Geant 4

L’esperienza di 20 anni e l’orizzonte del 2020

Maria Grazia Pia
INFN Sezione di Genova

INFN CNAF

Bologna, 4-5 febbraio 2014

This presentation includes material from several sources: thanks to all the authors!

1974-1994

R. Brun
R. Hagelberg
M. Hansroul
J.C. Lassalle

CERN - DATA HANDLING DIVISION
DD/78/2
January 1978

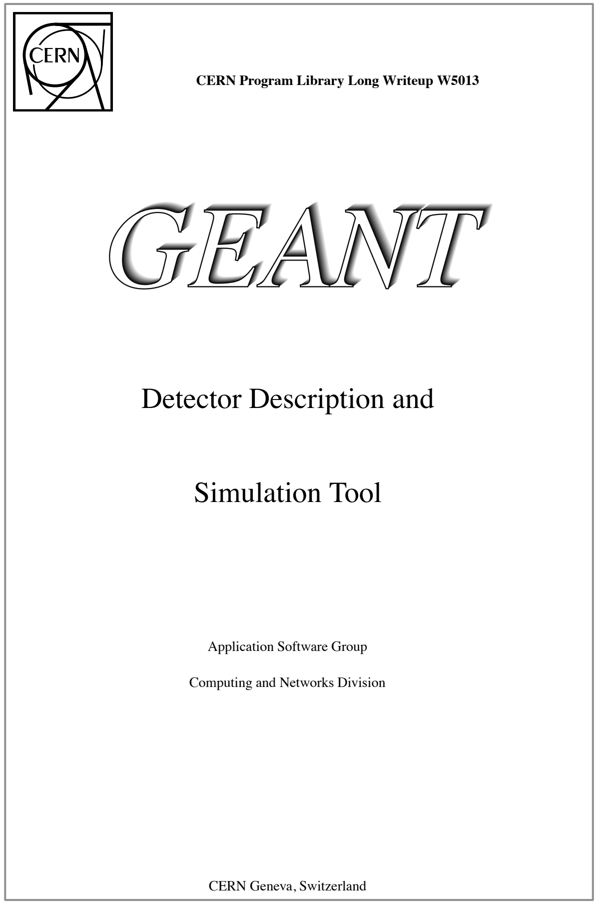
[redacted]

CM-P00059731

SIMULATION PROGRAM
FOR
PARTICLE PHYSICS EXPERIMENTS

GEANT

USER GUIDE
AND
REFERENCE MANUAL



CERN Program Library Long Writeup W5013

GEANT

Detector Description and

Simulation Tool

Application Software Group

Computing and Networks Division

CERN Geneva, Switzerland

- GEANT, GEANT2: bare framework
- GEANT 3: 1982

EGS physics…

GEANT 3.21, March 1994

+ *GHEISHA, FLUKA, GCALOR*

1993

“The main problem with GEANT 3 was that no documentation on its program design was available. Only, say, ten people in the world knew how it worked.”

Additionally, GEANT 3 was written in FORTRAN, which is a procedural programming language.

The extremely complicated nature of the simulation code, and the relative lack of structure inherent in most procedural languages, made it impossible for general users to add new components to the program.

Takashi Sasaki, KEK

http://legacy.kek.jp/intra-e/feature/2010/Geant4.html

e.g.~60 routines need to be modified in GEANT 3 to add a new geometrical shape

GEANT 3.20

CN Division Report, 1992

Together with this geometry, a new version of the graphics package has been developed which allows shadows, light processing and multiple light sources. All these developments will be introduced in GEANT version 3.20, which should be released at the end of 1993.

DRAFT DRAFT DRAFT DRAFT DRAFT

THE NEW GEOMETRICAL MODELLER OF GEANT 3.20

Jouko Vuoskoski

CERN, Geneva

June 29, 1993

ABSTRACT

The new geometrical modeller in GEANT 3.20 is entirely new with respect to the previous versions of GEANT. The internal representation is constructed solid geometry (CSG) following the half-space approach. The half-spaces are bounded by polynomial surfaces limited to 2^{nd} order. The user interface will also be extended. The new modeller allows users to construct more complicated and more accurate detector models. It offers also better possibilities to exchange geometrical information with CAD-systems.

Applying STEP Principles to Product Models in High Energy Physics Research

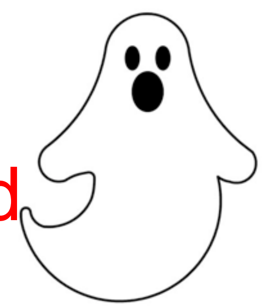
M. Dach et al., Report TKK-F-A724

1.2 GEANT

GEANT is a detector simulation program used in the design of detectors used in High Energy Physics (HEP) experiments. The simulation program has been developed at CERN by the HEP community and it is now in use in more than 600 research institutions in over 50 countries. Its applications are not limited to physics, but range from space science to medical research.

The GEANT version 3.20 to be released sometime in the future will have a new geometric modeler [9] which uses a constructive solid geometry (CSG) [10] approach. The internal geometric representation consists of half spaces. In GEANT a *solid object* composing a part of a detector is called a *volume*. Internally a volume is represented by a union of *caves* and a cave is represented by an intersection of half-spaces.

GEANT 3.20
was never released



MC93 Conference

STATUS AND FUTURE TRENDS OF THE GEANT SYSTEM

FEDERICO CARMINATI
CERN
1211 Geneva 23
Switzerland

p. 45

ABSTRACT

The GEANT simulation system is undergoing a constant development thanks to the feed-back and collaboration of its very large community of users. Version 3.15 has been released almost an year ago and it can be considered quite stable. Version 3.16 will be released soon and it will contain several improvements, both in the physics and in graphics and user interface. Little has been done in this version on the geometry and on the program structure, in order to preserve as much as possible backward compatibility.

In parallel with these developments, a completely new GEANT geometrical modeller has been developed and is now in an advanced testing phase. This will be released at the end of this year with GEANT Version 3.20. Following a series of discussions held at CERN on the evolution of the CERN Program Library in the LHC era, an experiment has been launched to evaluate C++ and Object Oriented languages for detector simulation.

TOWARDS OBJECT-ORIENTED GEANT
— ProdiG PROJECT —

pp. 329-338

YOSHINOBU TAKAIWA,
KATSUYA AMAKO, JUN-ICHI KANZAKI, and TAKASHI SASAKI
KEK (National Laboratory for High Energy Physics)
1-1 Oho, Tsukuba, Ibaraki 305, Japan

ABSTRACT

A project towards object-oriented design and implementation of GEANT (*ProdiG* project) is now under consideration and this is a brief report of current status. Viewing GEANT as a general purpose detector simulation package, motivations for making it object-oriented and possible issues for this end are discussed. Then, a preliminary attempt of analyzing and designing a detector simulation program is given. Also is discussed the possibility and necessity of the worldwide collaboration for it.

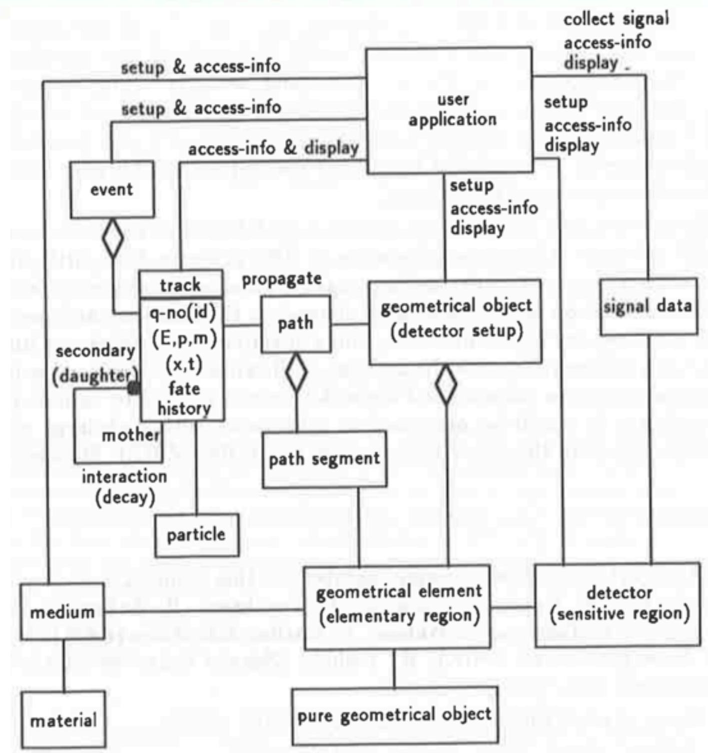


Figure 1: Class Diagram of Detector Simulation.

Steps into the future

Jouko Vuoskoski
27.08.1993

MINI-WORKSHOP ON OBJECT ORIENTED GEANT

Held 24-27 August 1993 at CERN/CN/AS

SLIDES

SPEAKERS:

Tuesday 24.08.1993

Katsuya Amako : The ProdiG project

Yoshi Takaiwa : Introduction of KEK activities on OO-GEANT

Rene Brun : The evolution of CERNLIB environment

Federico Carminati : GEANT status and plans for the geometry

Wednesday 25.08.1993

Simone Giani : Investigation of class hierarchy for GEANT

Alfred Nathaniel : General views on OOP. Ideas for I/O

Fons Rademakers : C++ evolution

Jouko Vuoskoski/
Janne Saarela : An OO method for manipulating geometries

Thursday 26.08.1993

Demonstrations

Friday 27.08.1993

Wrap-up

ProdiG and investigation of class hierarchy for GEANT at CERN merged

DRDC/94-28

Letter of intent to the DRDC

May 26, 1994

Proposal

to CERN Detector R&D Committee

EUROPEAN ORGANIZATION FOR NUCLEAR RESEARCH

CERN/DRDC/94-29
DRDC / P58
11 August 1994

GEANT 4 : an Object-Oriented toolkit for simulation in HEP

29 people, 19 institutes, 9 countries

Geant 4

R&D Project

RD44 (GEANT4)

GEANT 4: an Object-Oriented toolkit for simulation in HEP

ABSTRACT & FIGURES | HOME PAGE | NOTES & PUBLICATIONS

SPOKESPERSON: Simone GIANI

Experiment secretariat e-mail: Grey.Book@cern.ch

Beam:	
Approved:	24-11-1994
	07-12-1995
	01-07-1997
	21-10-1997
Completed	14-12-1998
Finished	14-12-2008
Status:	Finished

Geant4 today

S. Agostinelli et al.

Geant4: a simulation toolkit

NIM A, vol. 506, no. 3, pp. 250-303, 2003

4597 citations

Most cited publication in:	Total
Nuclear Science and Technology Instruments and Instrumentation	626356
Particle and Fields Physics	267891

Most cited **CERN** publication	26077
Most cited **INFN** publication	48779

Many papers that use Geant4 do not cite it

ISI WoS
Nuclear Science & Technology
Instruments & Instrumentation

1. **GEANT4-a simulation toolkit**
   By: Agostinelli, S; Allison, J; Amako, K; et al.
   NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT Volume: 506 Issue: 3 Pages: 250-303 Published: JUL 1 2003
   Full Text | View Abstract
   Times Cited: 4,597 *(from Web of Science Core Collection)*

2. **A MONTE-CARLO COMPUTER-PROGRAM FOR THE TRANSPORT OF ENERGETIC IONS IN AMORPHOUS TARGETS**
   By: BIERSACK, JP; HAGGMARK, LG
   NUCLEAR INSTRUMENTS & METHODS Volume: 174 Issue: 1-2 Pages: 257-269 Published: 1980
   Full Text
   Times Cited: 3,709 *(from Web of Science Core Collection)*

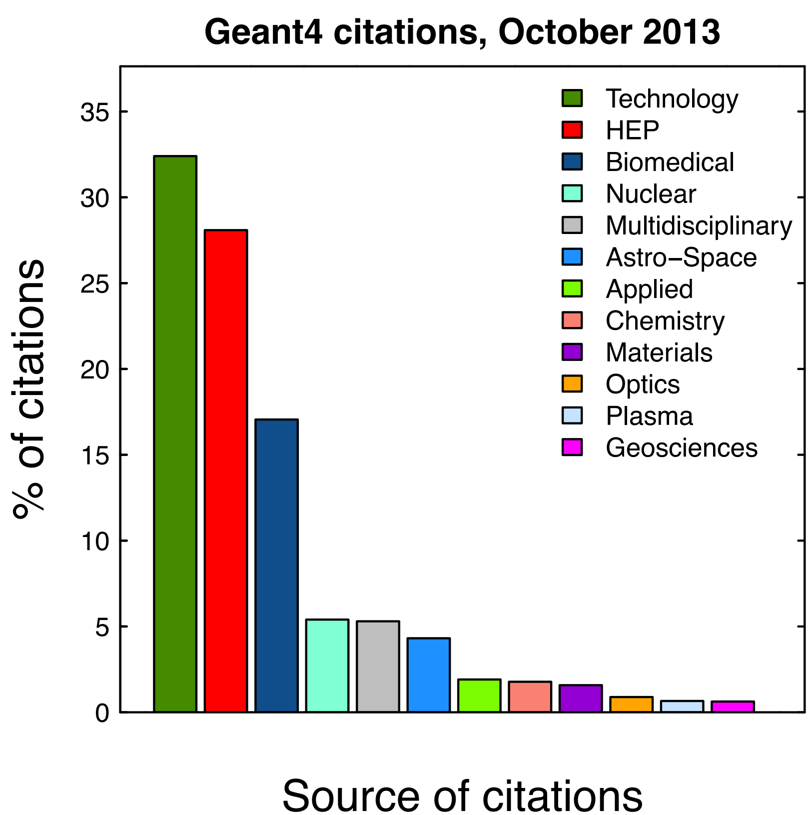
Software!

