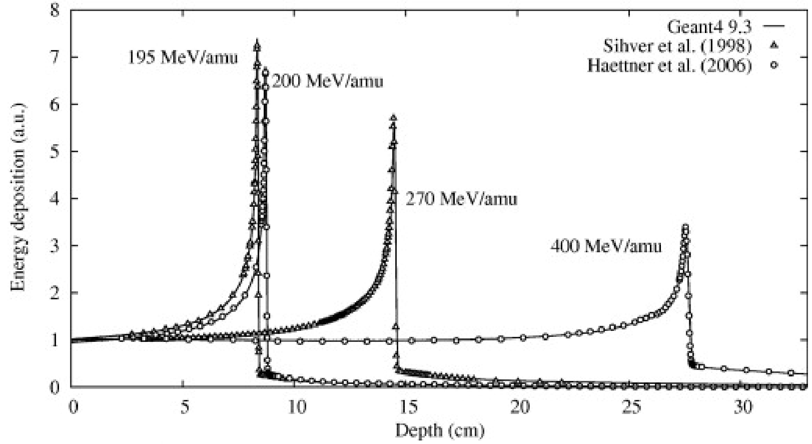

Nuclear stopping power

# Positive charged ions

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

- Effective charge model
- Nuclear stopping power

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



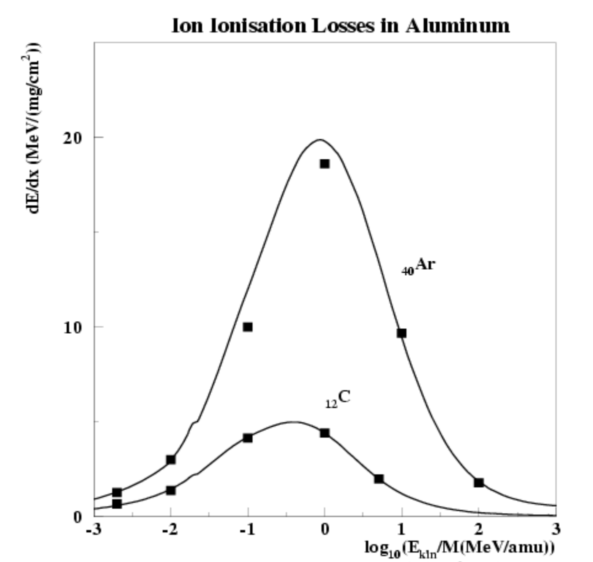
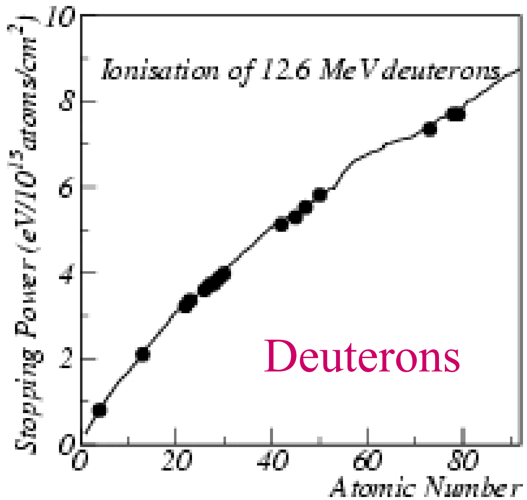




Figure 8: Ion electronic stopping power in aluminum. Points - the best fit on the data from Ref.[12], solid line - GEANT4 parameterisation. The accuracy of the data is about 5 %.




Comparison of simulated and measured $^{12}C$ depth-dose profiles in water (0.997 g/cm³). 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

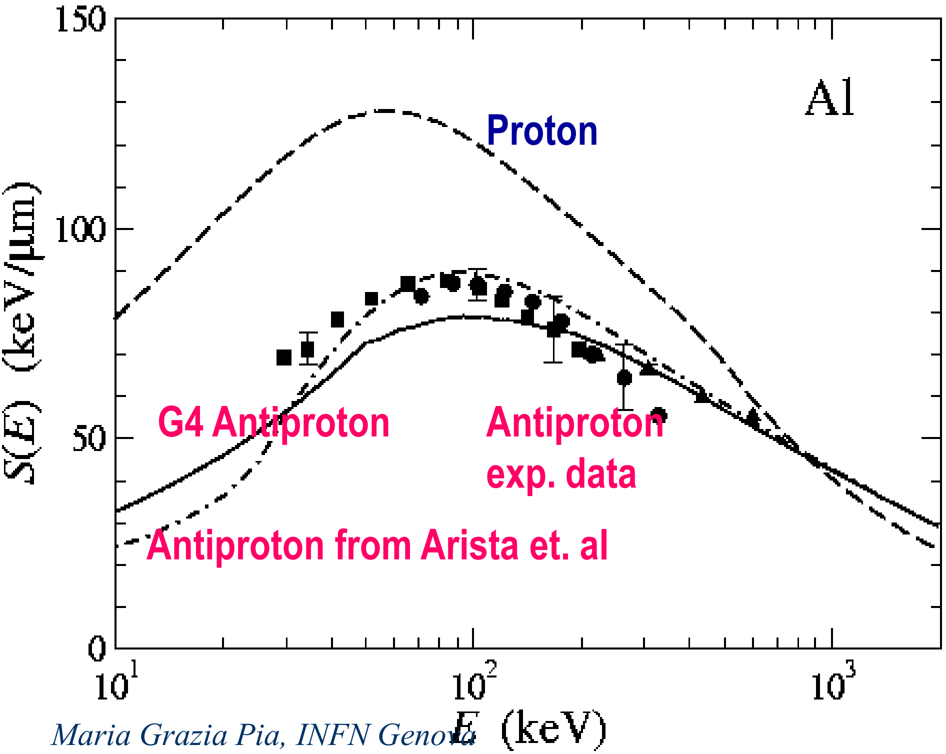
# Models for antiprotons

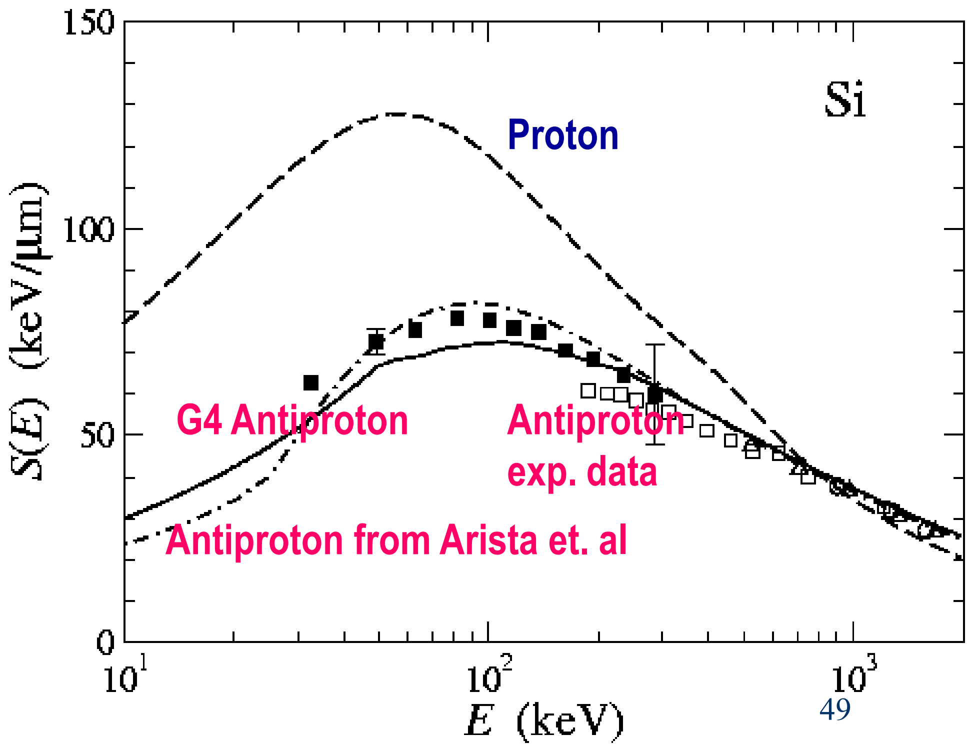
578 IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 54, NO. 3, JUNE 2007