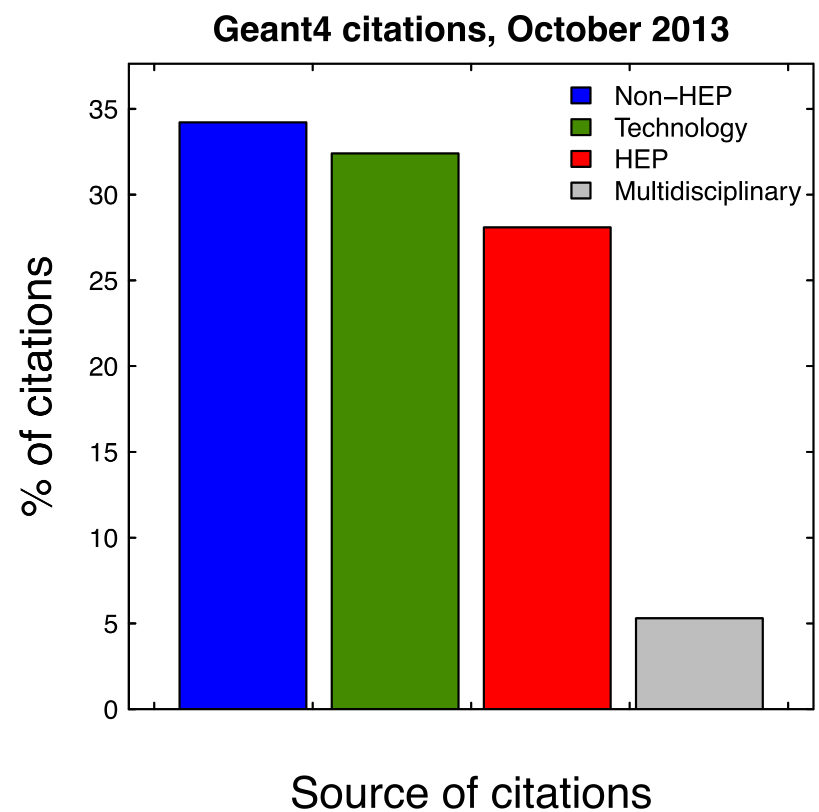
3. **ATHENA, ARTEMIS, HEPHAESTUS: data analysis for X-ray absorption spectroscopy using IFEFFIT**
   By: Ravel, B; Newville, M
   JOURNAL OF SYNCHROTRON RADIATION Volume: 12 Pages: 537-541 Part: 4 Published: JUL 2005
   Full Text | View Abstract
   Times Cited: 2,177 *(from Web of Science Core Collection)*

4. **ALGORITHMS FOR THE RAPID SIMULATION OF RUTHERFORD BACKSCATTERING SPECTRA**
   By: DOOLITTLE, LR
   NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION B-BEAM INTERACTIONS WITH MATERIALS AND ATOMS Volume: 9 Issue: 3 Pages: 344-351 Published: 1985
   Full Text
   Times Cited: 2,153 *(from Web of Science Core Collection)*

5. **WSXM: A software for scanning probe microscopy and a tool for nanotechnology**
   By: Horcas, I.; Fernandez, R.; Gomez-Rodriguez, J. M.; et al.
   REVIEW OF SCIENTIFIC INSTRUMENTS Volume: 78 Issue: 1 Article Number: 013705 Published: JAN 2007
   Times Cited: 2,146 *(from Web of Science Core Collection)*

Who uses Geant4?





Based on Thomson-Reuters' Web of Science data

Geant4-related publications by Geant4 developers

Geant4 core,
excluding applications
(early 2013 statistics)

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

Geant4 low energy electromagnetic physics
Geant4 advanced examples
Geant4 distributed simulation
Geant4 scientometrics
Uncertainty Quantification
Statistical Toolkit

Overview of Geant4 functionality

What is Geant 4 ?

OO Toolkit

for the simulation of next generation HEP detectors

...of the current generation

...not only of HEP detectors

Born from **RD44**, 1994 – 1998 (R&D phase)

1st release: 15 December 1998

1-2 new releases/year since then

RD44 was also an experiment of

- **distributed software production** and management
- application of rigorous **software engineering** methodologies
- introduction of the **object oriented technology** in the HEP environment

RD44 strategic vision

OO technology

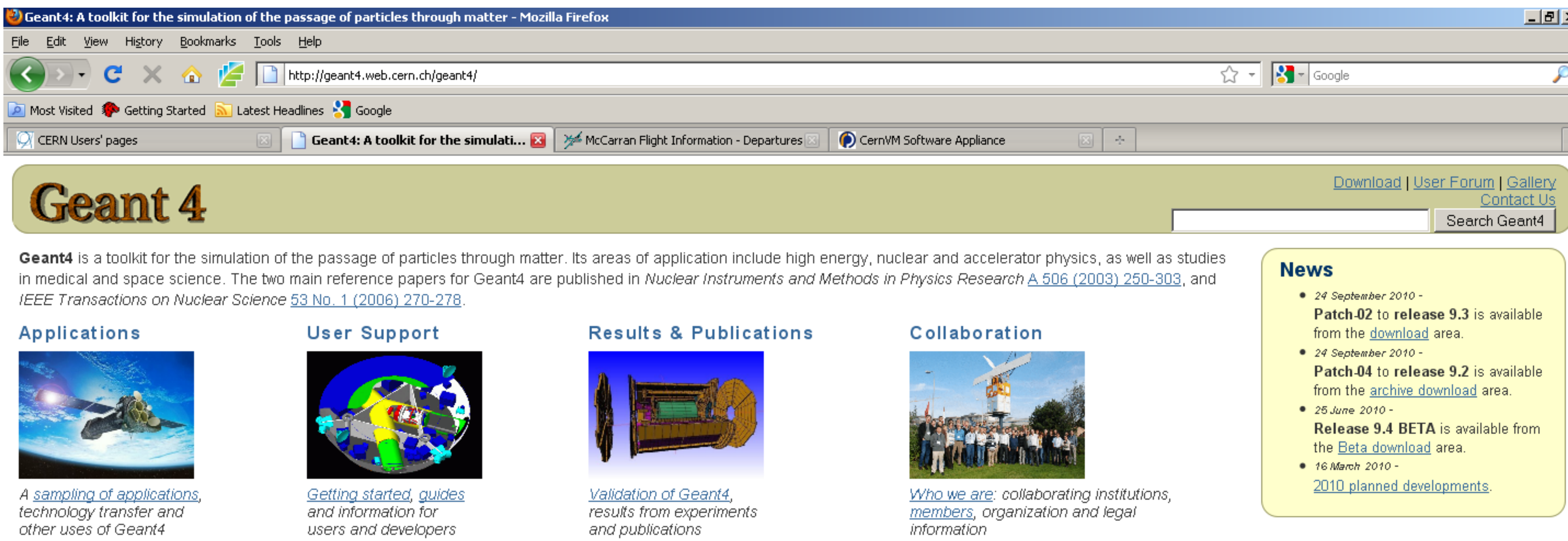
- Open to extension and evolution
  - new implementations can be added without changing existing code
- Robustness and ease of maintenance
  - protocols and well defined dependencies minimize coupling

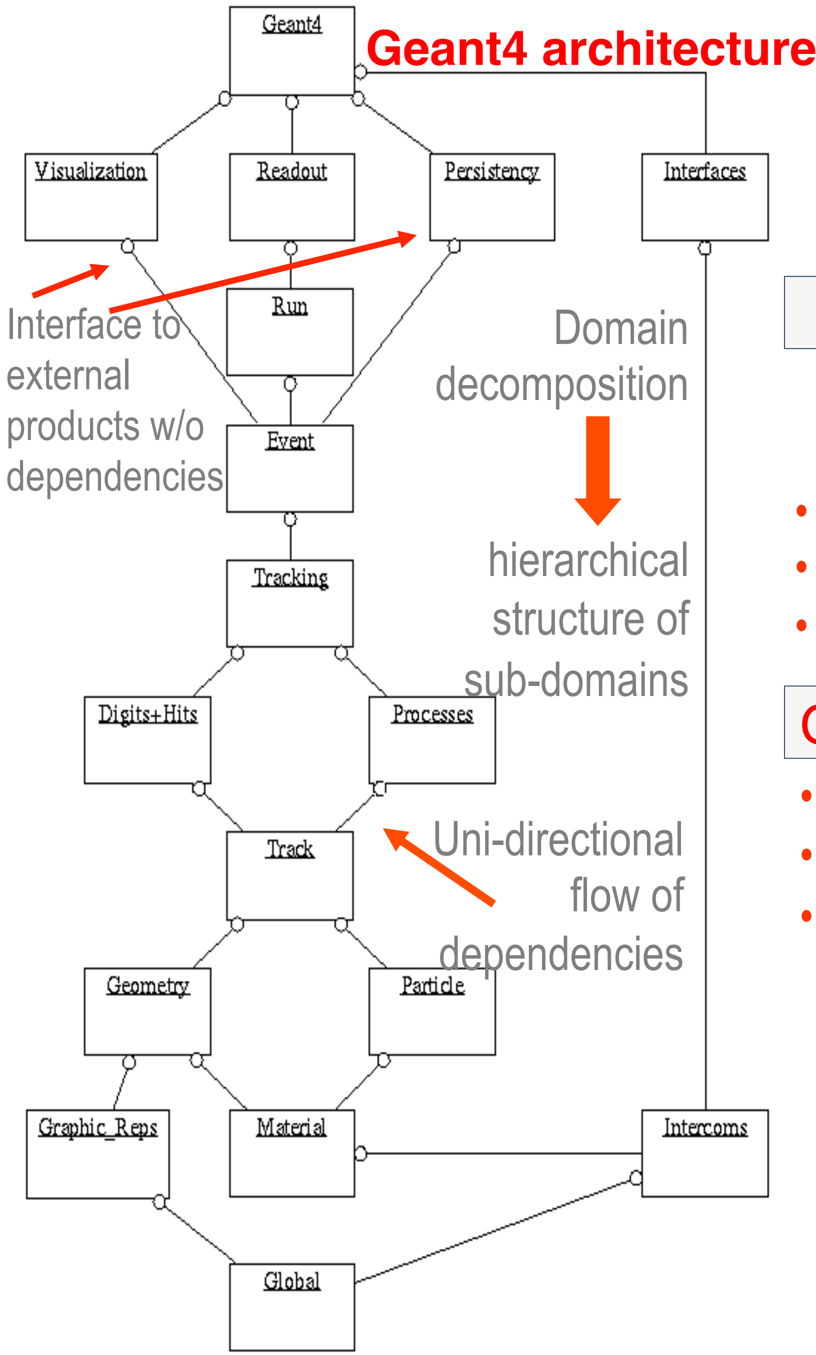
Toolkit

- A set of compatible components
  - each component is specialised for specific functionality
  - each component can be refined independently
- Components can cooperate at any degree of complexity
- Providing (and using) alternative components is easy
- User applications can be customised as needed

Distribution

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





Software Engineering

played a fundamental role in RD44

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

Geant4 functionality

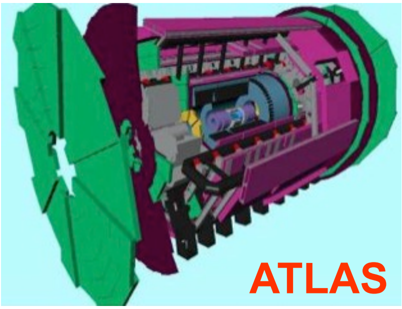
Geant4 provides tools for particle transport in matter:

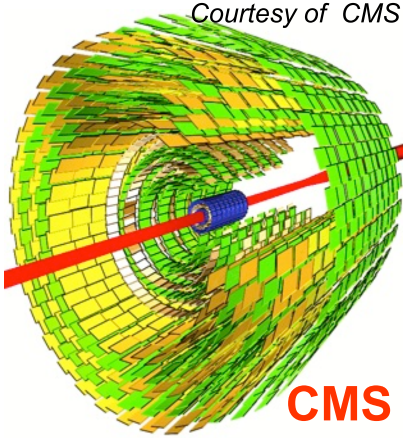
- Run — a collection of events that share the same detector conditions
- Event — multiple events: pile-up
- Tracking — decoupled from physics
  - no tracking cuts, but **secondary production thresholds**
- Particles
- Modeling experimental setups
  - Geometry and materials
  - Detector response
- Physics
- Visualisation
- User interface
- Persistency
- Parallel execution

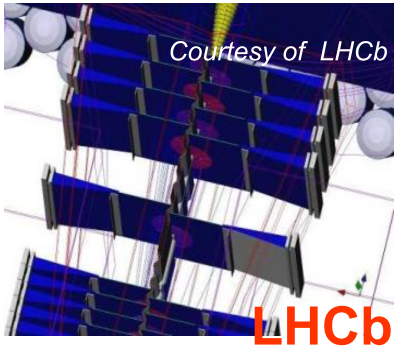
No time to review all Geant4 functionality in detail

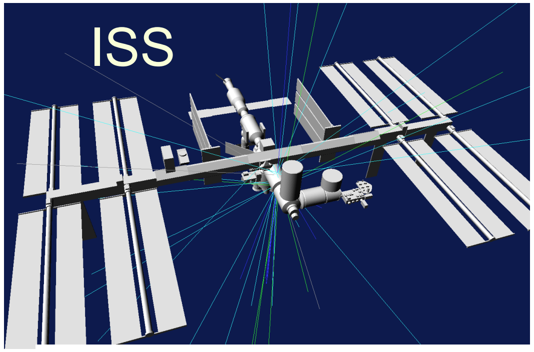
Geometry

- Role
  - detailed detector description
  - efficient navigation
- Three conceptual layers
  - **Solid**: shape, size
  - **LogicalVolume**: material, sensitivity, daughter volumes, etc.
  - **PhysicalVolume**: position, rotation