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

Stéphane Chauvie, Petteri Nieminen, and Maria Grazia Pia

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



IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 54, NO. 3, JUNE 2007 585

# 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

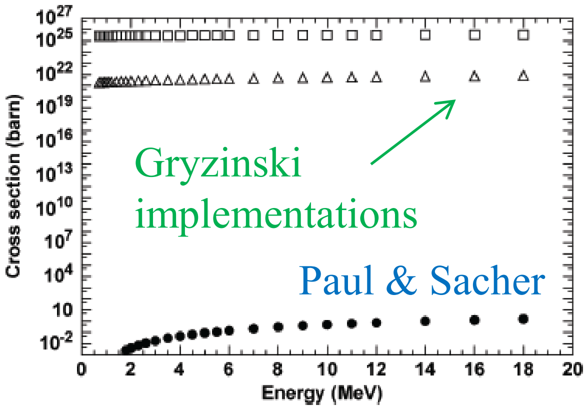
**36 pages**

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

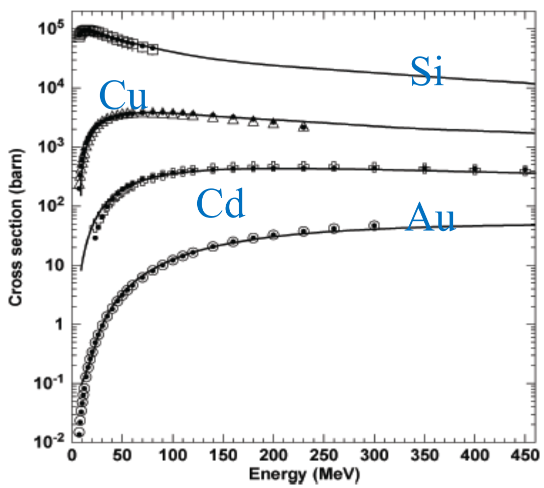
+ further ongoing activity and results

# Mishaps of Geant4 PIXE…

**1st development cycle**




K shell ionisation, Au




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

**Current low energy group's development**

Nuclear Instruments and Methods in Physics Research B 267 (2009) 37–44

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

ELSEVIER

New Geant4 cross section models for PIXE simulation

H. Ben Abdelouahed [a,*], S. Incerti [b], A. Mantero [c]

**Released in Geant4 9.2**

**Several flaws** documented in

*Pia et al., TNS 56(6), 3614-3649, 2003*

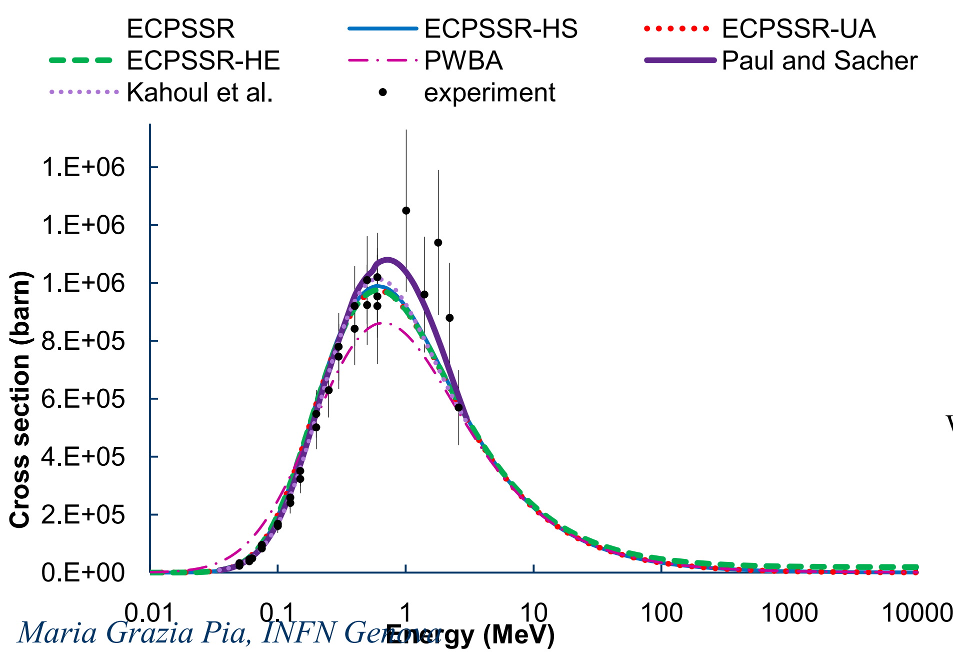
# PIXE now

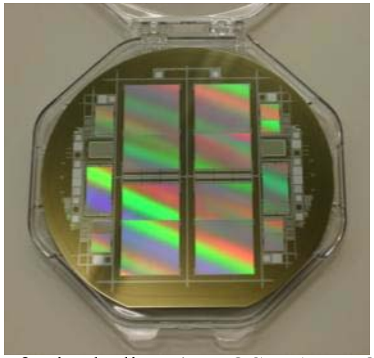
3614 IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 56, NO. 6, DECEMBER 2009

## 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

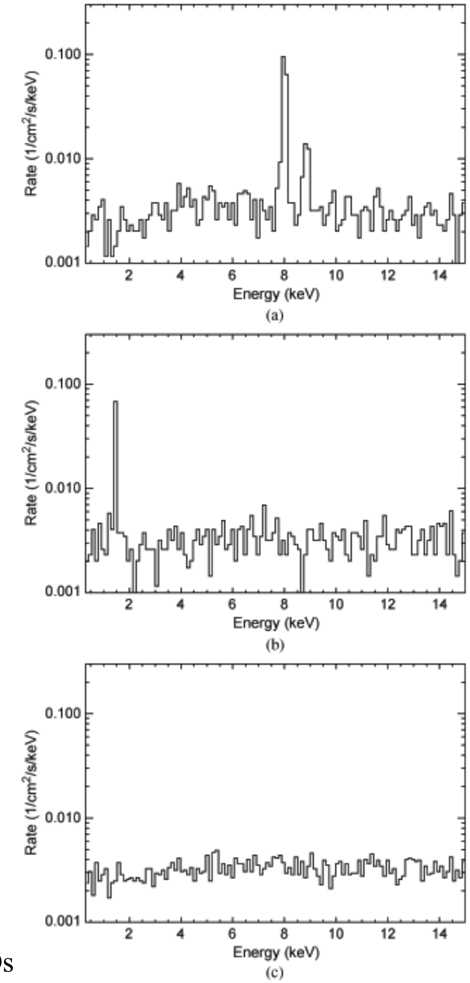



Fig. 12. A comparison of the fluorescence background due to ionization by cosmic-ray protons in an L2 orbit for three different graded Z shield designs for the eROSITA X-ray detectors. (a) Cu shield; (b) Cu-Al shield; (c) Cu – Al – $B_4C$ shield.

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

# Very-low energy extensions

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

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

# 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

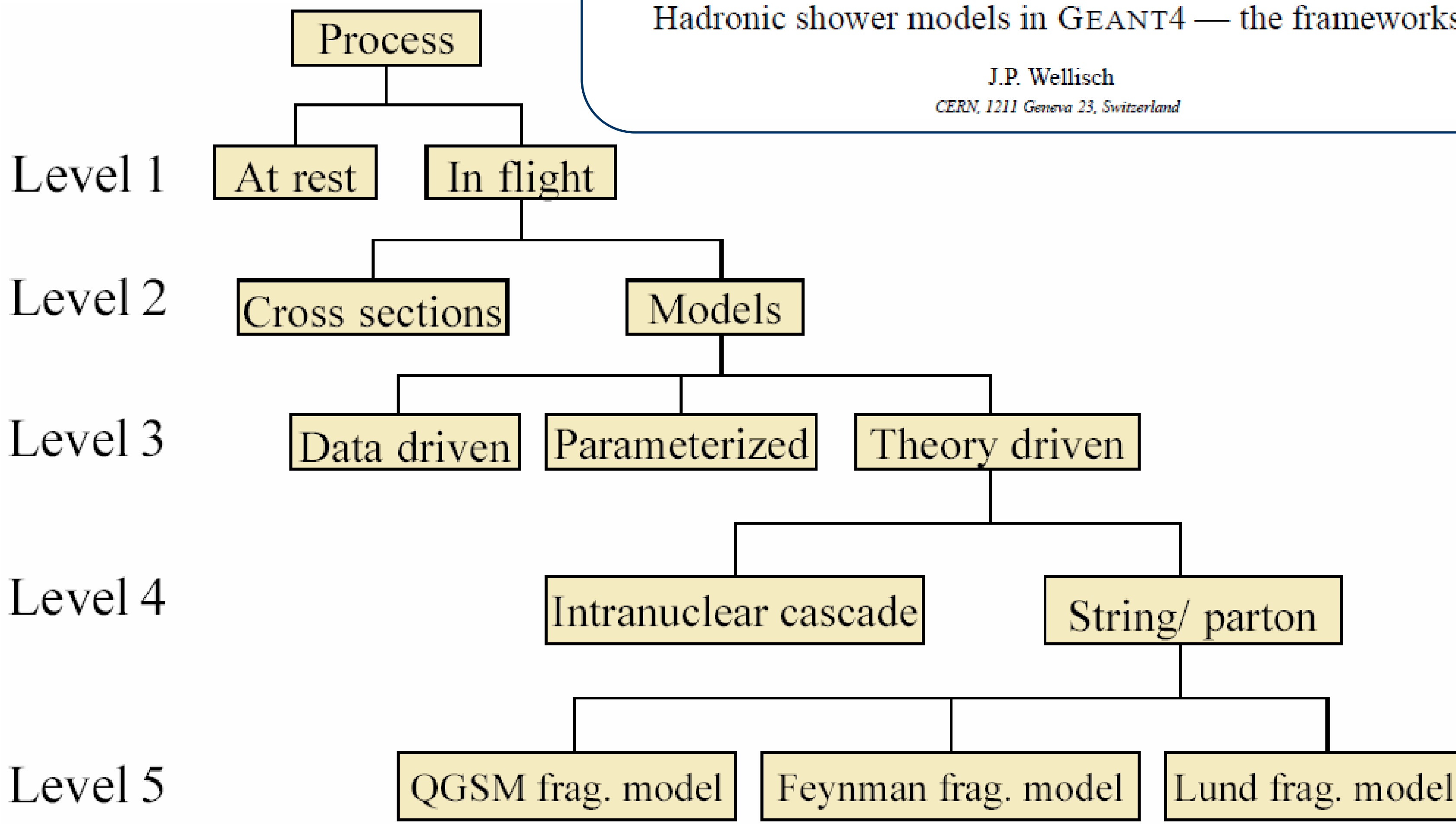
Computer Physics Communications

www.elsevier.com/locate/cpc

Hadronic shower models in GEANT4 — the frameworks

J.P. Wellisch

*CERN, 1211 Geneva 23, Switzerland*



# 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 MeV < E < 20 GeV
- **Ion-nucleus reaction** cross sections (several models)
  - Good for E/A < 1 GeV
- **Isotope production** data
  - E < 100 MeV
- **Photo-nuclear** cross sections

# Nuclear elastic scattering

G4HadronElasticDataSet

G4HadronElasticProcess

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"*

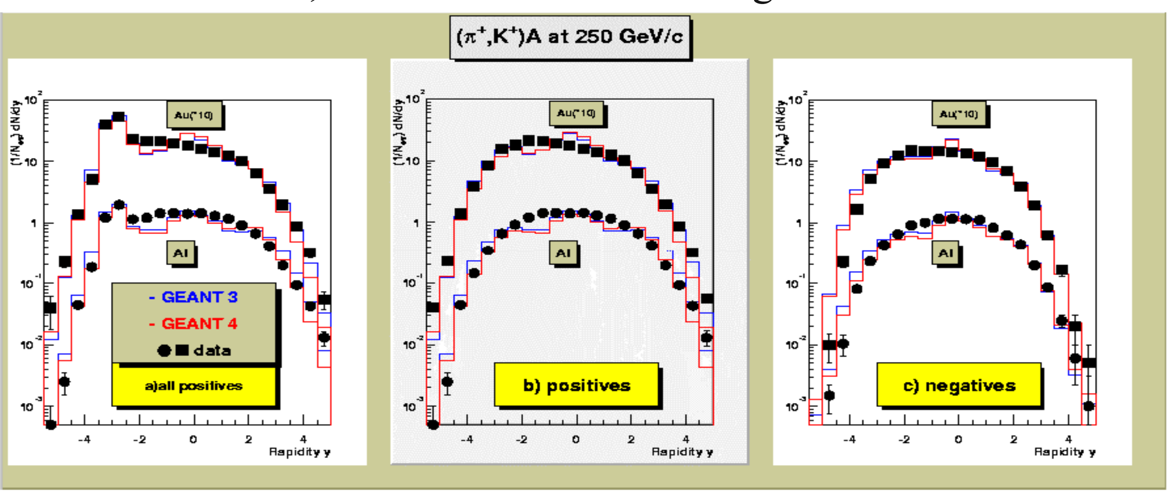
G4QElasticCrossSection

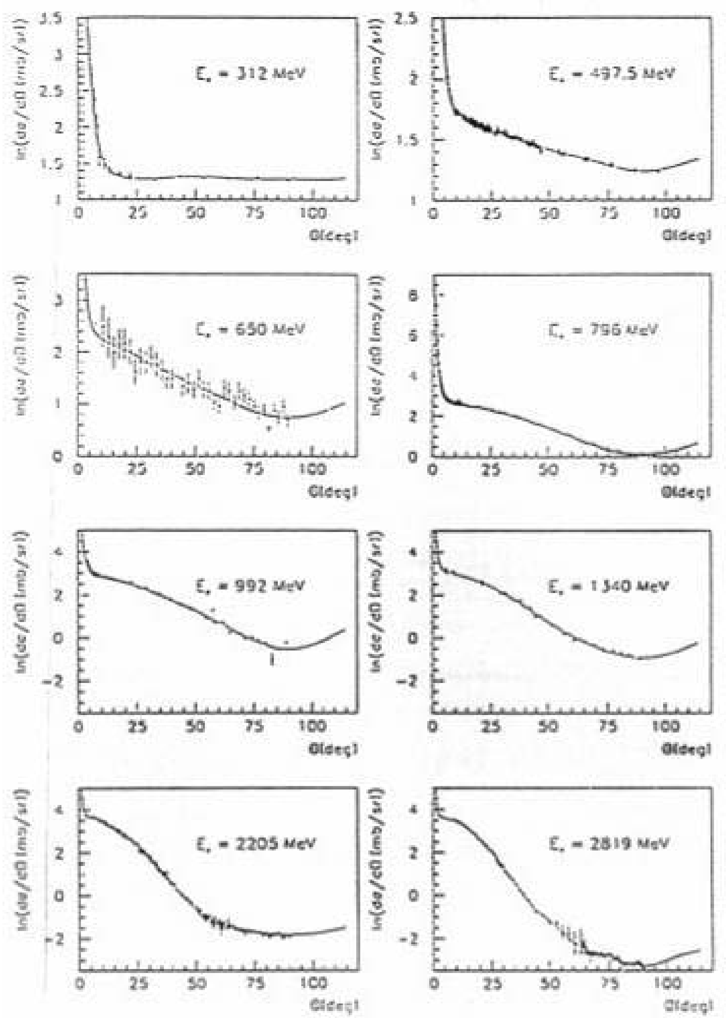
**Validation?**

# 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
  - πN, total cross section
  - πN, coherent elastic scattering



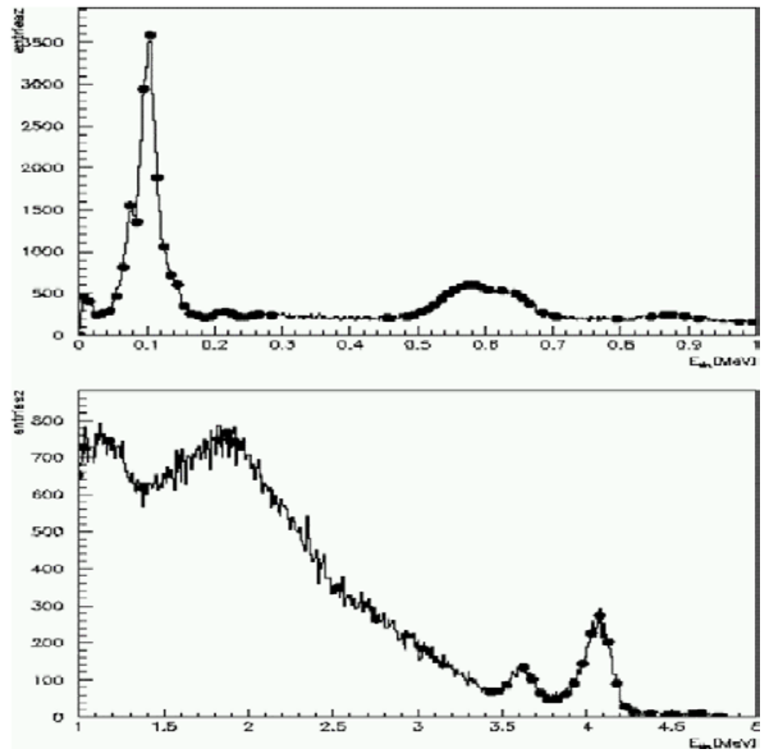
# Theory-driven hadronic non-elastic models

- Complementary and alternative models
  - **Evaporation** phase
  - Low energy range, O(100 MeV): **pre-equilibrium**
  - Intermediate energy, O(100 MeV -5 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)

# 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**




Geant4 simulation of γ-rays from 14 MeV neutron capture on uranium

# 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)

# 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**

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research A

journal homepage: www.elsevier.com/locate/nima

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

G.A.P. Cirrone [a], G. Cuttone [a], F. Di Rosa [a], L. Pandola [b,*], F. Romano [a], Q. Zhang [a,c,**]

## 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 [26)] 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

Vladimir IVANCHENKO[1,2,3*], John APOSTOLAKIS[1], Alexander BAGULYA[4], Haifa Ben ABDELOUAHED[5], Rachel BLACK[6], Alexey BOGDANOV[7], Helmut BURKHARD[1], Stéphane CHAUVIE[8], Pablo CIRRONE[9], Giacomo CUTTONE[9], Gerardo DEPAOLA[10], Francesco Di ROSA[9], Sabine ELLES[11], Ziad FRANCIS[12], Vladimir GRICHINE[4], Peter GUMPLINGER[13], Paul GUEYE[6], Sebastien INCERTI[14], Anton IVANCHENKO[14], Jean JACQUEMIER[11], Anton LECHNER[1,15], Francesco LONGO[16], Omrane KADRI[5], Nicolas KARAKATSANIS[17], Mathieu KARAMITROS[14], Rostislav KOKOULIN[7], Hisaya KURASHIGE[18], Michel MAIRE[11,19], Alfonso MANTERO[20], Barbara MASCIALINO[21], Jakub MOSCICKI[1], Luciano PANDOLA[22], Joseph PERL[23], Ivan PETROVIC[9], Aleksandra RISTIC-FIRA[9], Francesco ROMANO[9], Giorgio RUSSO[9], Giovanni SANTIN[24], Andreas SCHAELICKE[25], Toshiyuki TOSHITO[26], Hoang TRAN[14], Laszlo URBAN[19], Tomohiro YAMASHITA[27] and Christina ZACHARATOU[28]

# 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

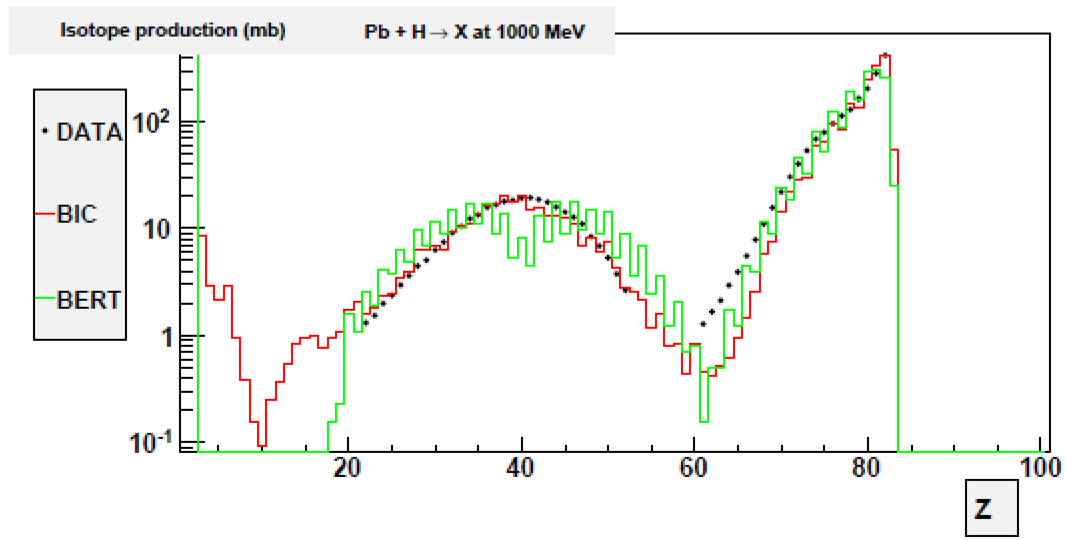
# Hadronic simulation validation

- 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**



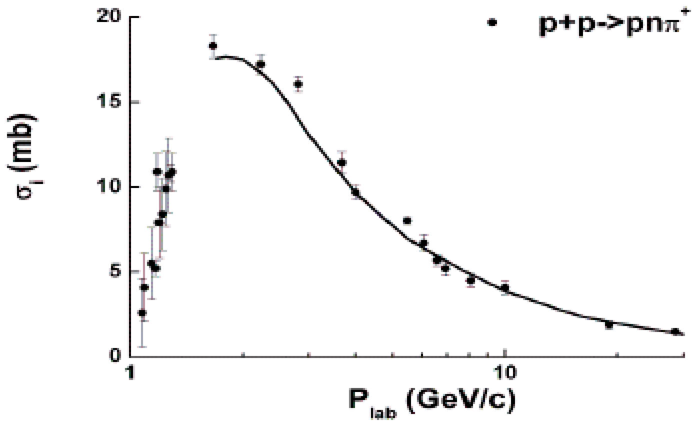

## Calibration or validation?

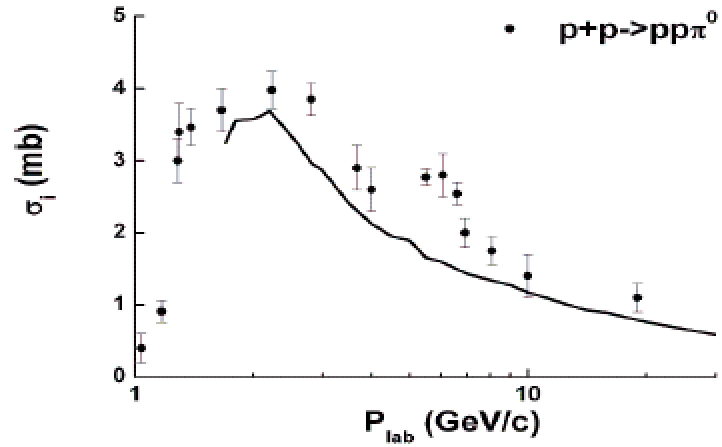

*Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2010 (SNA + MC2010)*
Hitotsubashi Memorial Hall, Tokyo, Japan, October 17-21, 2010


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


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

# Experimental comparisons - **FRITIOF**




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

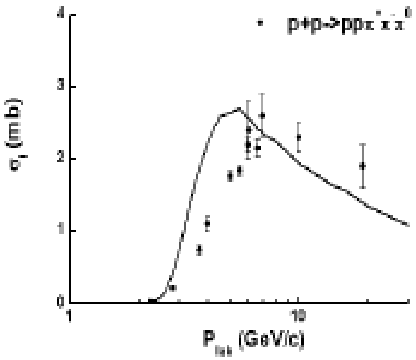
More in

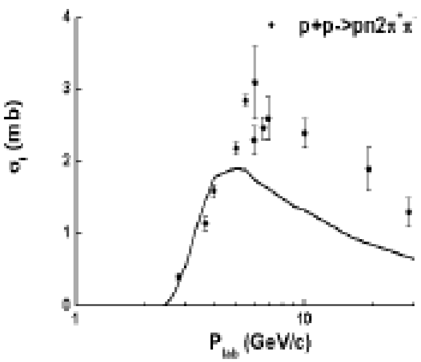
*Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2010 (SNA + MC2010)*
Hitotsubashi Memorial Hall, Tokyo, Japan, October 17-21, 2010

**Development of the Fritiof Model in Geant4**

Vladimir UZHINSKY [1,2*]
On behalf of the Geant4 Hadronics Working Group

*[1] CERN, CH-1211, Geneva 23, Switzerland*
*[2] LIT, JINR, 141980 Dubna, Russia*