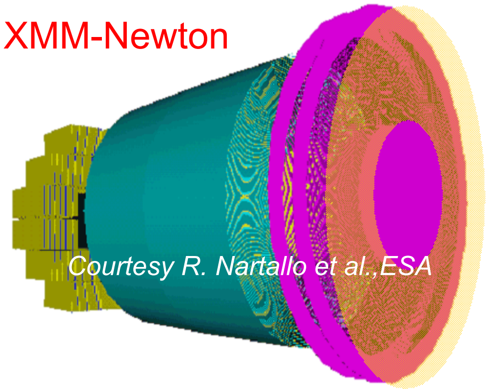


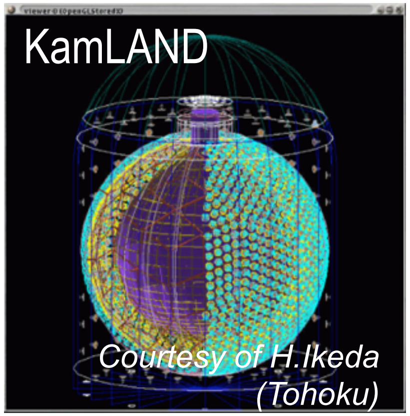


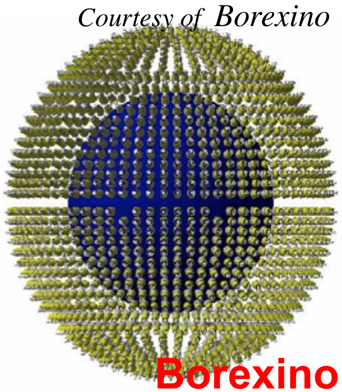




Courtesy T. Ersmark, KTH Stockholm



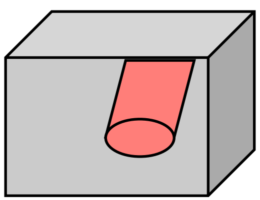




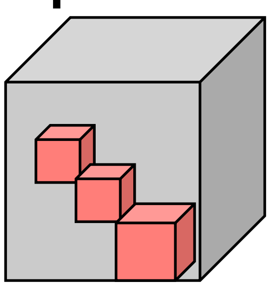
Solids

- **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

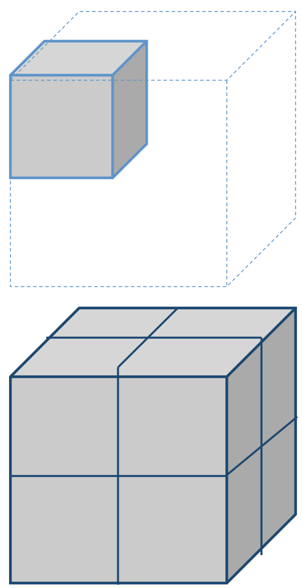
Physical Volumes



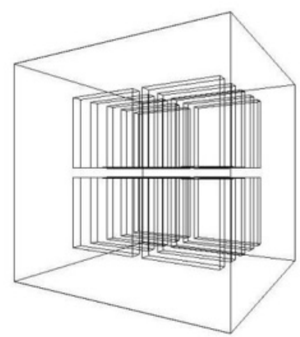
placement



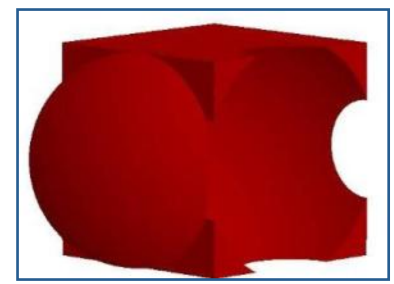
parameterised



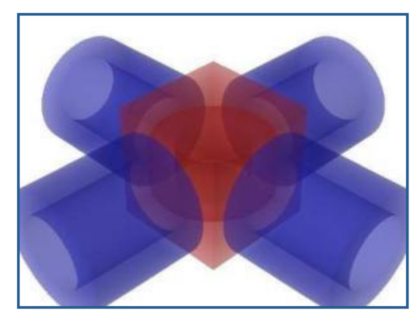
replica



assembled



Boolean operations



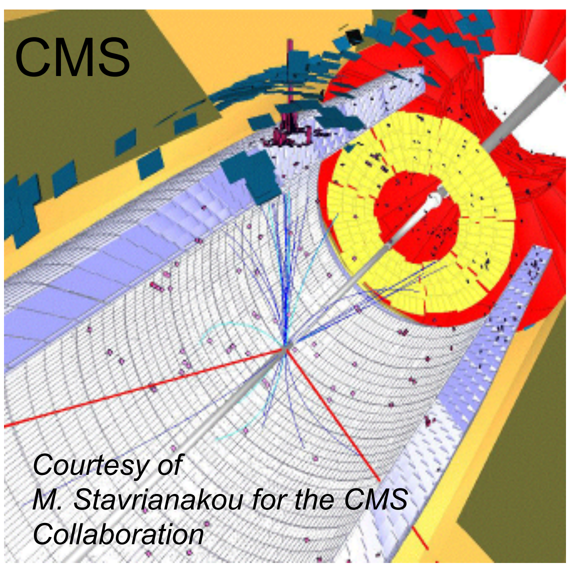
Transparent solids

Materials

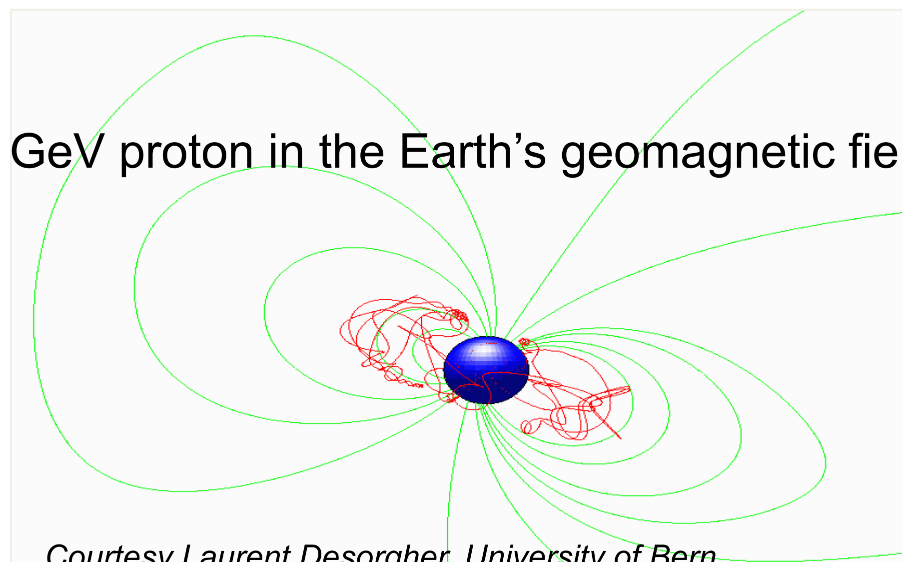
- Different kinds can be defined
  - **isotopes**
  - **elements**
  - **molecules**
  - **compounds** and **mixtures**
- Associated attributes:
  - temperature
  - pressure
  - state
  - density

Electric and magnetic fields

of variable non-uniformity and differentiability



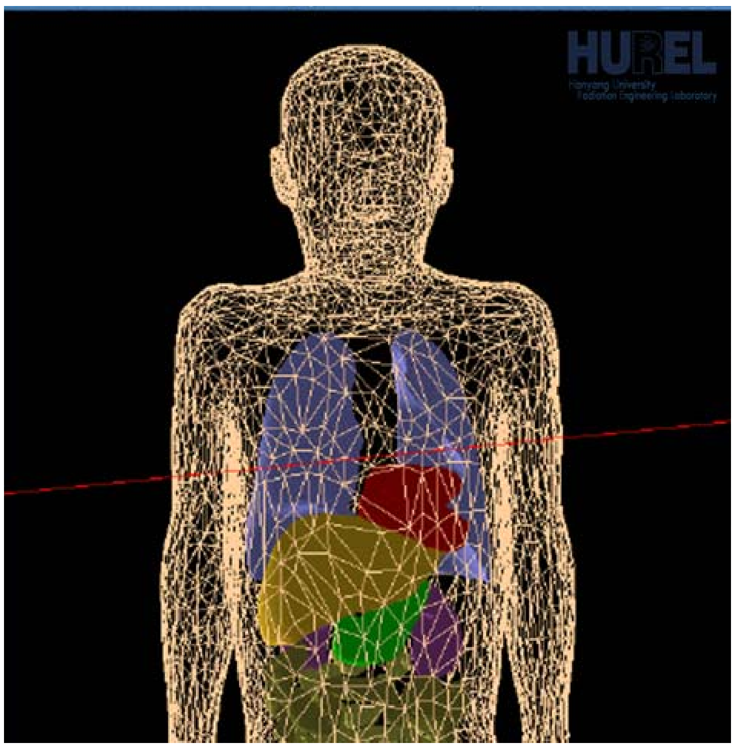
Courtesy of M. Stavrianakou for the CMS Collaboration


1 GeV proton in the Earth's geomagnetic field

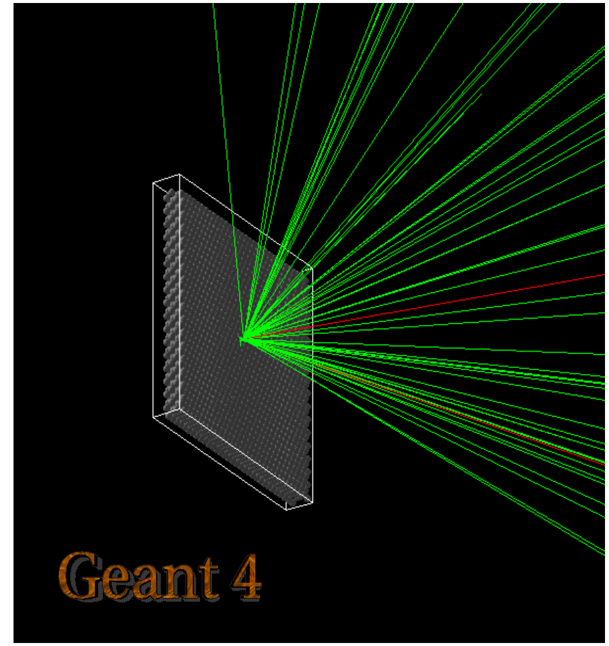
Courtesy Laurent Desorgher, University of Bern

Not only large scale, complex detectors…

anthropomorphic phantoms

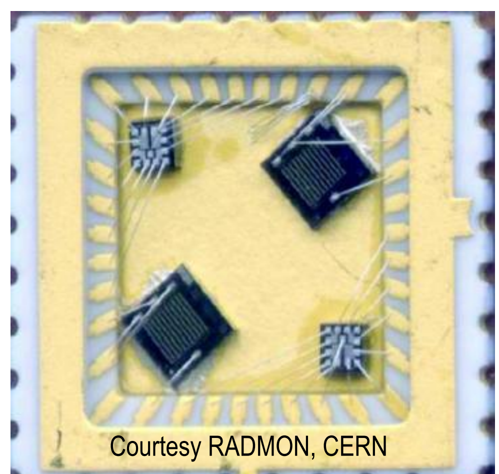


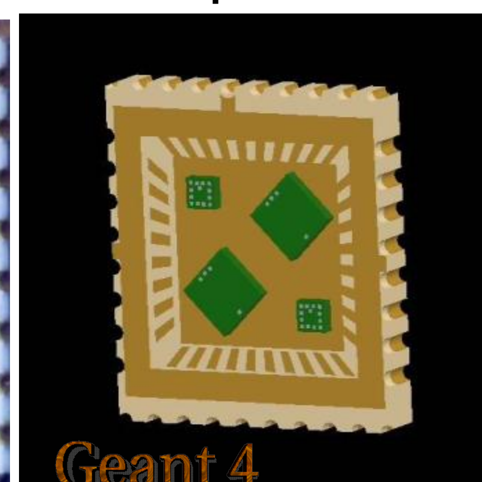
Courtesy Min Cheol Han, Hanyang Univ.



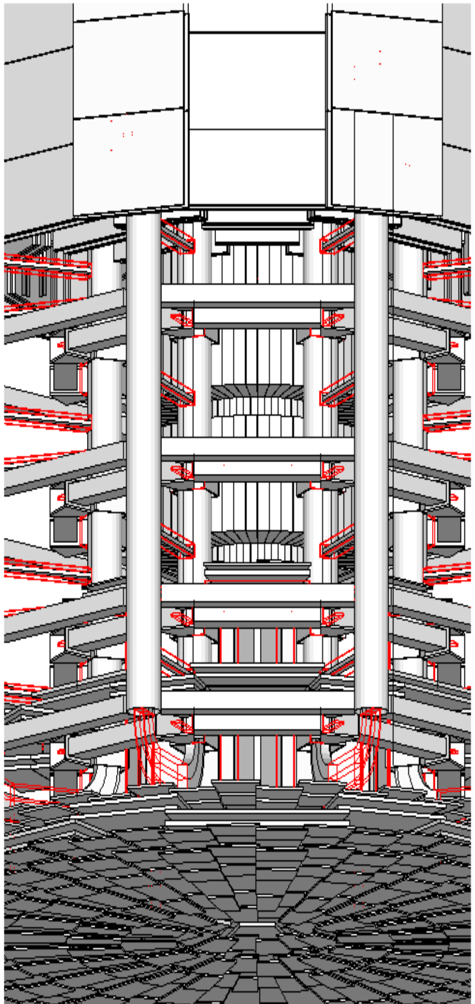
simple geometries

small scale components





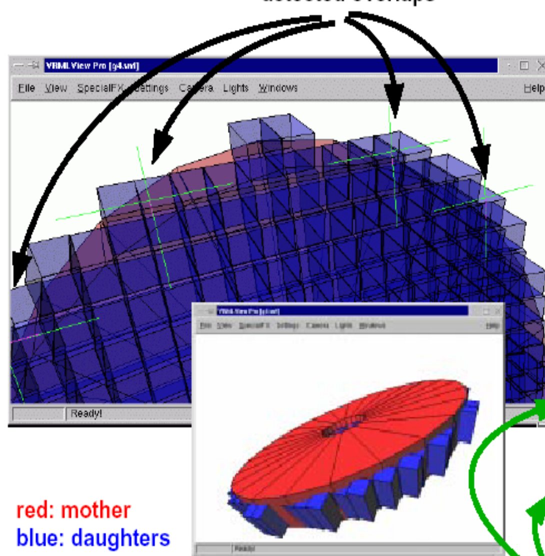
One may also do it wrong…



DAVID

Tools to detect badly defined geometries

graphical indication of detected overlaps



red: mother
blue: daughters

daughters are protruding their mother

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

"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

⇩

RD44 physics vision and design

RD44 physics vision and design

- 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

- Comparable to GEANT 3 already in 1997 α release
- 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 ν experiments, antimatter spectroscopy, radiation effects on components etc.