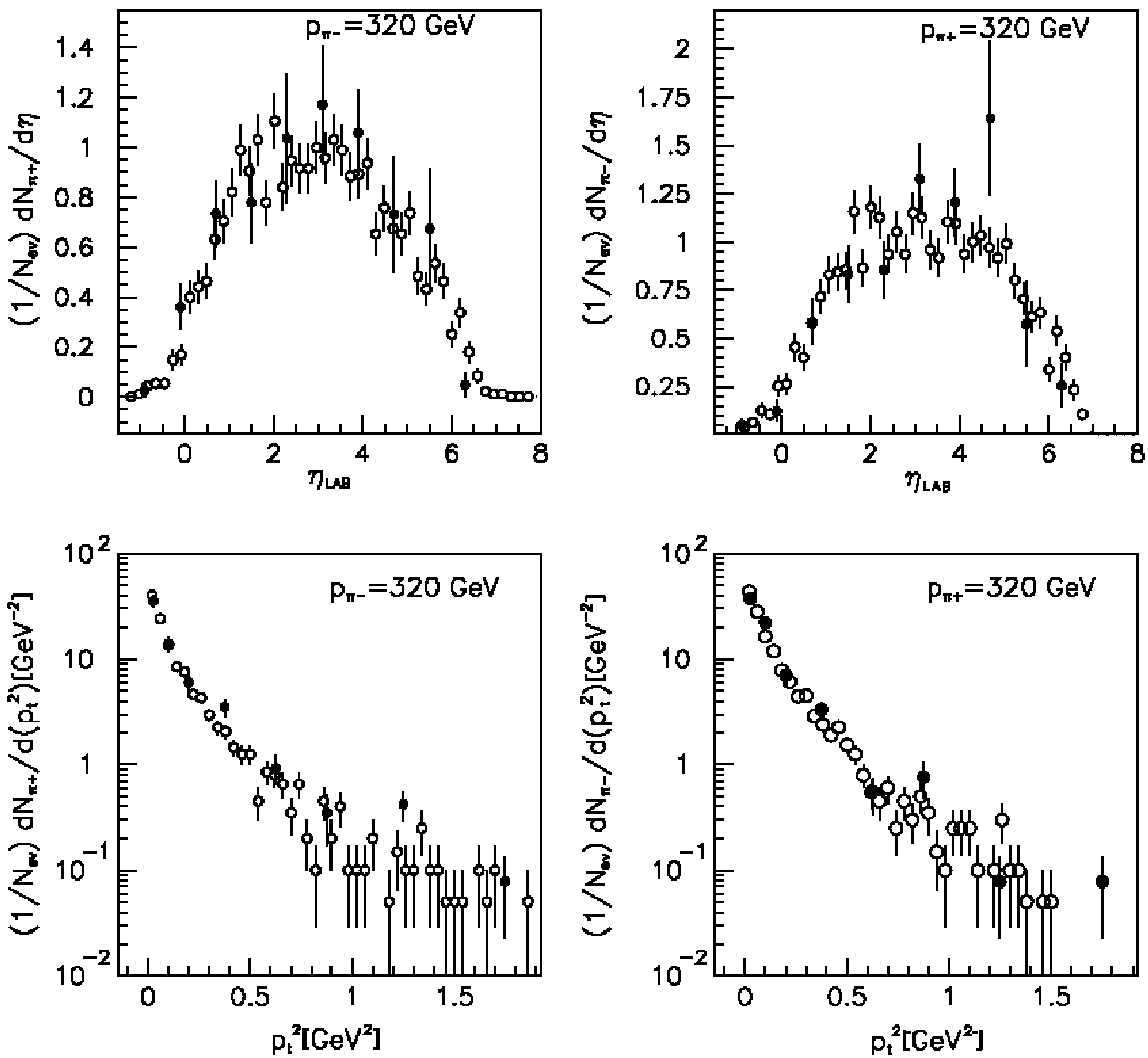



Validation? “Tuning”?

# Experimental comparisons: **QGS**

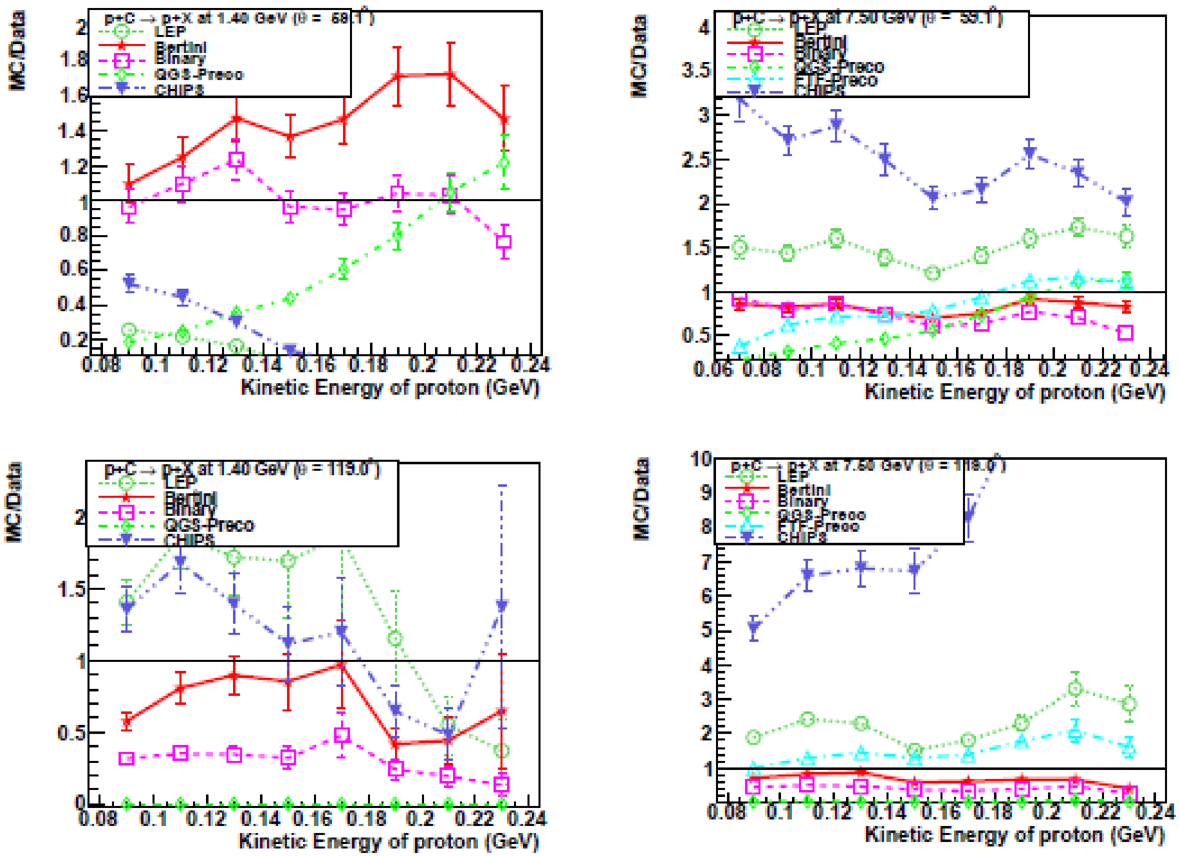
Scattering off Mg (Whitmore et al, Z.P. C62, p.199ff, 1994)




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




Lorentz invariant cross section for **inclusive proton production** at 59° (top row) and 119° (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

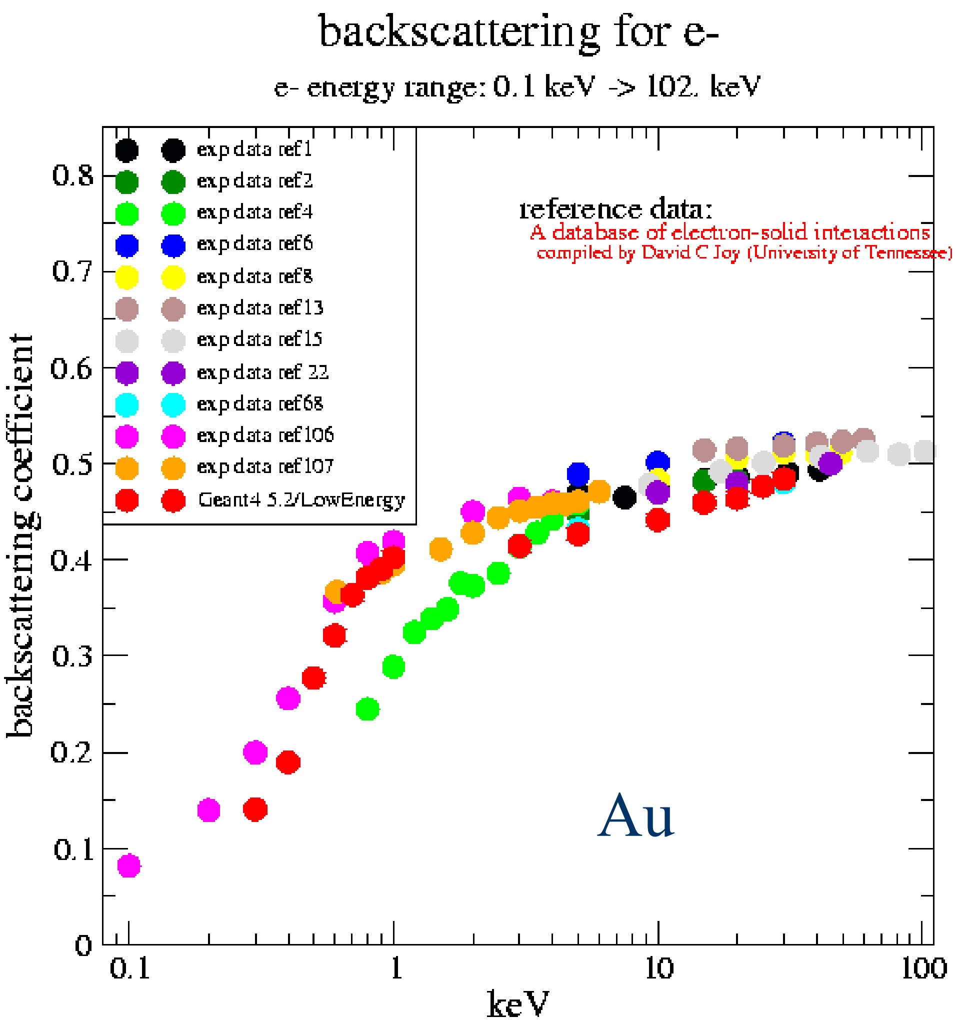
**Bertini cascade**
**Binary cascade**
**LEP**
**QGS+Precompound**
**CHIPS**

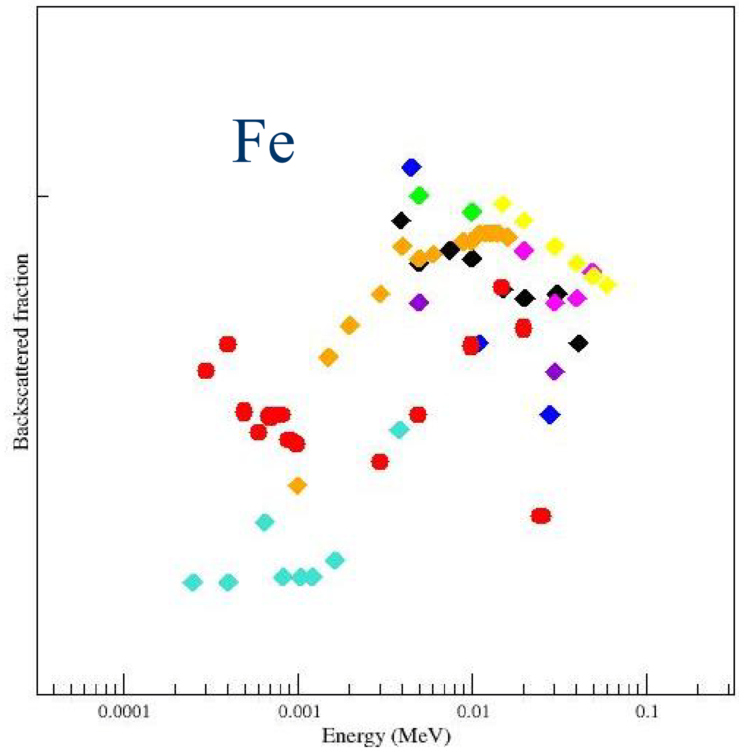
*Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2010 (SNA + MC2010)*
Hitotsubashi Memorial Hall, Tokyo, Japan, October 17-21, 2010

**Validation of GEANT4 Hadronic Generators versus Thin Target Data**

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

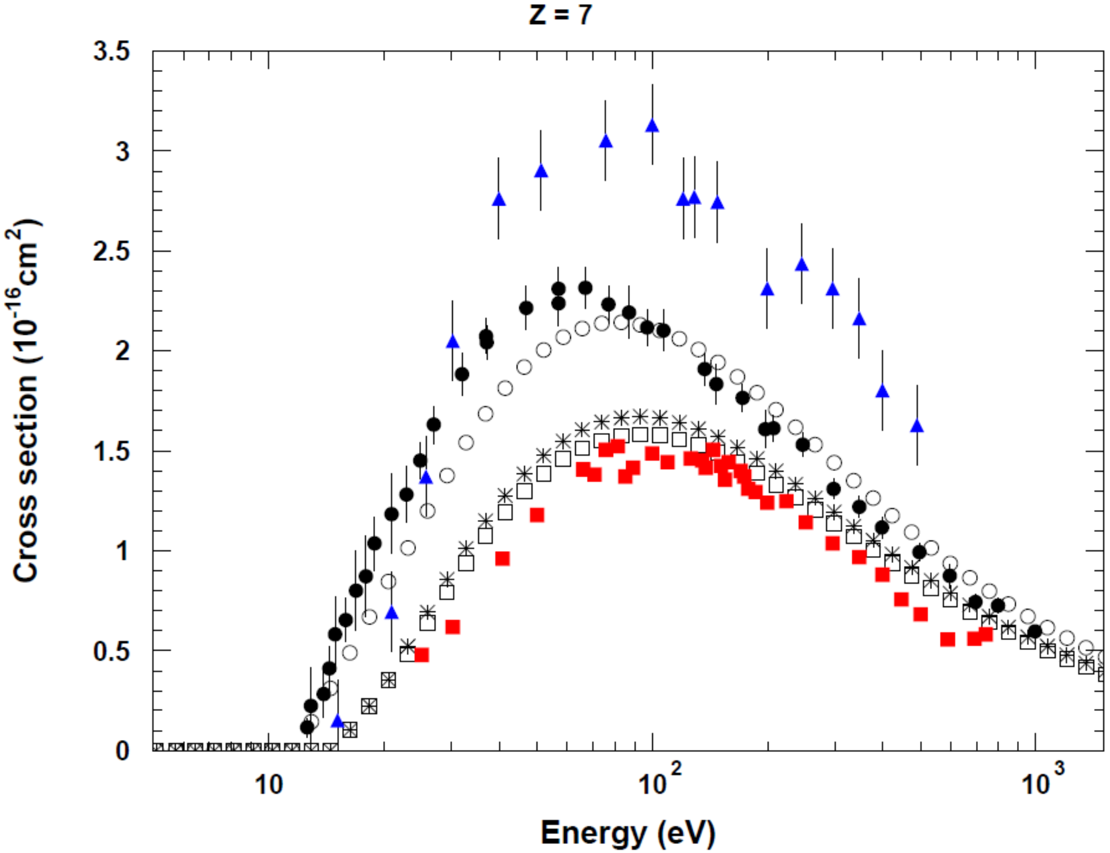
# The main problem of validation: experimental data!




Experimental data often exhibit large differences!

# Which one is right?




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

Paper with full results in progress

Often and 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)*

# 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**


*The launch of STS-107 on January 16,2003*

Columbia Space Shuttle accident, 2003

# R&D

*Novel ideas*
*Experimental motivations*

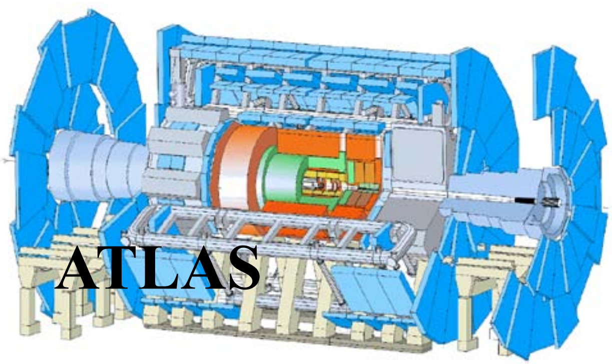
**Physics:** new developments, rigorous validation
**Software technology** (in support to physics)
**Fundamental issues** in particle transport

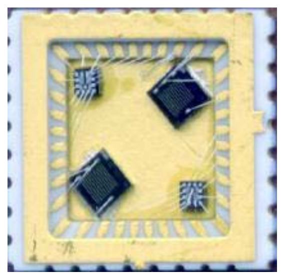
# Two worlds…

## Condensed-random-walk OR "discrete" régime

Characterizing choice in a Monte Carlo system

**What does it mean in practice?**



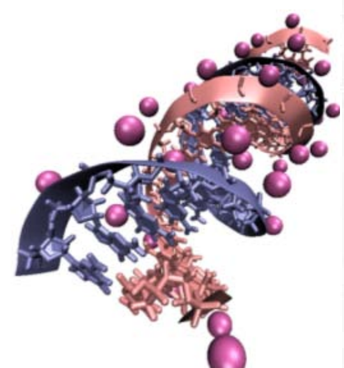



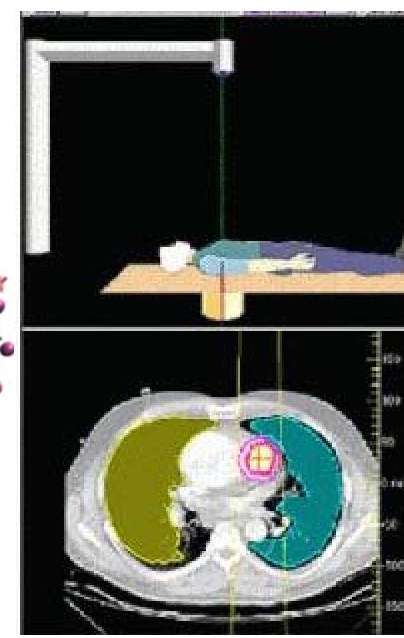
How does one estimate radiation effects on components exposed to LHC + detector environment?

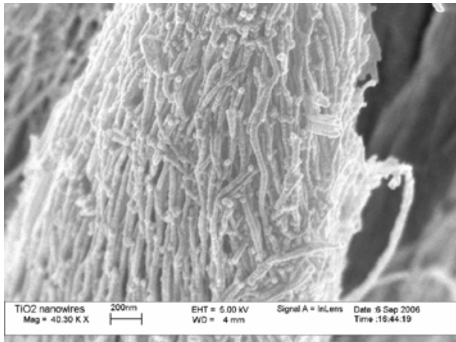
And what about **nanotechnology**-based detectors for HEP?
And tracking in a **gaseous detector**?

*And **plasma** facing material in a fusion reactor?*

How does one relate **dosimetry** to **radiation biology**?

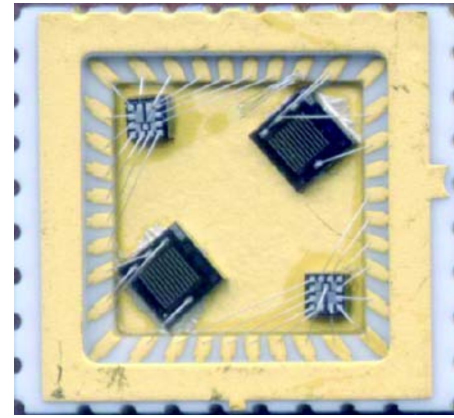


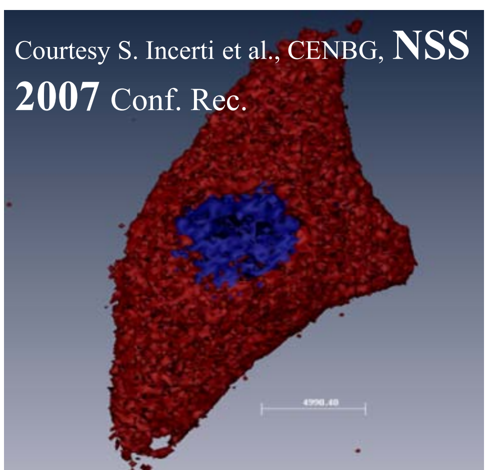




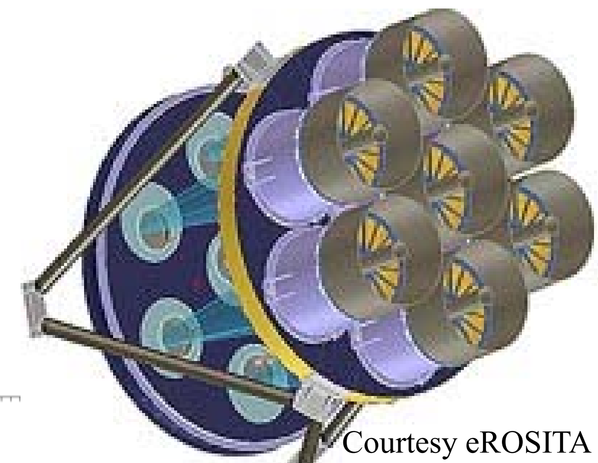

Courtesy A. Montanari et al., INFN Bologna **NSS 2006** Conf. Rec.

Courtesy RADMON (M. Moll et al.) Team, CERN, **NSS 2006** Conf. Rec.

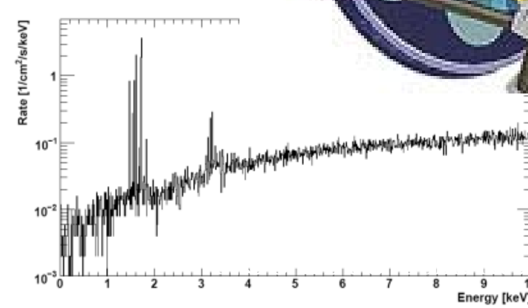




Courtesy S. Incerti et al., CENBG, **NSS 2007** Conf. Rec.