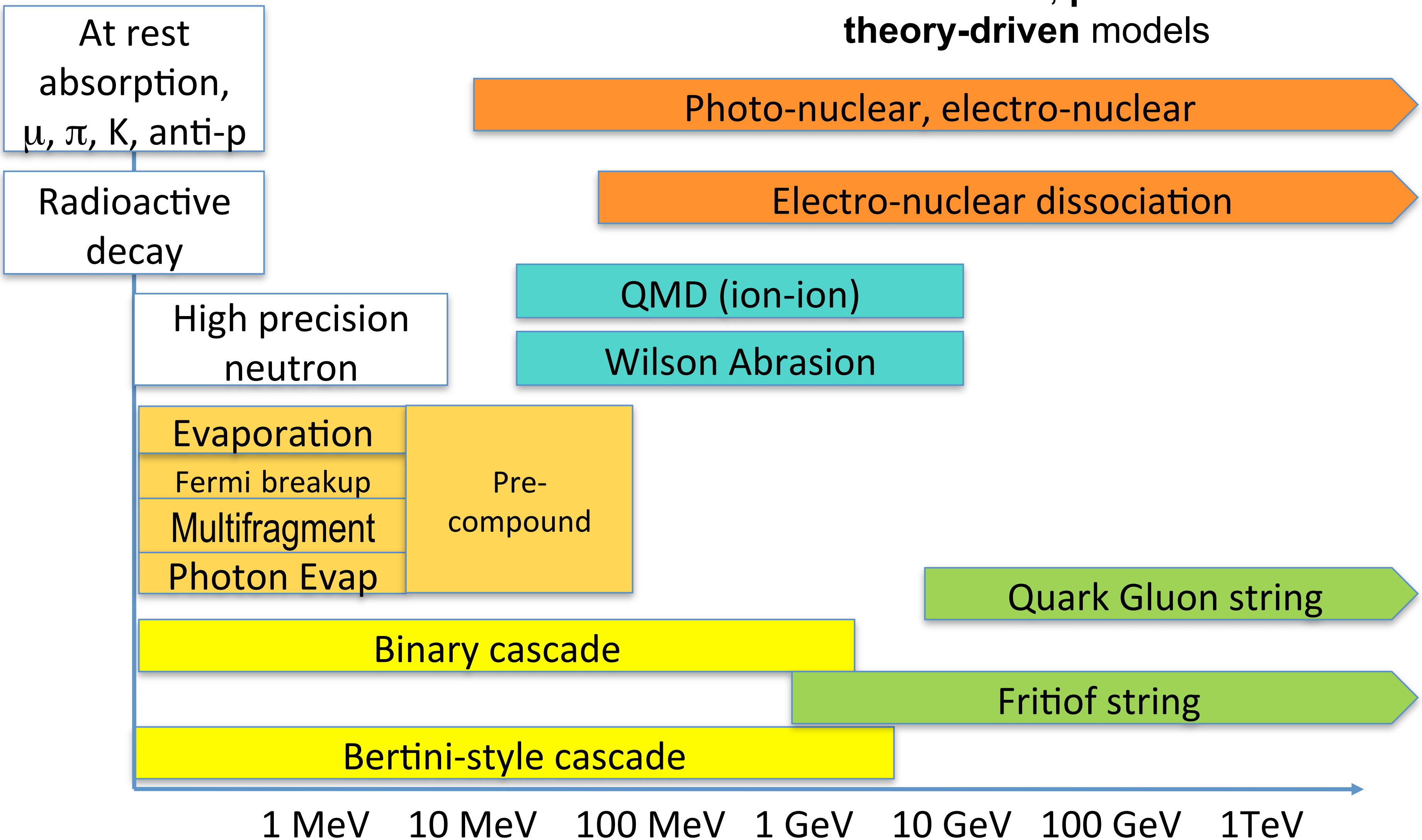
- Alternative models for the same process

- Multiple scattering
- Bremsstrahlung
- Ionisation
- Annihilation
- Photoelectric effect
- Compton scattering
- Rayleigh scattering
- γ conversion
- Synchrotron radiation
- Transition radiation
- Cherenkov
- Refraction
- Reflection
- Absorption
- Scintillation
- Fluorescence
- Auger emission

Hadronic physics

Ample variety of models

- Alternative/complementary
- **Data-driven**, **parameterised** and **theory-driven** models

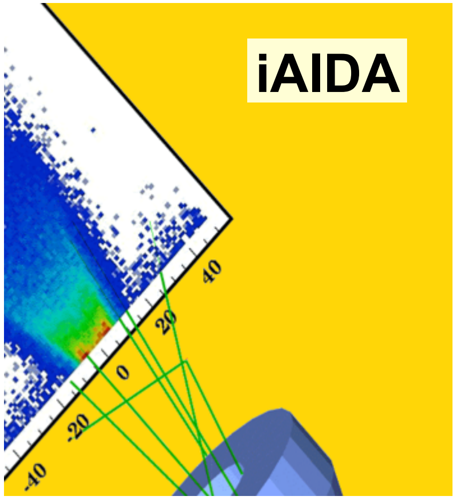


Other features

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

No time to review them in detail

Interface to external tools



Through abstract interfaces (when they exist…)
➔ No dependency

Similar approach
- Visualisation
- (G)UI
- Persistency
- [Analysis]

Visualisation

- Detector geometry
- Particle trajectories
- Hits in detectors

Drivers

- OpenGL
- OpenInventor
- Postscript
- DAWN
- OPACS
- HepRep
- VRML…

User interface

- Several implementations
- Command-line
  - batch and terminal
- GUIs
  - X11/Motif, GAG, MOMO, OPACS…
- Automatic code generation for geometry and physics through a GUI
  - GGE (Geant4 Geometry Editor)
  - GPE (Geant4 Physics Editor)

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 **choose** which Geant4 tools to use
  - To describe the experimental scenario
  - To input primary particles
  - To select physics processes and models, to set secondary production thresholds
- Geant4 tools for user interaction are **base classes**
  - **Abstract base classes** (detector construction, physics, primary generation)
  - **Concrete base classes** (with *virtual* dummy methods) for optional actions
- Guidance: **examples** are distributed with Geant4

GATE

Simulations of Preclinical and Clinical Scans in Emission Tomography, Transmission Tomography and Radiation Therapy

GOBIERNO DE ESPAÑA MINISTERIO DE CIENCIA E INNOVACIÓN

Ciemat Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas

Geant 4

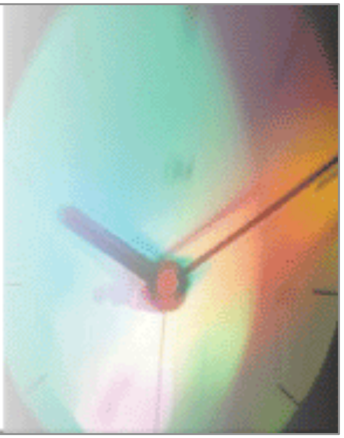
GAMOS

Geant4-based Architecture for Medicine-Oriented Simulations

独立行政法人科学技術振興機構(JST)
戦略的基礎研究推進事業(CREST)
「シミュレーション技術の革新と実用化基盤の構築」研究領域

高度放射線医療のためのシミュレーション基盤の開発

研究代表者 高エネルギー加速器研究機構　計算科学センター 教授　佐々木 節



GRAS – Geant4 Radiation Analysis for Space

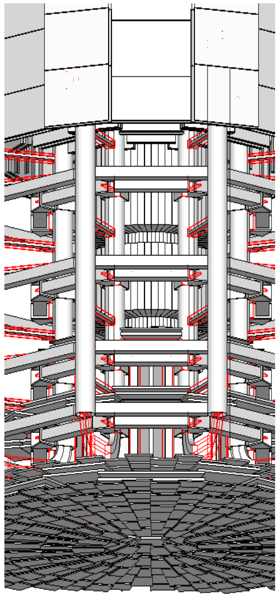
Introduction

GRAS is a Geant4-based tool that deals with common radiation analyses types (TID, NIEL, fluence, SEE, path length, charge deposit, dose equivalent, equivalent dose, ...) in generic 3D geometry models.

esa

QinetiQ

MUlti-LAyered Shielding SImulation Software (MULASSIS)



The user must implement a class derived from
G4VUserPhysicsList
to configure the physics for his/her application

No DAVID for physics!

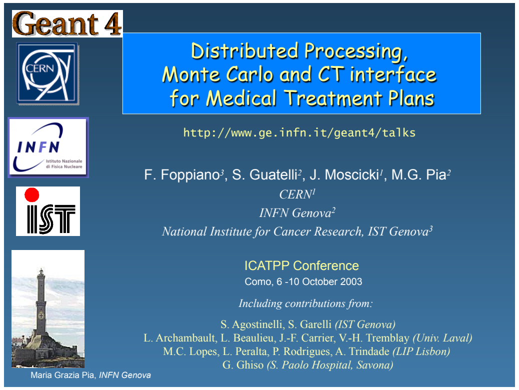
- Automated tools to detect badly defined geometries
- No such tools to detect badly defined physics!

Knowledge of the **capabilities** and **accuracy** of Geant4 physics options is essential to select the most appropriate ones for an experimental application

Geant4 physics validation

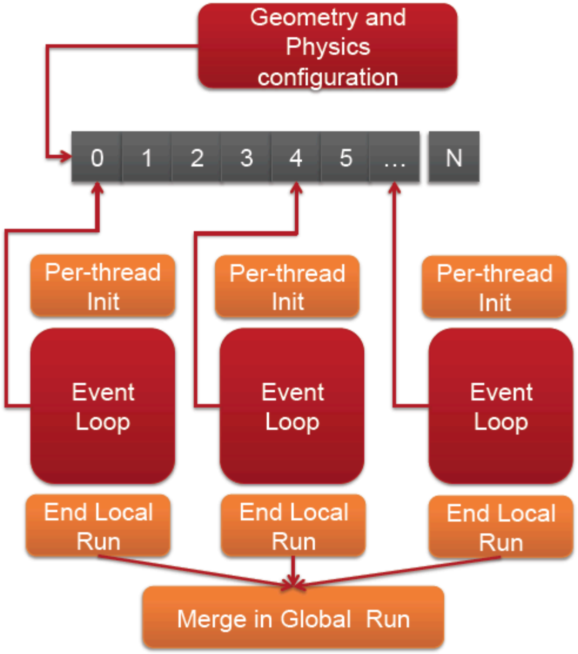
Parallel execution

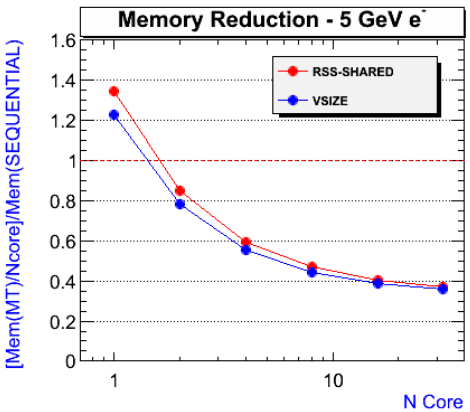
- Activity since early Geant4 releases
- Multi-threading released in Geant4 10.0
  - Event-level parallelism

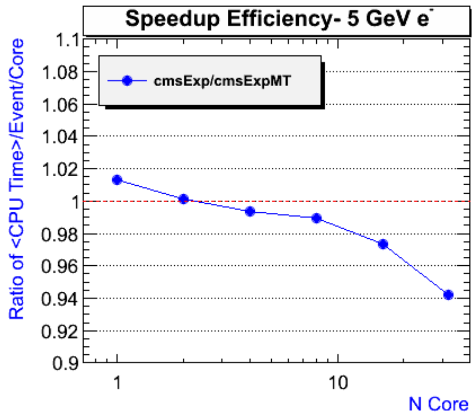


Each worker thread proceeds independently

- Initializes its state from a master thread
- Identifies its part of the work (events)
- Generates hits in its own hits-collection
- Uses thread-private objects and state
- Shares read-only data structures *(e.g. geometry, cross-sections, …)*
- Has its own read-write part in a few 'shared/split' objects







No time to show detailed results

Further benchmarks would be useful

Thanks to G. Cosmo for material borrowed from his CHEP 2013 talk!

Perspectives

All done?

Perspectives for the next 20 years…

- **Reviving sound software methods**
- **Geant4 validation**
- **Detector simulation**
- **New experimental challenges**
  - Beyond IPA and IA
  - Multi-scale simulation
- **Computational resources**
- **Uncertainty Quantification**
  - Predictive simulation

largely inter-related

Software

If it stinks, change it.