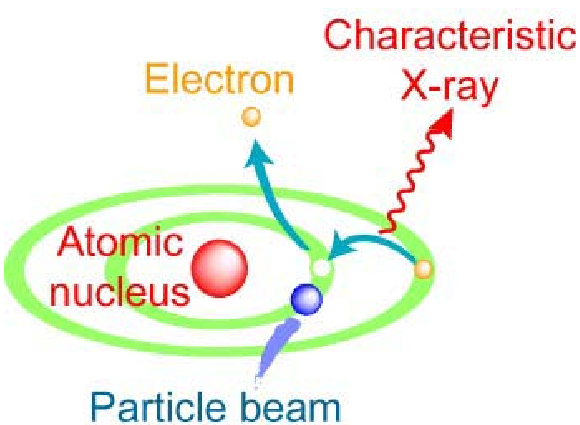


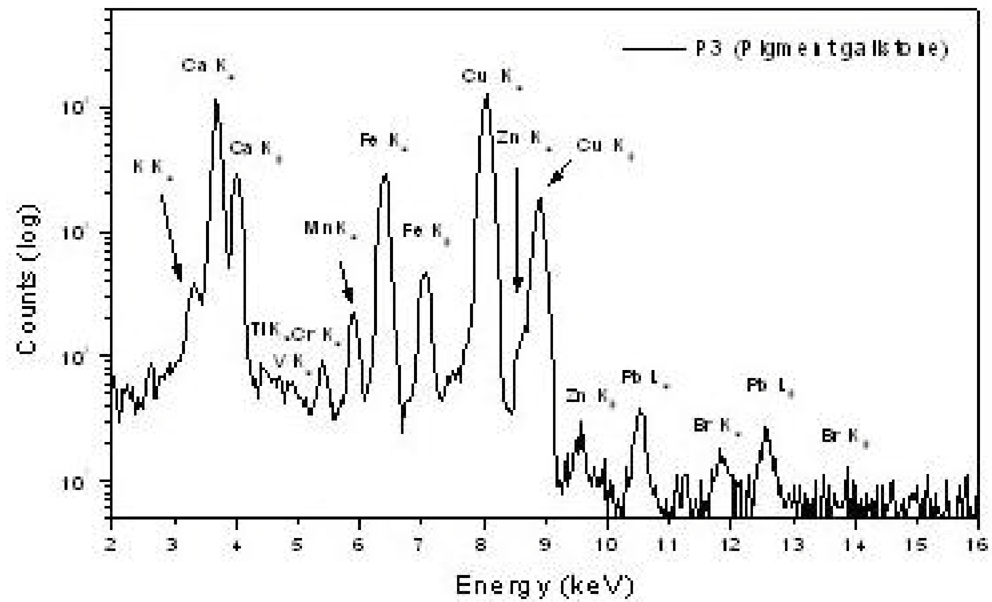
Courtesy eROSITA



# Clashing worlds…

## PIXE - Particle Induced X-ray Emission




**ionization**

*condensed*

**atomic relaxation**

*discrete*

Subtle consequences

- e.g. X-ray fluorescence emission (PIXE) by impact ionisation has a dependence on the **secondary production cut** introduced to handle **infrared divergence**!
- can affect macroscopic applications: material analysis, precise dosimetry etc.

# Condensed-random-walk simulation Discrete

- **Condensed-random-walk approximation**
  - all general-purpose Monte Carlo codes (EGS, FLUKA, GEANT 3, Geant4, MCNP)
  - charged particle tracks divided into many steps, several interactions occur in a step
  - one energy loss and one deflection are calculated for each step
    - further simplification of Continuous Slowing Down Approximation: energy loss rate determined by stopping power
  - collisions are treated as binary processes
    - target electrons free and at rest (or binding accounted only in an approximated way)
  - adequate as long as the discrete energy loss events are » electronic binding energies
- **Discrete simulation**
  - all collisions are explicitly simulated as single-scattering interactions
  - prohibitively time-consuming on large scale
  - many "track structure" codes documented in literature
    - single-purpose, not public, maintenance not ensured, lack general functionality

# NANO5

# R&D on transport schemes

- Project launched at INFN (2009)
  - International, multi-disciplinary team
  - **R&D** = research **study**, exploration of novel ideas
- Motivated by concrete **experimental requirements**
- Response to **current limitations** of Geant4
  - of all major Monte Carlo systems, not only Geant4
- Address **experimental use cases**
  - by going to the very **core of Monte Carlo methods**

R&D on
**complementary, co-working transport methods**

| | |
|---|---|
| **Condensed-random-walk** scheme<br>**Discrete** scheme | **Monte Carlo** method<br>**Deterministic** methods |

# 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[1], Maria Grazia PIA[2*], Paolo SARACCO[2], Chan-Hyeung KIM[1]

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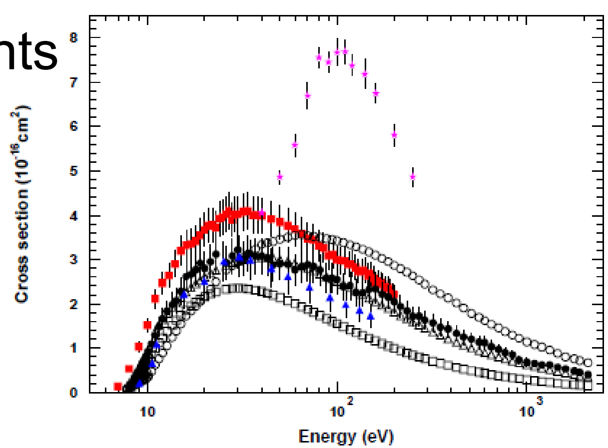
**Student Paper Award**
**Monte Carlo 2010**

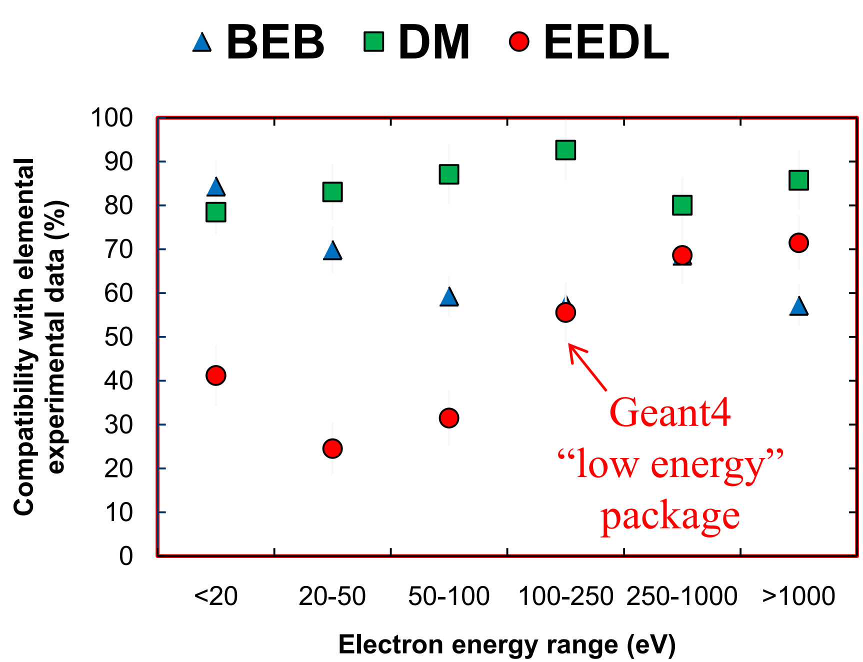
**Cross section models:**

- 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**

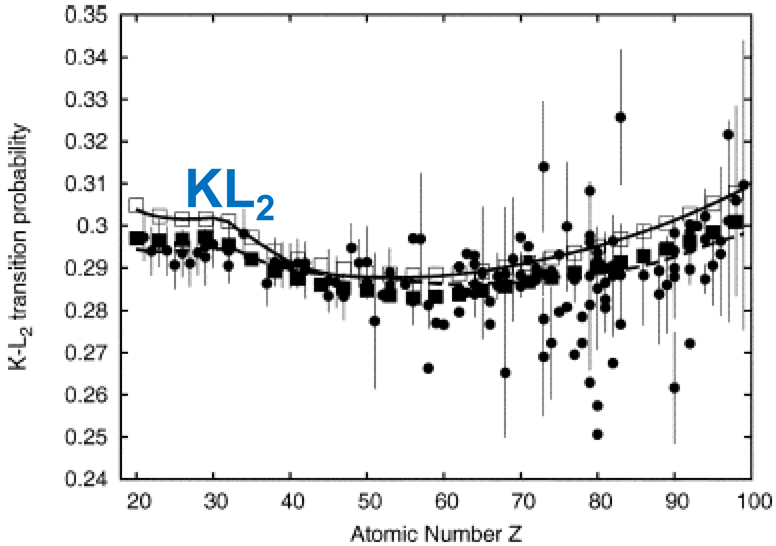
# Progress with XRF and PIXE

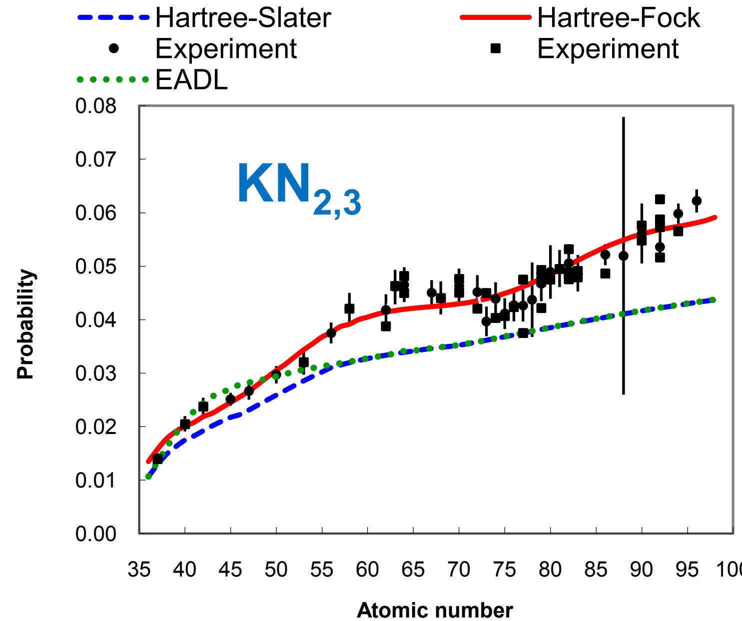
- **PIXE data library** in progress
  - To be publicly released by RSICC, ORNL

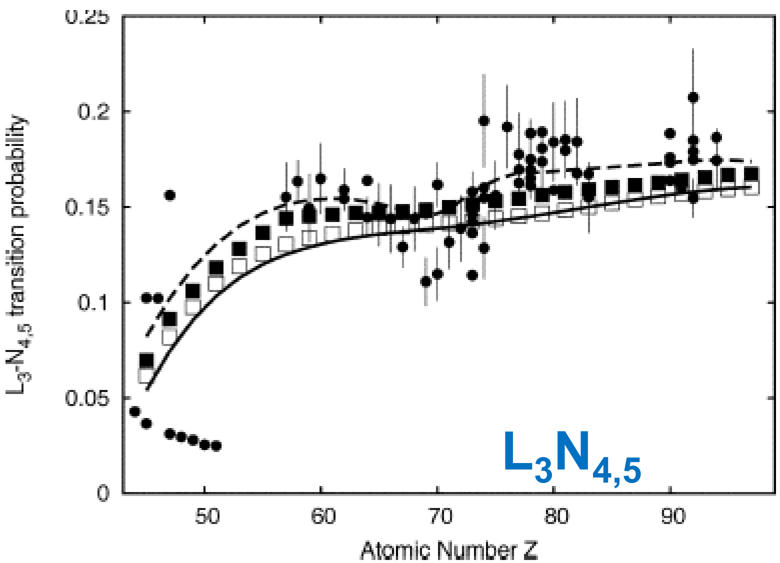
# Simulation reliability and accuracy

- **Radiative transition probabilities**
  - Extensive comparison with experimental data
- **Atomic binding energies**
  - Extensive validation of binding energies used by Geant4, GEANT 3, EGS (5/NRC), MCNP and Penelope
  - Effects on X-ray energy accuracy
  - Effects on ionisation cross sections