Grandma Beck, discussing child-rearing philosophy

Post-RD44 electromagnetic software

Coupling

total cross section

whether a process occurs

final state generation

how a process occurs

Dependencies

on other parts of the software

One needs a geometry
(and a full scale application)
to test a cross section

Difficult to test ➔ no testing
often

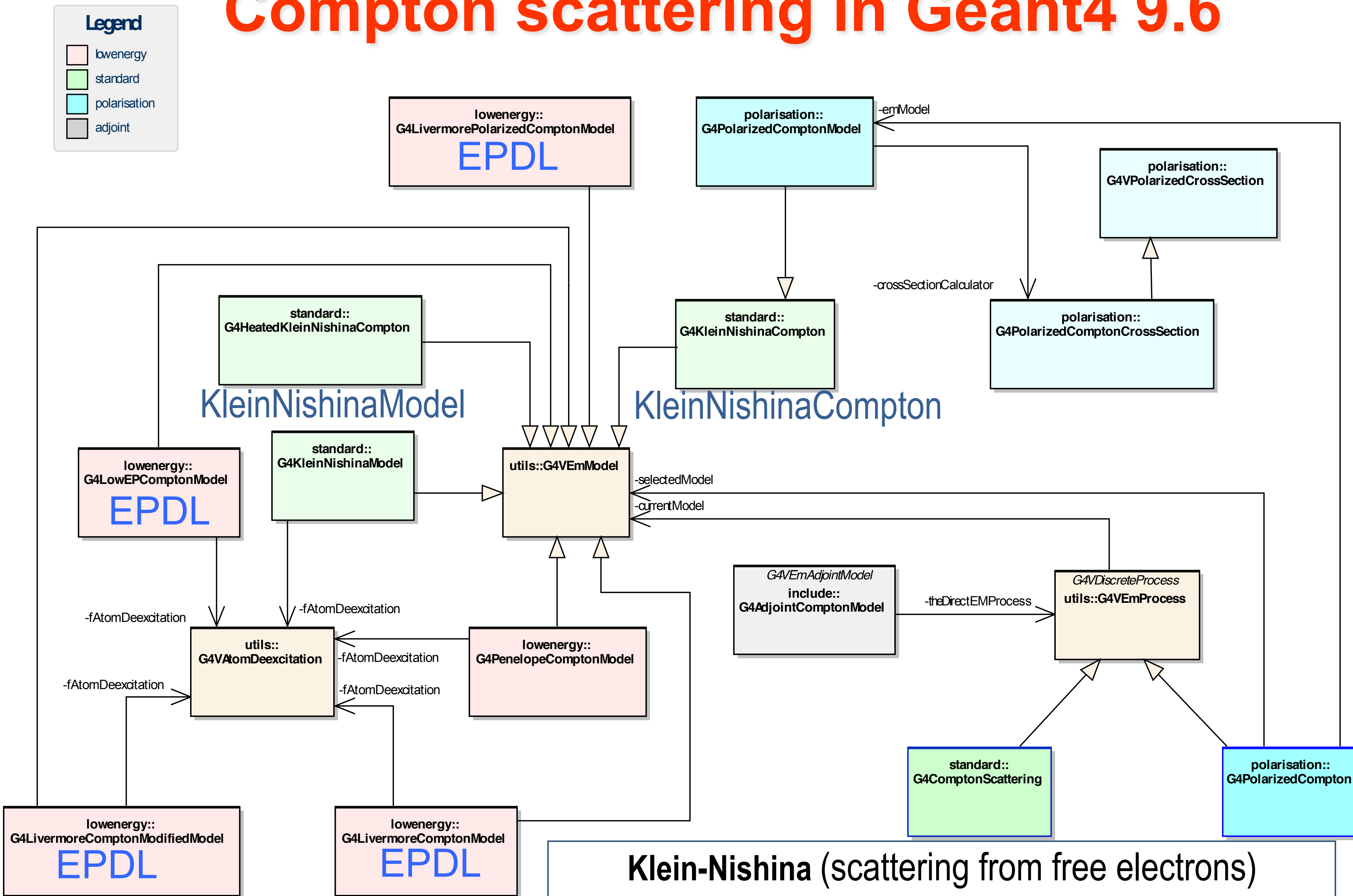
Reverse engineered

No UML diagrams exist
No design peer reviews

ENTERPRISE ARCHITECT

Maria Grazia Pia, INFN Genova

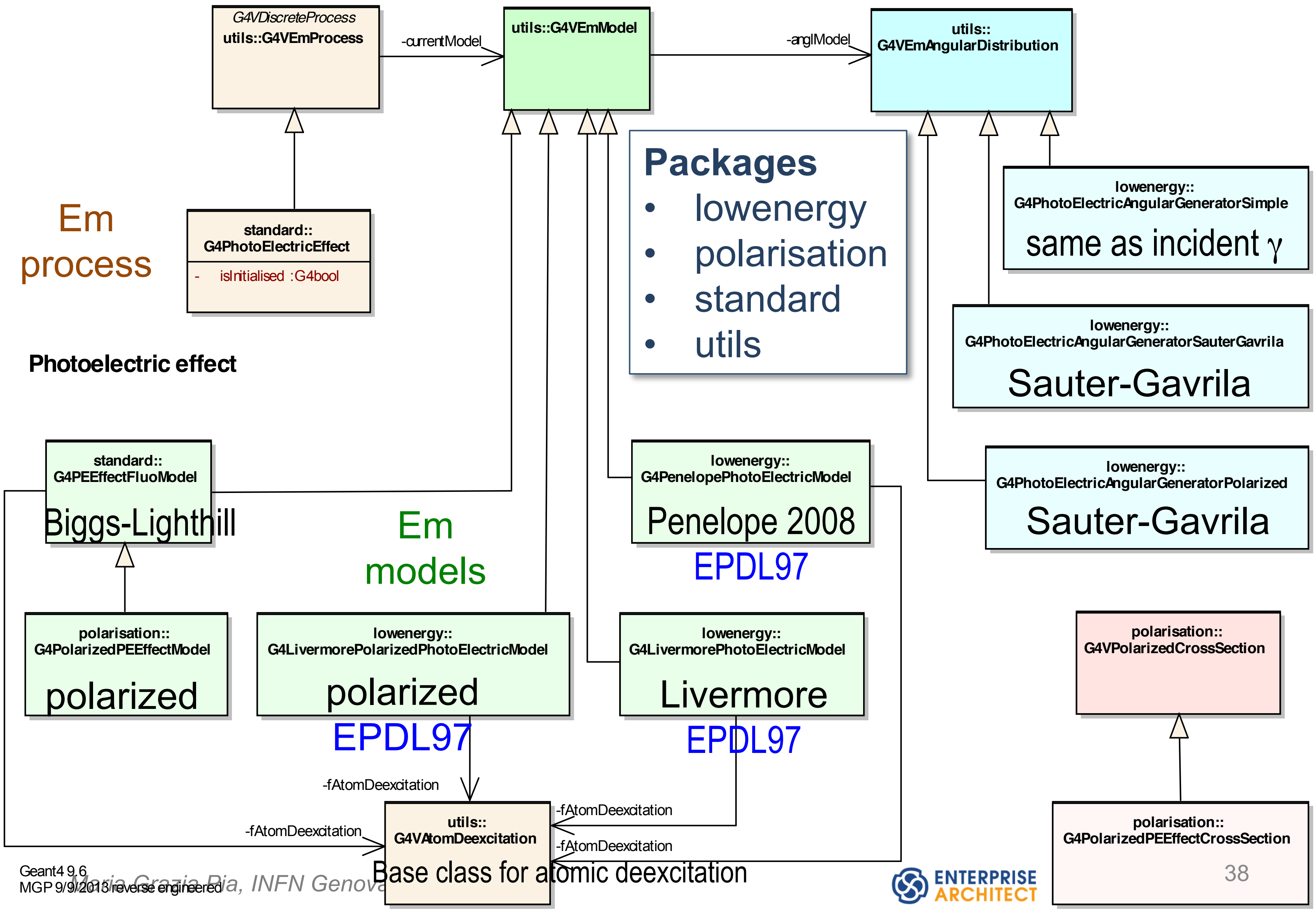
Compton scattering in Geant4 9.6



Klein-Nishina (scattering from free electrons)
EPDL (Hubbell’s scattering functions),Doppler broadening

Maria Grazia Pia, INFN Genova

Photoelectric effect in Geant4 9.6

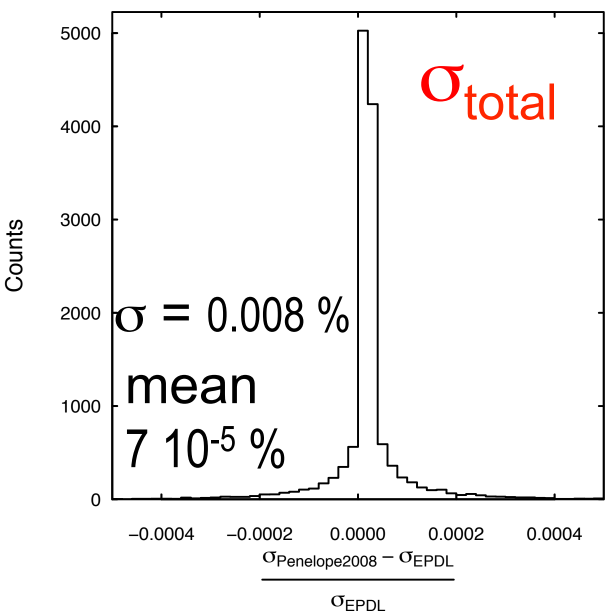


Duplication

Number one in the stink parade is duplicated ~~code~~ physics

Two Geant4 models:
different code, identical underlying physics content
(it used to be different physics)

Photon elastic scattering total cross section



"Livermore"	Penelope
EPDL97	EPDL97
0.38 ± 0.06	0.38 ± 0.06

← Efficiency w.r.t. experiment

Code bloat

Burden on
- Software design
- Maintenance
- User support

Unnecessary complexity

Maria Grazia Pia, INFN Genova

Bremsstrahlung, evaporation, proton elastic scattering etc.

Duplication

Number one in the stink parade is duplicated ~~code~~ numbers

1. Bearden & Burr (1967)
2. Carlson
3. EADL
4. Sevier
5. Tol 1978 (Shirley)
6. Tol 1996 (Larkins)
7. Williams

Atomic binding energies

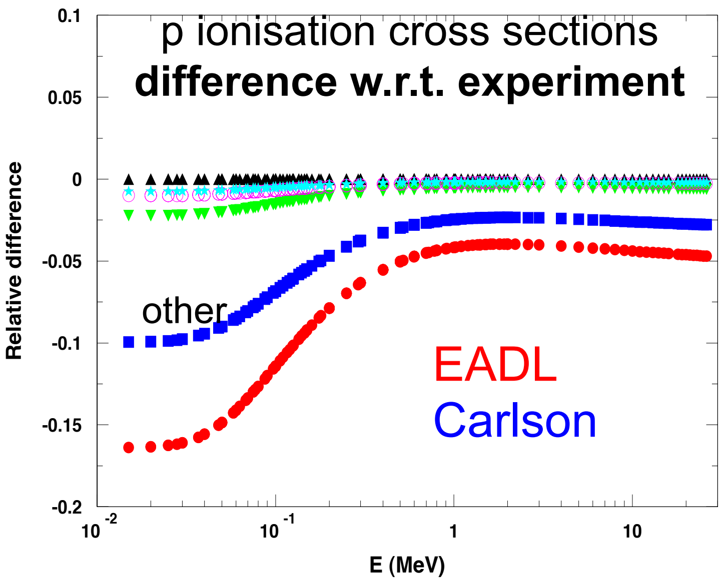
Geant 4 { Carlson + Williams / EADL

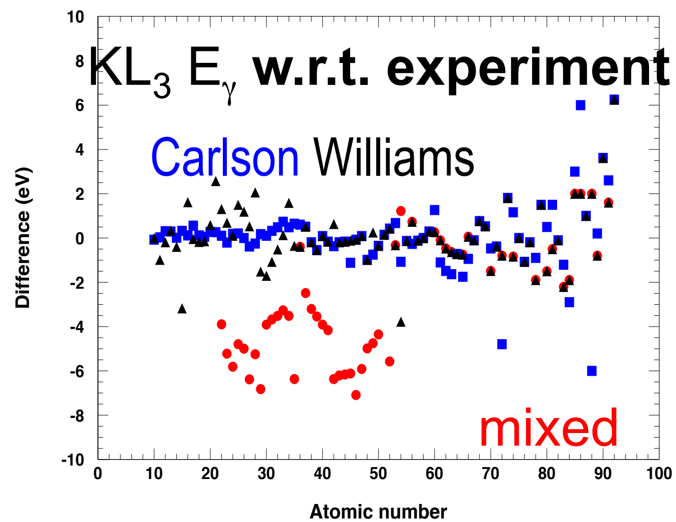
Vacuum
Fermi level

3246 IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 58, NO. 6, DECEMBER 2011

Evaluation of Atomic Electron Binding Energies for Monte Carlo Particle Transport

Maria Grazia Pia, Hee Seo, Matej Batic, Marcia Begalli, Chan Hyeong Kim, Lina Quintieri, and Paolo Saracco