# Radiative transition probabilities




Radiative transition probabilities in Geant4 are based on EADL, i.e. **Hartree-Slater** calculations

Extensive comparison with experimental data shows that **Hartree-Fock** calculations are more accurate than Hartree-Slater ones

**EADL is NOT the state-of-the-art!**

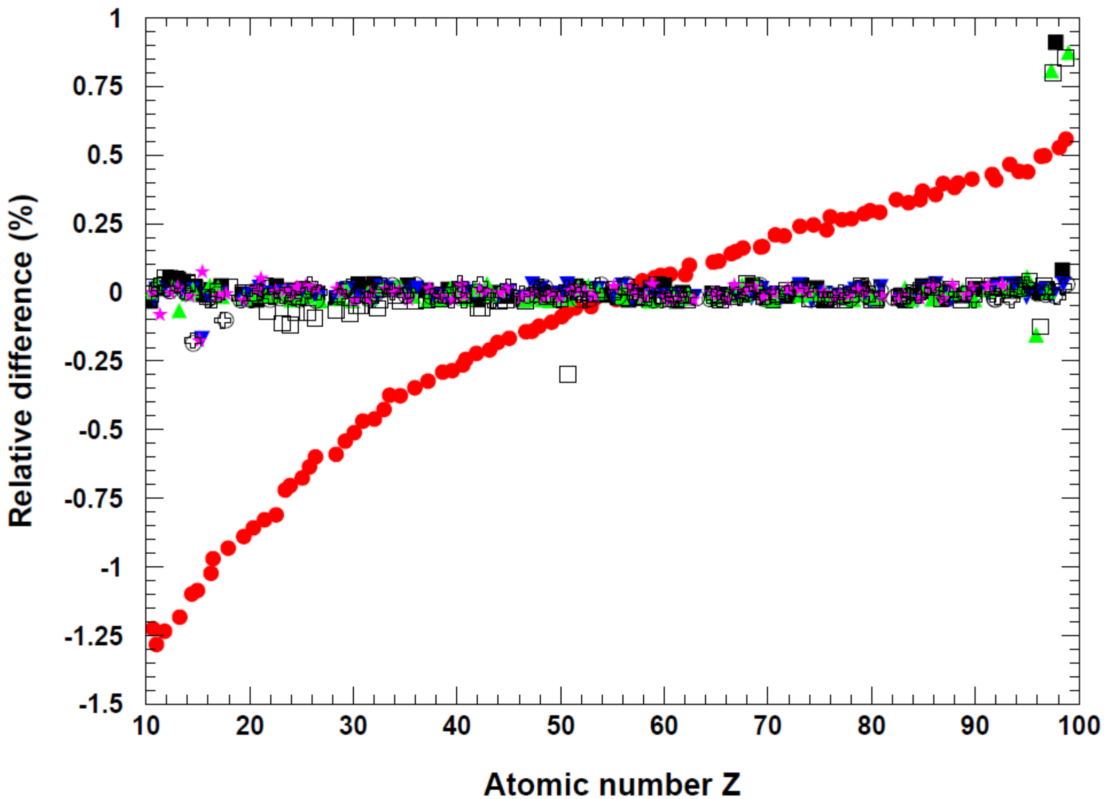
# X-ray energies

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

*well, it can be worse…*

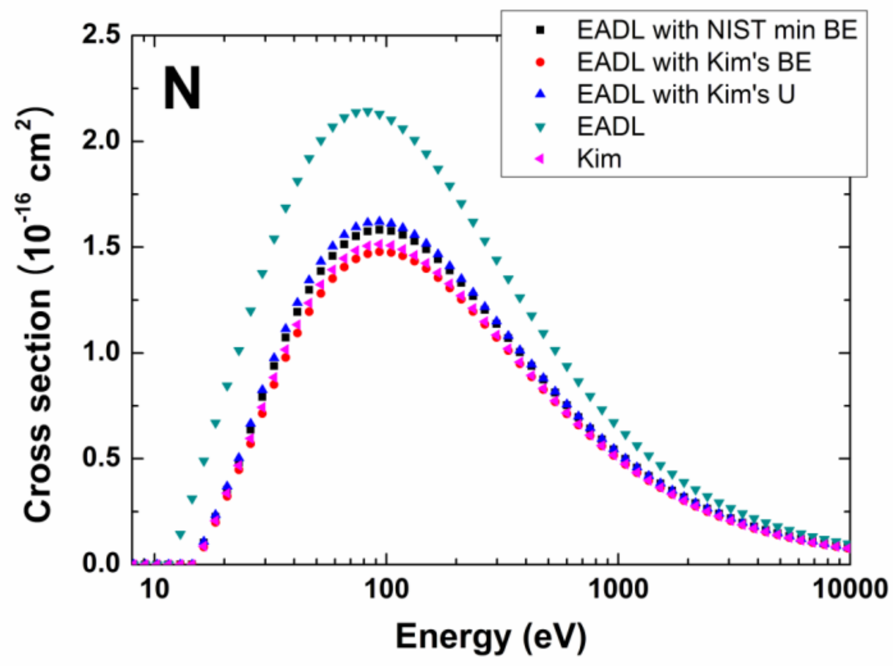



Extensive set of tests
Comparisons with experimental data

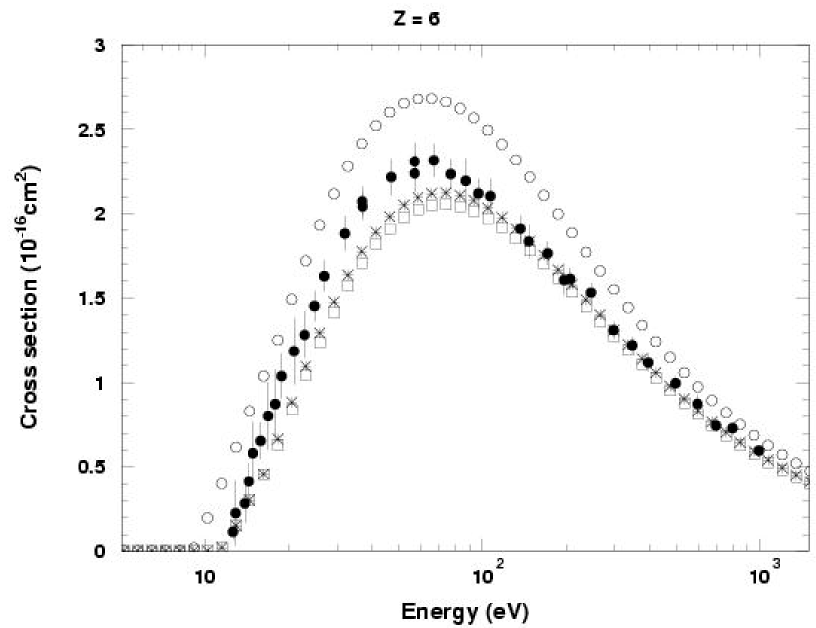
Rigorous statistical methods for quantitative evaluations

*Paper in preparation*

# Effect of atomic parameters on ionisation cross sections




**Comparison with experimental data**



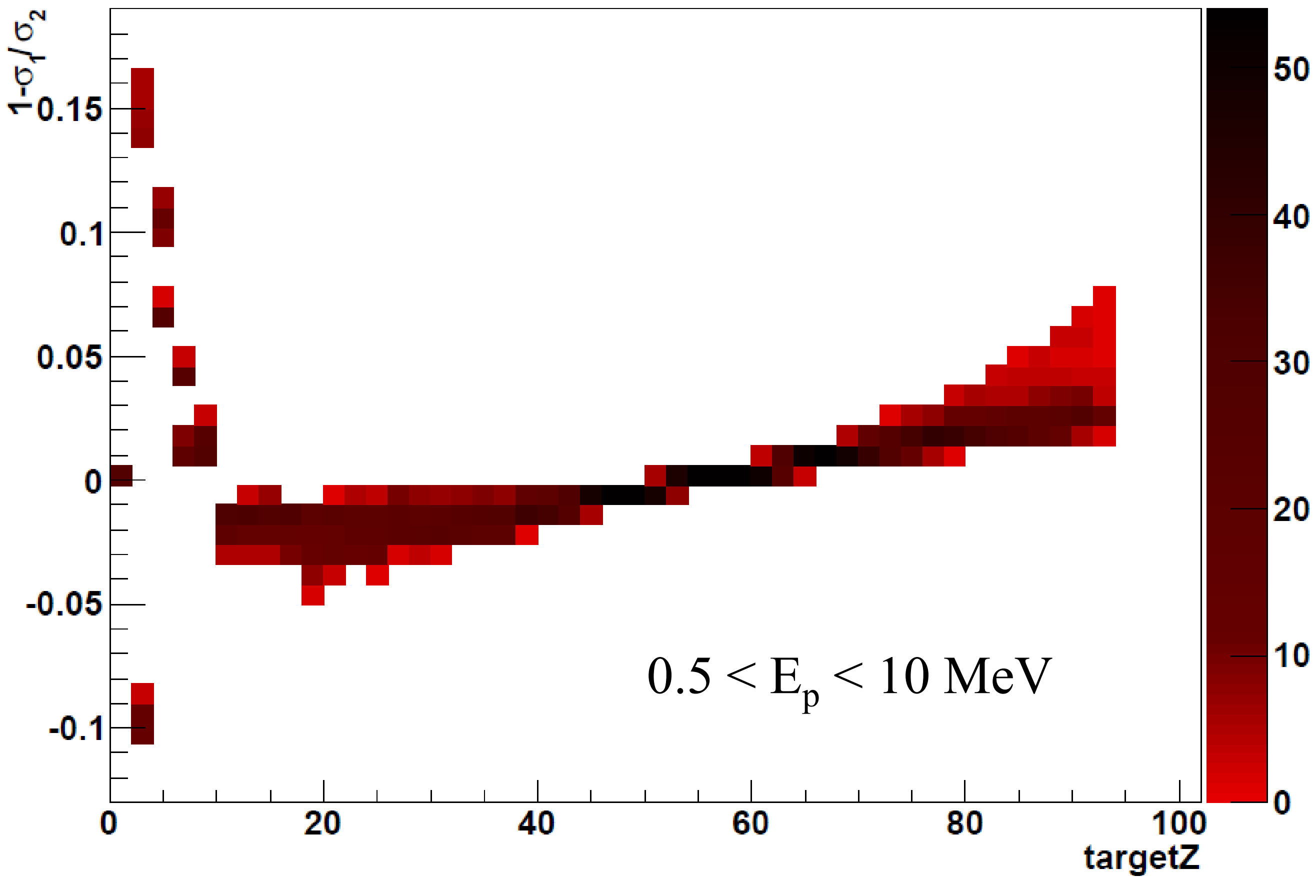

Significant effect of outer shell binding energies on electron ionisation cross sections

**BEB cross section**
○ with EADL binding energies
⁎ with Lotz binding energies
□ with EADL (inner shells) b.e. and NIST ionisation energy

*Full set of results and references to experimental data in a forthcoming publication*