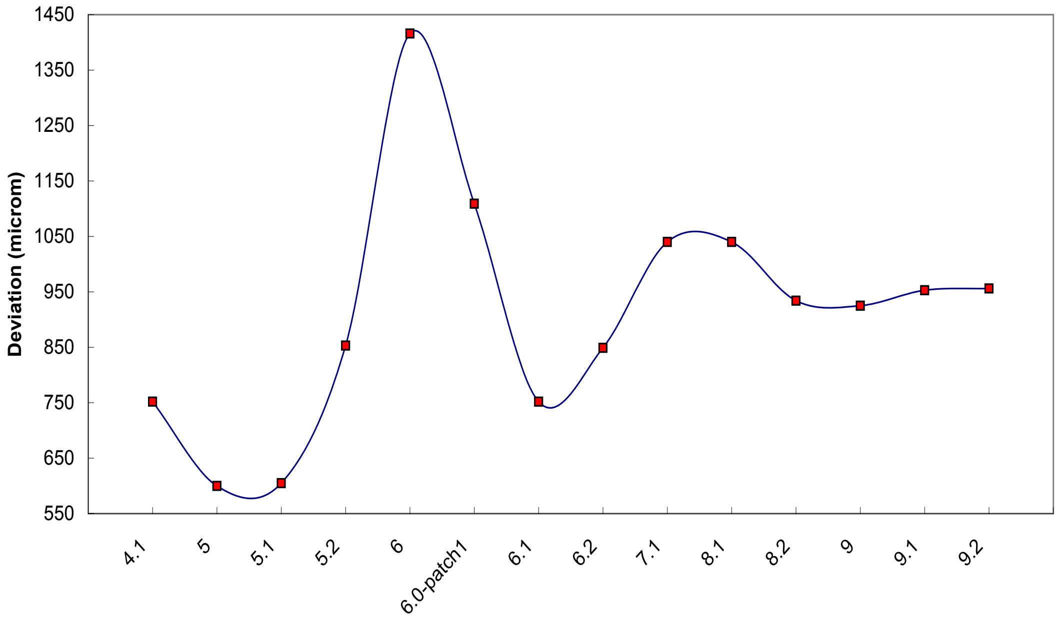
XRF

Maria Grazia Pia, INFN Genova

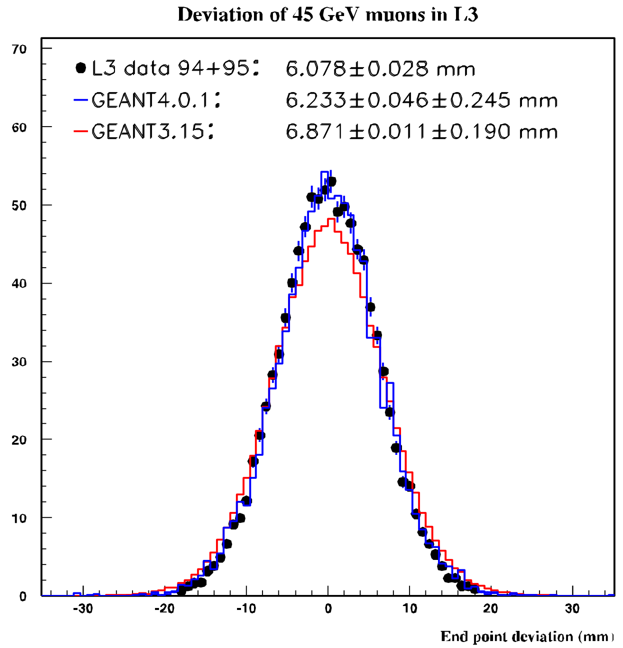
Change management

Traceability
Test

100 GeV muons, 1 m thick iron
Lateral deviation at end point



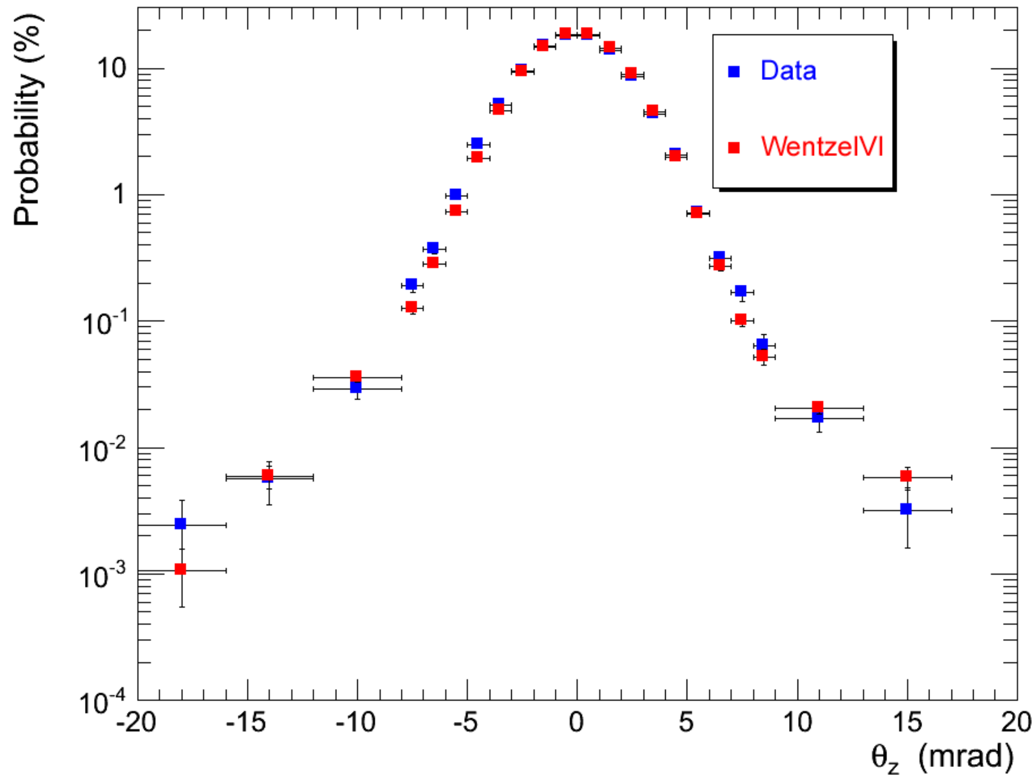
Geant4 version



P. Arce and M. Wadhwa, Deviation in matter of 45 GeV muons in GEANT3 and GEANT4. A comparison with L3 data. CMS Note 2000/16, 2000

Muons

Geant4 electromagnetic physics for the LHC and other HEP applications Proc. CHEP 2010



Muon scattering angular distribution for 7.3 Gev/c muon on a copper target (1 radiation length thick) in comparison with the **Wentzel-VI** MSC model.

Comparison with experimental data limited to stopping power in two materials

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 53, NO. 2, APRIL 2006 513

Geant4 Simulation of Production and Interaction of Muons

A. G. Bogdanov, H. Burkhardt, V. N. Ivanchenko, S. R. Kelner, R. P. Kokoulin, M. Maire, A. M. Rybin, and L. Urban

High energy extensions based on theoretical models (**PeV** scale): data?

software changes…

What you validated yesterday, is still valid today?

398 Best Student paper, IEEE NSS 2007

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 56, NO. 2, APRIL 2009

Validation of Geant4 Low Energy Electromagnetic Processes Against Precision Measurements of Electron Energy Deposition

Anton Lechner, Maria Grazia Pia, and Manju Sudhakar

2934

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 60, NO. 4, AUGUST 2013

Validation of Geant4 Simulation of Electron Energy Deposition

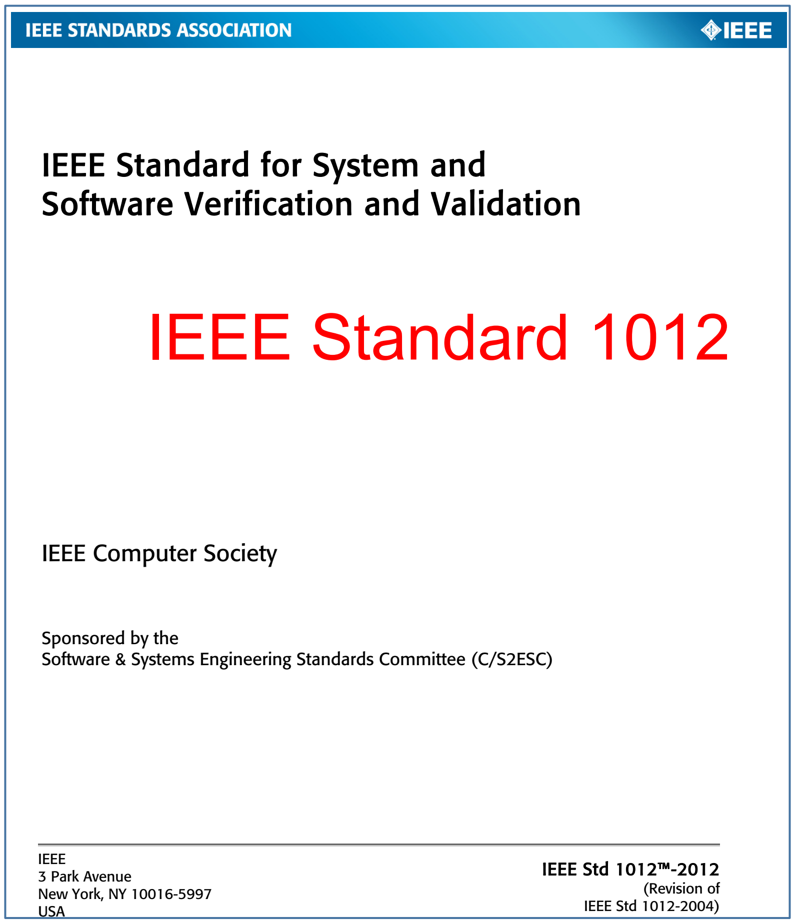
Matej Batič, Gabriela Hoff, Maria Grazia Pia, Paolo Saracco, and Georg Weidenspointner

How does it look like 4 years later?

Geant4 physics validation

What is what

- **Verification**
- **Validation**
- **Calibration**


IEEE STANDARDS ASSOCIATION ◆IEEE

IEEE Standard for System and
Software Verification and Validation

IEEE Standard 1012

IEEE Computer Society

Sponsored by the
Software & Systems Engineering Standards Committee (C/S2ESC)

IEEE
3 Park Avenue
New York, NY 10016-5997
USA

IEEE Std 1012™-2012
(Revision of
IEEE Std 1012-2004)

Conforms to

- **ISO/IEC 15288** (IEEE Std 15288)
  Systems and Software Engineering – System Life Cycle Processes
- **ISO/IEC 12207** (IEEE Std 12207)
  Systems and Software Engineering – Software Life Cycle Processes
- **IEEE Std 1074**
  IEEE Standard for Developing a Software Project Life Cycle Process

Verification

A. The process of evaluating a system or component to determine whether the products of a given development phase satisfy the conditions imposed at the start of that phase.

B. The process of providing objective evidence that the system, software, or hardware and its associated products **conform to requirements** *(e.g., for correctness, completeness, consistency, and accuracy)* for all life cycle activities during each life cycle process (acquisition, supply, development, operation, and maintenance); satisfy standards, practices, and conventions during life cycle processes; and successfully complete each life cycle activity and satisfy all the criteria for initiating succeeding life cycle activities.

e.g. in the context of Monte Carlo simulation

Requirement:
Compton scattering cross section shall be described by the Klein-Nishina formula

Verification: the software calculates

$$\frac{d\sigma_{KN}(\theta)}{d\Omega} = \frac{r_e^2}{2}[1+k(1-\cos\theta)]^{-2}\left[1+\cos^2\theta + \frac{k^2(1-\cos\theta)^2}{1+k(1-\cos\theta)}\right]$$

consistently, correctly,
with adequate numerical precision…

Validation

A. The process of evaluating a system or component during or at the end of the development process to determine whether it satisfies specified requirements.

B. The process of providing evidence that the system, software, or hardware and its associated products satisfy requirements allocated to it at the end of each life cycle activity, **solve the right problem** *(e.g., **correctly model physical laws**, implement business rules, and use the proper system assumptions),* and **satisfy intended use and user needs**.

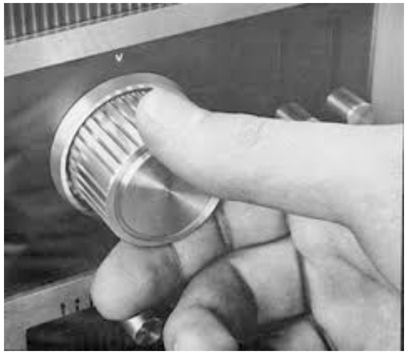
In the context of Monte Carlo simulation

validation = consistency with experimental measurements

e.g. does the Klein-Nishina formula reproduce measured differential cross sections of photon inelastic scattering?

Calibration

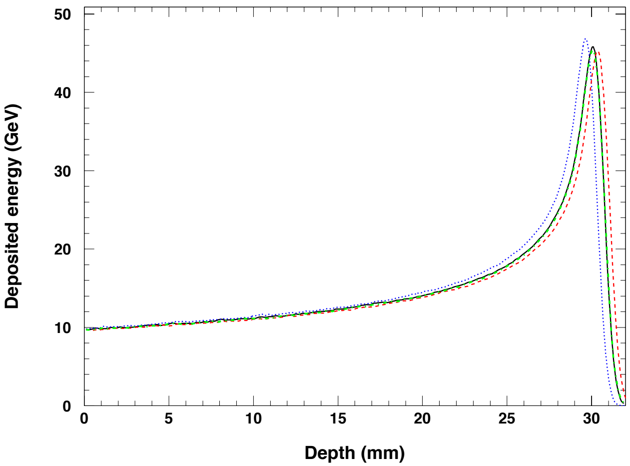
AKA "tuning"



- 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
- Calibration **is not** validation
  - 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

M. G. Pia et al, **Physics-related epistemic uncertainties of proton depth dose simulation**, *IEEE Trans. Nucl. Sci.*, vol. 57, no. 5, pp. 2805-2830, 2010



What is NOT validation

- Comparison of simulations with different Monte Carlo codes
  - Or comparison of different physics models in the same Monte Carlo system
- Comparison of simulation with theory
- Comparison with non-pertinent experimental data
- Calibration

Oenology

Mozart opera

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!

cited in

Progress in NUCLEAR SCIENCE and TECHNOLOGY, Vol. 2, pp.898-903 (2011)

REVIEW

"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]

Comparisons of Monte Carlo codes

Phys. Med. Biol. **56** (2011) 811–827 doi:10.1088/0031-9155/56/3/017

Comparison of GATE/GEANT4 with EGSnrc and MCNP for electron dose calculations at energies between 15 keV and 20 MeV

Phys. Med. Biol. **57** (2012) 6381–6393 doi:10.1088/0031-9155/57/20/6381

Comparison of MCNPX and Geant4 proton energy deposition predictions for clinical use

Phys. Med. Biol. **57** (2012) 1231–1250 doi:10.1088/0031-9155/57/5/1231

Comparison of nanodosimetric parameters of track structure calculated by the Monte Carlo codes Geant4-DNA and PTra

Applied Radiation and Isotopes 83 (2014) 137–141

Dose point kernels in liquid water: An intra-comparison between GEANT4-DNA and a variety of Monte Carlo codes

C. Champion [a,*], S. Incerti [a], Y. Perrot [b], R. Delorme [c], M.C. Bordage [d], M. Bardiès [e], B. Mascialino [f], H.N. Tran [a], V. Ivanchenko [g], M. Bernal [h], Z. Francis [i], J.-E. Groetz [j], M. Fromm [j], L. Campos [k]

Comparison of  and 

Comparison of GEANT4 very low energy cross section models with experimental data in water

S. Incerti, A. Ivanchenko, M. Karamitros, A. Mantero, P. Moretto, H. N. Tran, B. Mascialino, C. Champion, V. N. Ivanchenko, M. A. Bernal, Z. Francis, C. Villagrasa, G. Baldacchino, P. Guèye, R. Capra, P. Nieminen, and C. Zacharatou

Citation: Medical Physics **37**, 4692 (2010); doi: 10.1118/1.3476457

Simulation models: **liquid water**
Experimental data: **water vapour**

Validation is holistic

One has to 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

Columbia Space Shuttle disaster

The Columbia Space Shuttle wing failed during re-entry due to hot gases entering a portion of the wing damaged by a piece of foam that broke off during launch

— NASA Columbia Shuttle Accident Report

Boeing did an analysis with the CRATER code (designed to study the effects of micrometeorite impacts, validated only for projectiles less that 1/400 the size and mass of the piece of foam that struck the wing), did not use a code like LS-DYNA that was the industry standard for assessing impact damage

What is validated

- Validation of the "**ingredients**" of Geant4
  - Foundation of Geant4 physics models
  - Cross sections (total, partial, differential)
    - angular distributions, secondary particle energy spectra etc.
  - Modeling assumptions

very limited coverage!