# 2nd round of the "beast"?

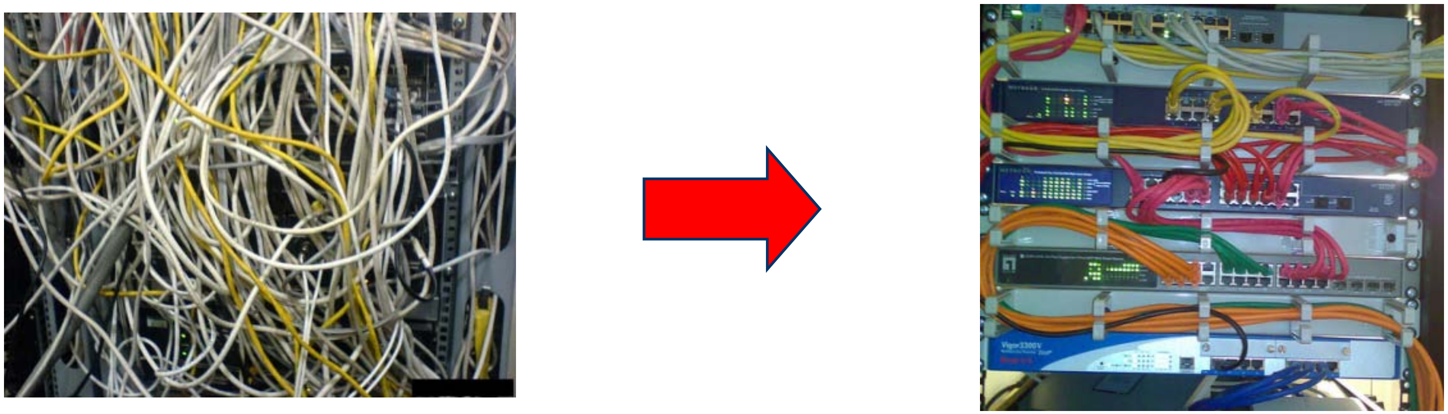
Analysis in progress




Relative difference between K-shell cross-sections versus $Z_{target}$

# R&D in physics design

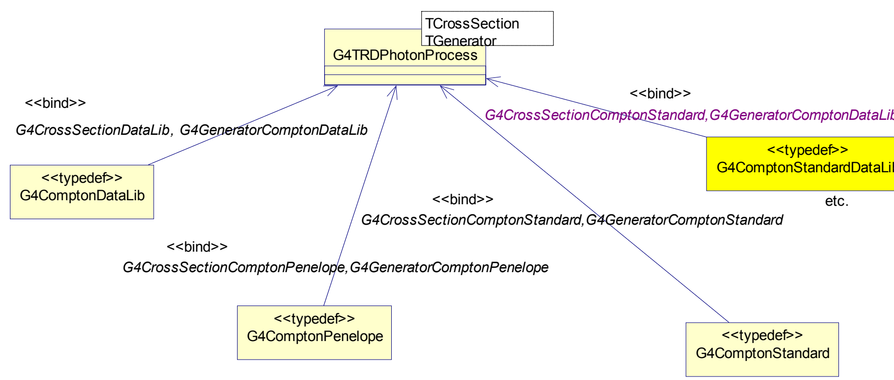
Evolutions since RD44 have fogged some of the pristine Geant4 transparency



New technology is available, that was not yet established at the time of RD44, or not supported by compilers

## Prototype:
## R&D in photon physics design

Preliminary indications: gain **performance** and **agility of testing**

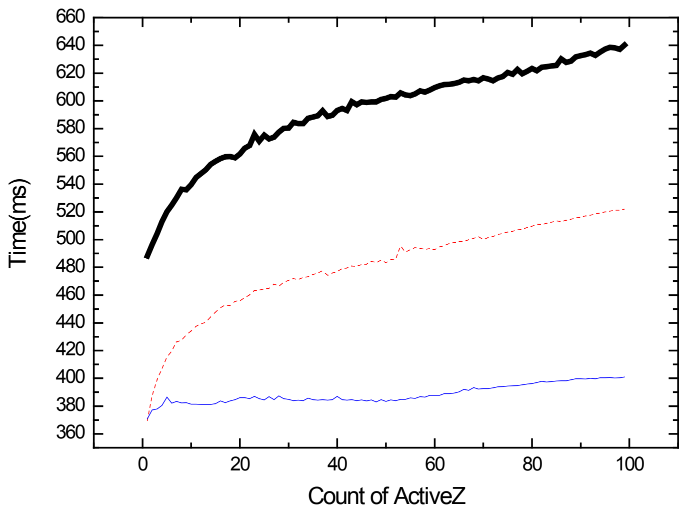


# Physics data management

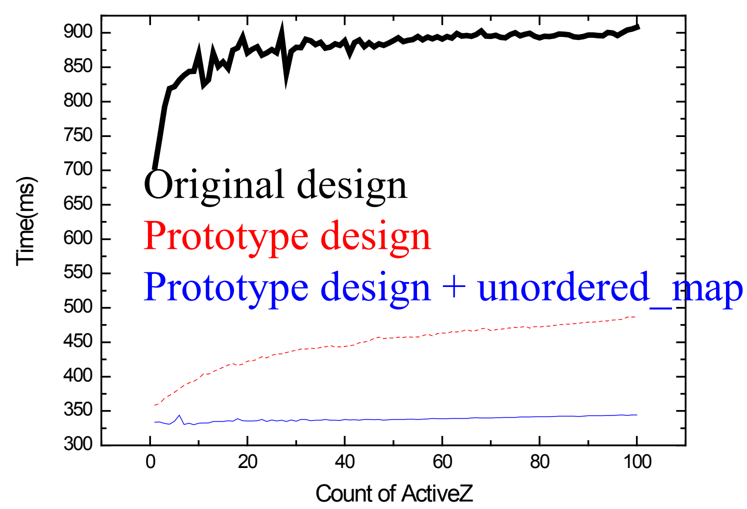
## Performance improvement

*Mincheol Han, Hanyang Univ., Seoul*

**Pair production cross sections**




**Bremsstrahlung spectrum data**




**time** (ms) to **retrieve** data

vs. number of elements present in the experimental set-up

# 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 estimate them?

No generally accepted method of measuring epistemic uncertainties

**Interval analysis**

**Dempster-Shafer theory of evidence**

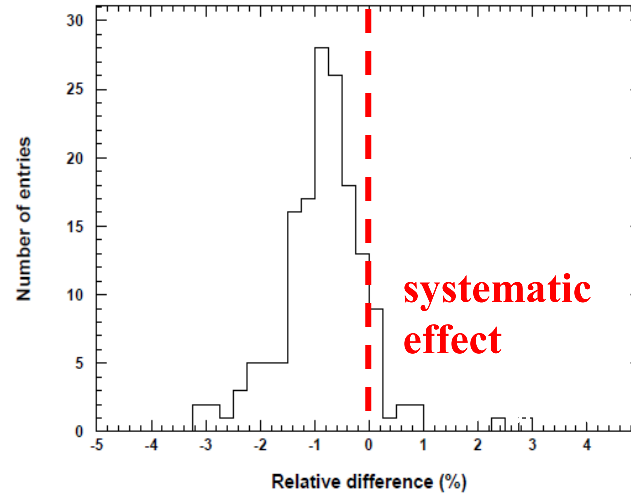
IEEE Trans. Nucl. Sci., vol. 57, no. 5, pp. 2805-2830, October 2010

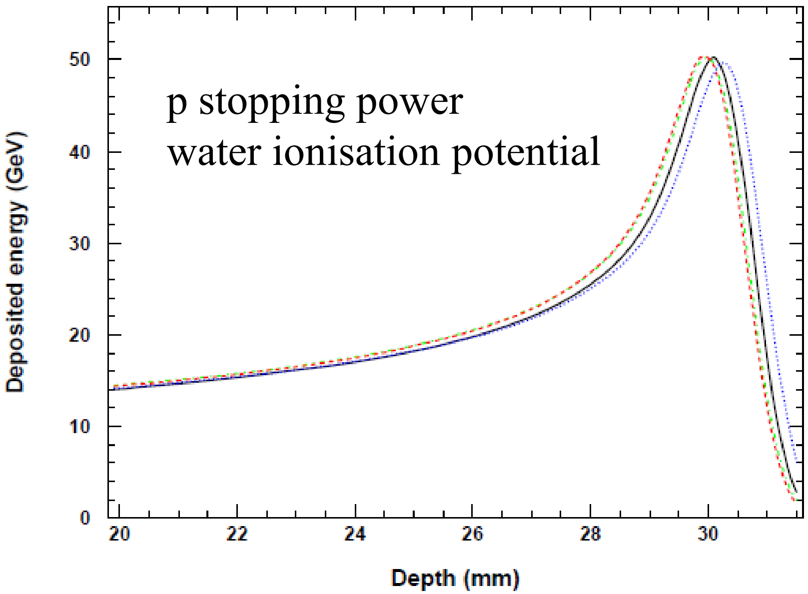
IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 57, NO. 5, OCTOBER 2010 2805

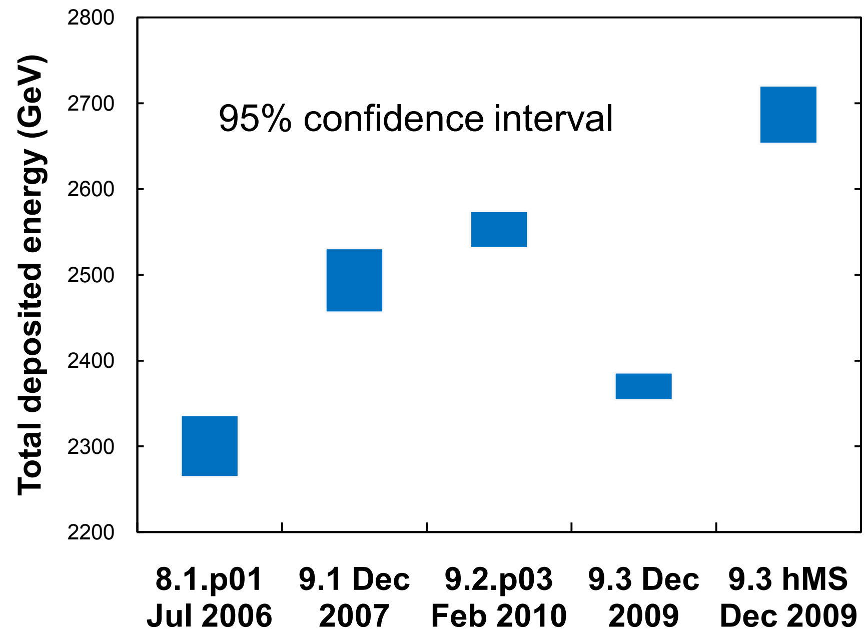
# Physics-Related Epistemic Uncertainties in Proton Depth Dose Simulation

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

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




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

# Geant4 Collaboration

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103. Douglas Wright (Lawrence Livermore National Laboratory )
104. Julia Yarba (Fermilab)
105. Hajime Yoshida (Naruto University of Education)
106. Christina Zacharatou (Niels Bohr Institute, Copenhagen)

Der gerade ist der Mächtigste, der möglichst wenig selber tun, möglichst viel von dem, wofür er den Namen hergibt und den Vorteil einstreicht, anderen aufbürden kann.

*T.W. Adorno, Minima Moralia*

# Conclusion

- Geant4 is a rich and powerful tool for experimental research
- Widely used in multi-disciplinary applications

- **Validation** is ongoing
- **R&D** for challenging experimental domains
- Large investment still needed in both areas
- Thinning resources

- **Collaboration** between Geant4 developers and the experimental community is fundamental

# Further info

Slides available at
http://www.ge.infn.it/geant4/seminar/geant4_xfel2011.pdf

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

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

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

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