- Validation of **simulated observables** in **use cases**
  - Largely represented in the literature
  - Often **qualitative** only
  - Resulting from **Geant4 + user application**
  - Often lacking traceability *(e.g. no configuration documentation)*

Establishing validity

Agreement
Good agreement
Excellent agreement
Satisfactory agreement
…

- Comparison of simulation and experimental data in the literature mainly rests on
  - qualitative visual appraisal of figures
  - indicators (%) deprived of any statistical relevance
- **Statistics** is the mathematical foundation of Monte Carlo validation
- Rigorous statistical methods assess
  - Whether a **simulation model is consistent with nature**
  - Whether different simulation models produce (or do not produce) equivalent results in terms of compatibility with experiment

Conference papers

- J. Apostolakis et al., Recent Progress of Geant4 Electromagnetic Physics and Readiness for the LHC Start, *XII Workshop Advanced Computing and Analysis Techniques in Physics Research (ACAT)*, 2008
- J. Apostolakis et al., Validation and verification of Geant4 standard electromagnetic physics, *J. Phys.: Conf. Series* 219 (2010) 032044 (CHEP 2009)
- A. Schälicke et al., Geant4 electromagnetic physics for the LHC and other HEP applications, J. Phys.: Conf. Series 331 (2011) 032029 (CHEP 2010)
- V. Ivanchenko et al., Recent Improvements in Geant4 Electromagnetic Physics Models and Interfaces*, Progr. Nucl. Sci. Technol.*, 2 (2011) 898-903 (SNA+Monte Carlo 2010)
- J. Allison et al., Geant4 electromagnetic physics for high statistic simulation of LHC experiment, *J. Phys.: Conf. Series*, 396 (2012) 022013 (CHEP 2012)

…etc.

An example:

*"The Urban93 MSC model was introduced and **validated** within Geant4 release 9.3 and made default in Geant4 release 9.4. With this model simulation results for low Z materials **have improved**.*
*In general the accuracy of the Urban model is **of the order of a few percent**, **sufficient** for most HEP applications."*

Multiple scattering

J. Allison et al., Geant4 electromagnetic physics for high statistic simulation of LHC experiment, *J. Phys.: Conf. Series*, 396 (2012) 022013

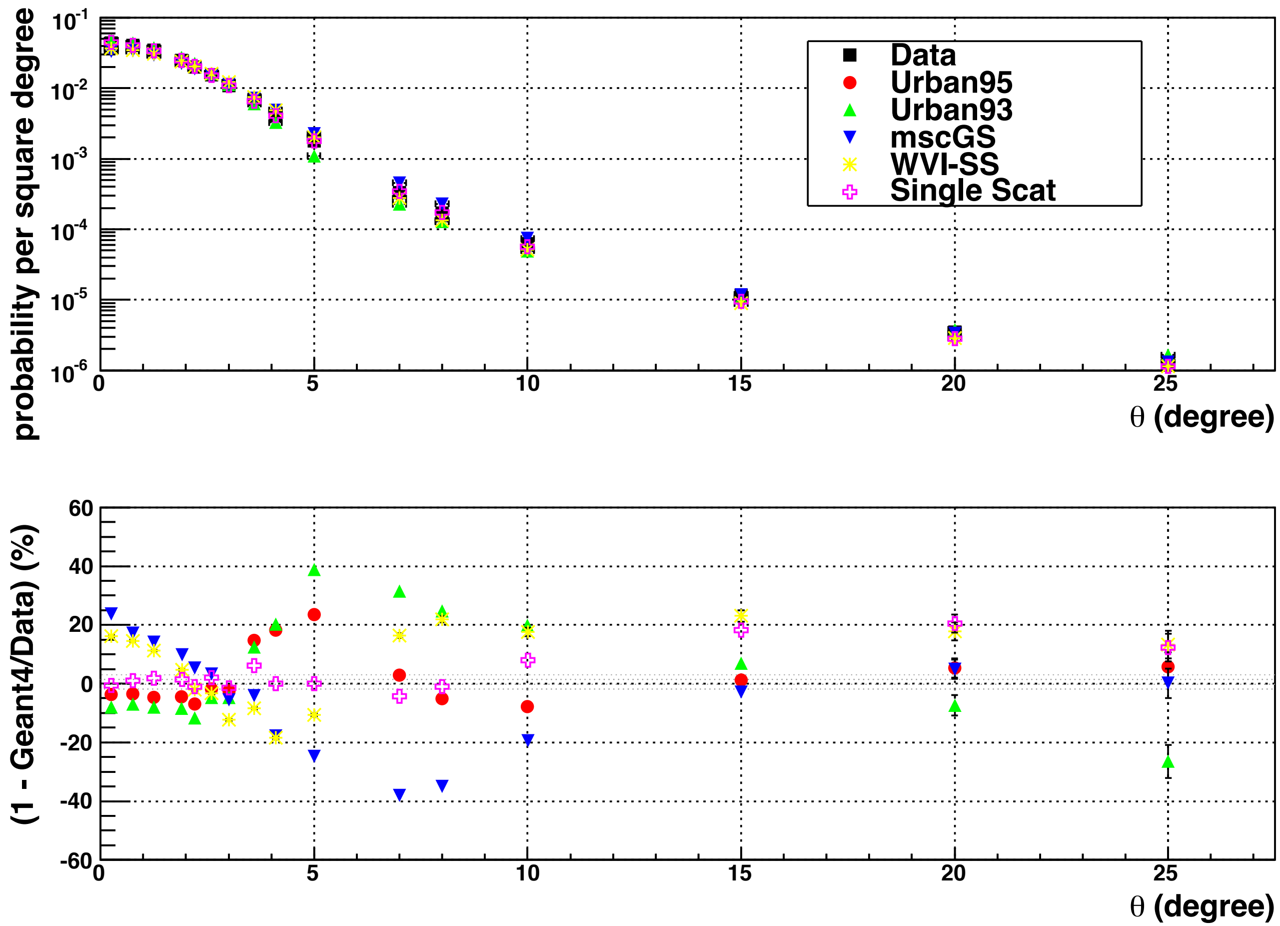


Figure 4. Comparison of different Geant4 MSC model predictions and experimental data [23] for 15.7 MeV electrons scattering off 9.68 um Gold foil: angular distribution (top); Monte Carlo over data (bottom). Urban model 95 and the single scattering model provides overall better agreement with the data.

J. Allison et al., Geant4 electromagnetic physics for high statistic simulation of LHC experiment, *J. Phys.: Conf. Series*, 396 (2012) 022013

Electron energy loss

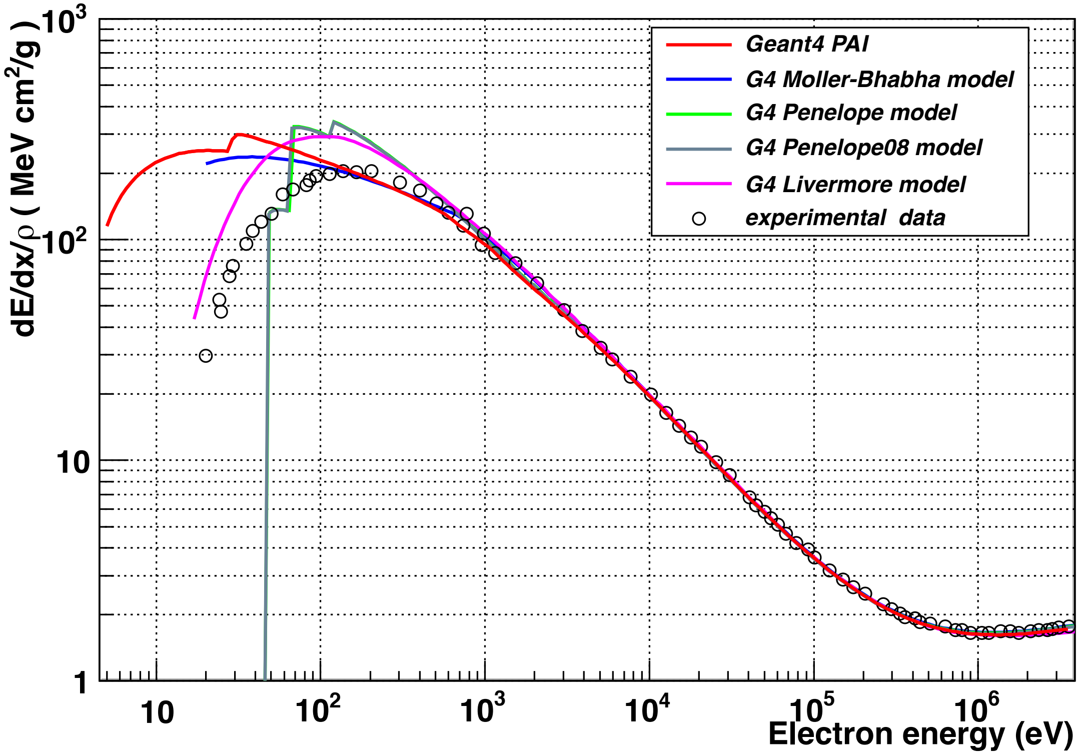


Figure 5. Electron mean energy loss in CO_2 vs. electron energy: points are data [30], solid lines - different Geant4 models. Moller-Bhabha and PAI model follow the date down to 100 eV. Below 200 eV Penelope and Livermore models show effects caused by the treatment of atomic shell effects.

PROCEEDINGS OF SCIENCE

V. Ivanchenko et al., Recent **Progress** of Geant4 Electromagnetic Physics and Readiness for the LHC Start, *XII Advanced Computing and Analysis Techniques in Physics Research, Erice, Italy, 3-7 November 2008*

Improvements

Progress in NUCLEAR SCIENCE and TECHNOLOGY, Vol. 2, pp.898-903 (2011)

REVIEW

SNA+Monte Carlo 2010

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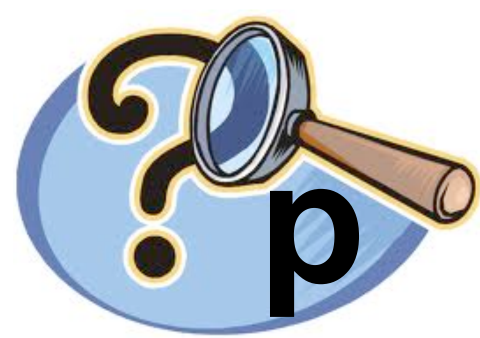
Vladimir IVANCHENKO[1,2,3*], John APOSTOLAKIS[1], Alexander BAGULYA[4], Haifa Ben ABDELOUAHED[5], Rachel BLACK[6], Alexey BOGDANOV[7], Helmut BURKHARD[1], Stéphane CHAUVIE[8], Pablo CIRRONE[9], Giacomo CUTTONE[9], Gerardo DEPAOLA[10], Francesco Di ROSA[9], Sabine ELLES[11], Ziad FRANCIS[12], Vladimir 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]

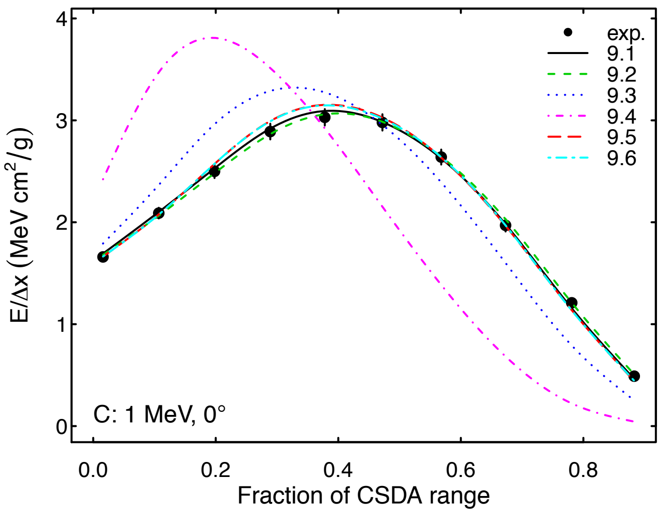
RADECS 2011 Proceedings - PA-19 115

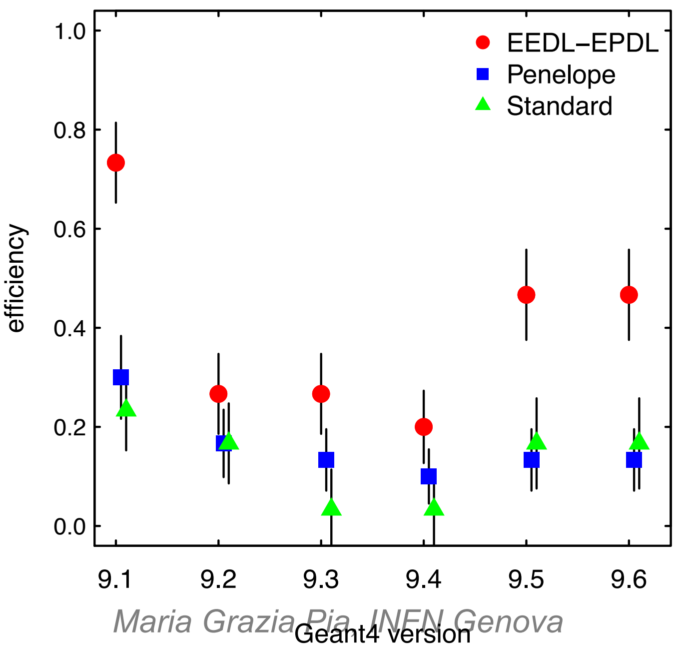
New Geant4 Model and Interface Developments for Improved Space Electron Transport Simulations: First results

John Allison, Juan Cueto, Vladimir Grichine, Alexander Howard, Sergio Ibarmia, Vladimir Ivanchenko, Michel Maire, Giovanni Santin and Laszlo Urban



Negative improvements





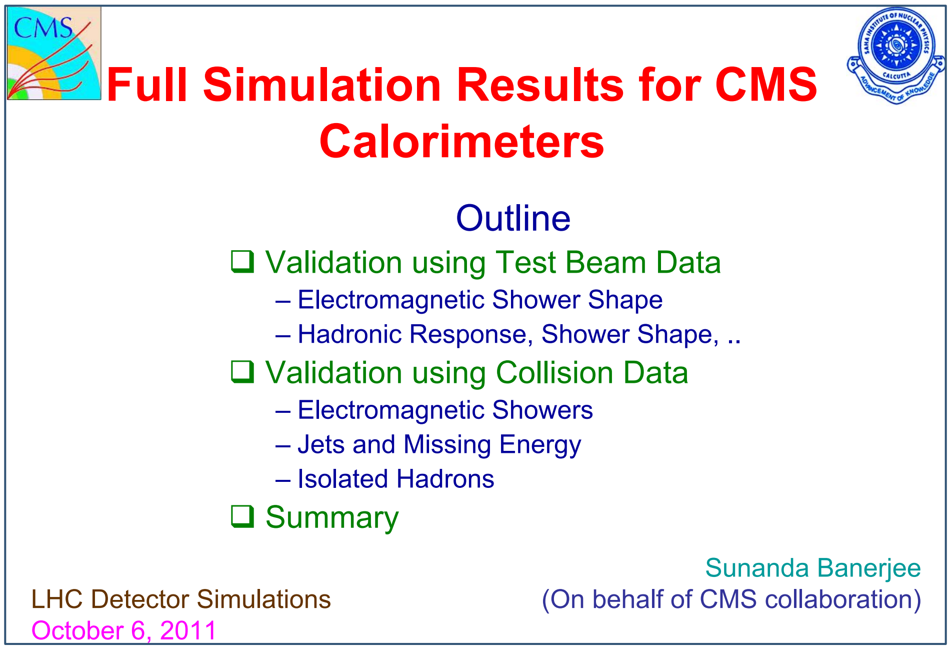
2934 IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 60, NO. 4, AUGUST 2013

Validation of Geant4 Simulation of Electron Energy Deposition

Matej Batič, Gabriela Hoff, Maria Grazia Pia, Paolo Saracco, and Georg Weidenspointner

Target	Z	E (kev)	angle (degrees)	Geant4 version 9.1	9.2	9.3	9.4	9.5	9.6
Be	4	58	0	0.071	0.014	0.124	0.311	0.149	0.156
Be	4	109	0	0.021	< 0.001	< 0.001	< 0.001	0.015	0.013
Be	4	314	0	0.015	0.764	< 0.001	< 0.001	0.013	0.014
Be	4	521	0	0.092	0.967	< 0.001	< 0.001	0.832	0.793
Be	4	1033	0	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
C	6	1000	0	0.917	0.994	< 0.001	< 0.001	0.290	0.346
Al	13	314	0	0.182	< 0.001	< 0.001	< 0.001	0.004	0.007
Al	13	521	0	0.574	< 0.001	< 0.001	< 0.001	0.091	0.089
Al	13	1033	0	0.484	0.123	< 0.001	< 0.001	< 0.001	< 0.001
Al	13	314	60	0.396	0.596	< 0.001	< 0.001	0.001	0.002
Al	13	521	60	0.137	0.011	0.001	< 0.001	0.056	0.086
Al	13	1033	60	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
Fe	26	300	0	0.832	< 0.001	0.351	0.741	0.787	0.742
Fe	26	500	0	0.055	< 0.001	0.314	0.003	0.814	0.808
Fe	26	1000	0	< 0.001	< 0.001	0.169	0.003	< 0.001	< 0.001
Cu	29	300	0	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
Cu	29	500	0	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
Mo	42	100	0	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
Mo	42	300	0	0.062	< 0.001	0.001	< 0.001	0.008	0.002
Mo	42	500	0	0.020	< 0.001	< 0.001	0.001	0.128	0.115
Mo	42	1000	0	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
Mo	42	300	60	0.023	0.002	0.049	0.043	0.029	0.022
Mo	42	500	60	0.022	< 0.001	0.011	0.006	0.003	0.007
Mo	42	1000	60	0.037	< 0.001	0.010	0.028	0.001	0.002
Ta	73	300	0	0.043	0.511	0.242	0.272	0.364	0.294
Ta	73	500	0	0.025	0.003	< 0.001	< 0.001	0.012	0.019
Ta	73	1000	0	0.030	< 0.001	< 0.001	< 0.001	0.002	0.001
Ta	73	500	60	0.011	0.003	0.040	0.042	0.010	0.007
Ta	73	1000	60	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
Ta	73	500	30	0.034	0.005	0.004	0.006	0.020	0.017

CMS simulation



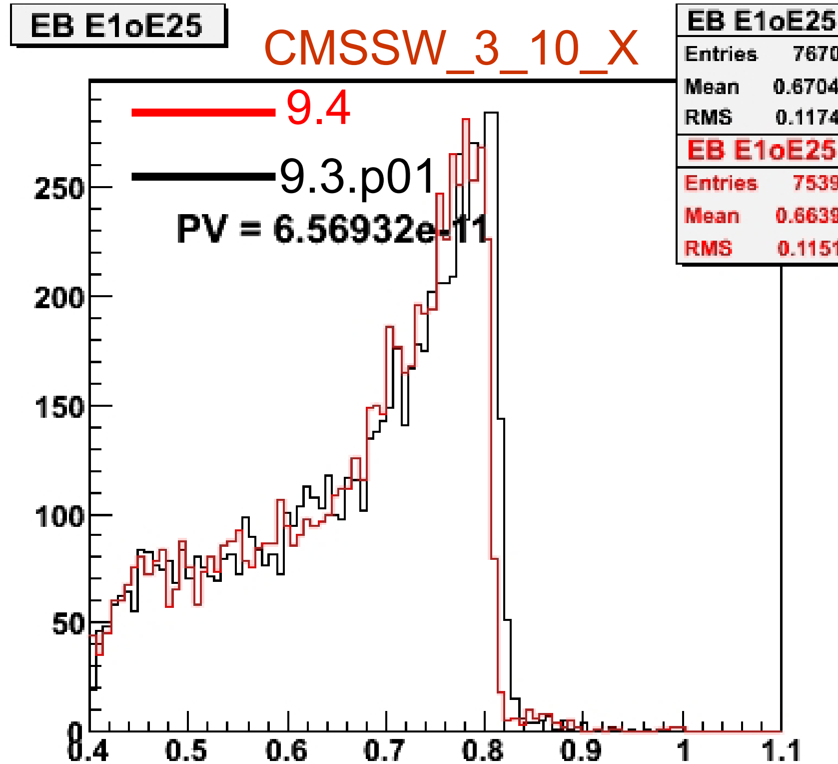
Full Simulation Results for CMS Calorimeters

Outline

- Validation using Test Beam Data
  - Electromagnetic Shower Shape
  - Hadronic Response, Shower Shape, ..
- Validation using Collision Data
  - Electromagnetic Showers
  - Jets and Missing Energy
  - Isolated Hadrons
- Summary

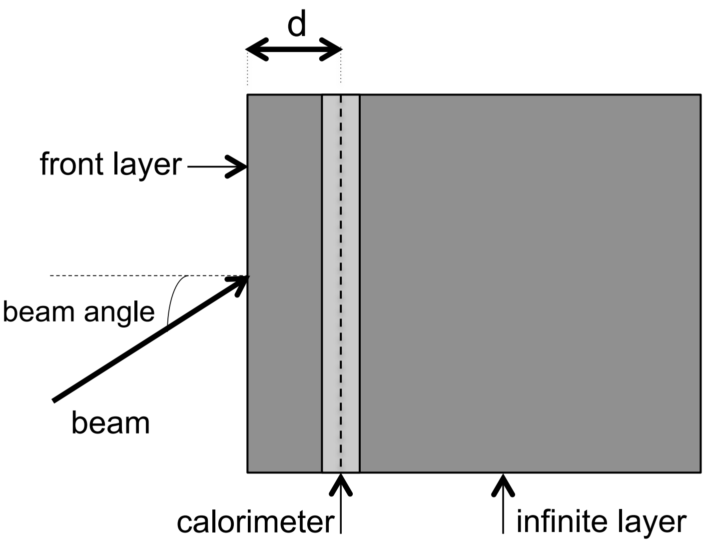
Sunanda Banerjee
(On behalf of CMS collaboration)

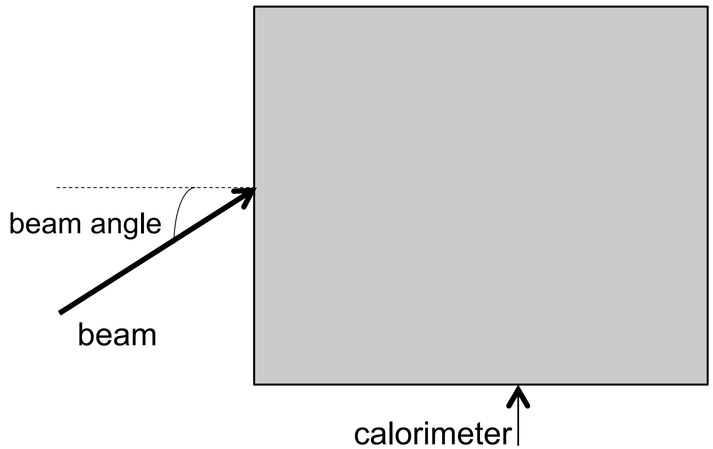
LHC Detector Simulations
October 6, 2011

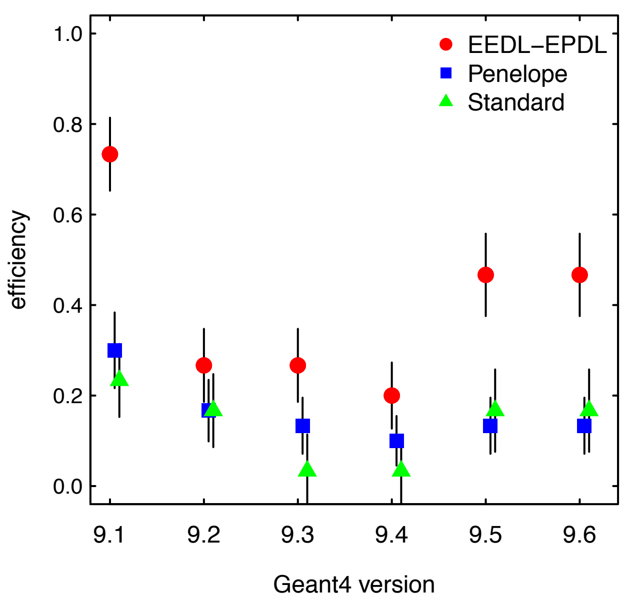


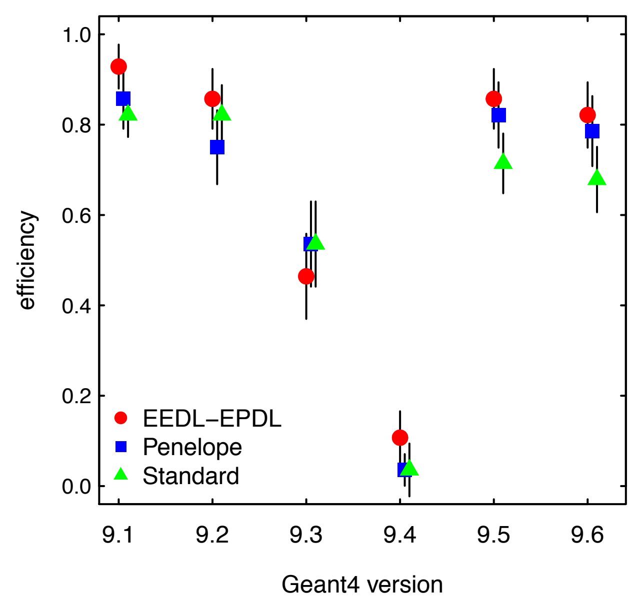
- The lateral shower profile for photons (and $e^{\pm}$) is changing with the Geant4 version from 9.3.p01 to 9.4 to 9.4.p02. This is not yet understood and we need some help to get some of the key distributions agreeing better with the data.

What is bad may be good









IEEE Standard 1012

validation: (A) [...] **(B)** The process of providing evidence that the system, software, or hardware and its associated products satisfy requirements allocated to it at the end of each life cycle activity, solve the right problem (e.g., correctly model physical laws, implement business rules, and use the proper system assumptions), and **satisfy intended use and user needs**.

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Hadronic physics validation

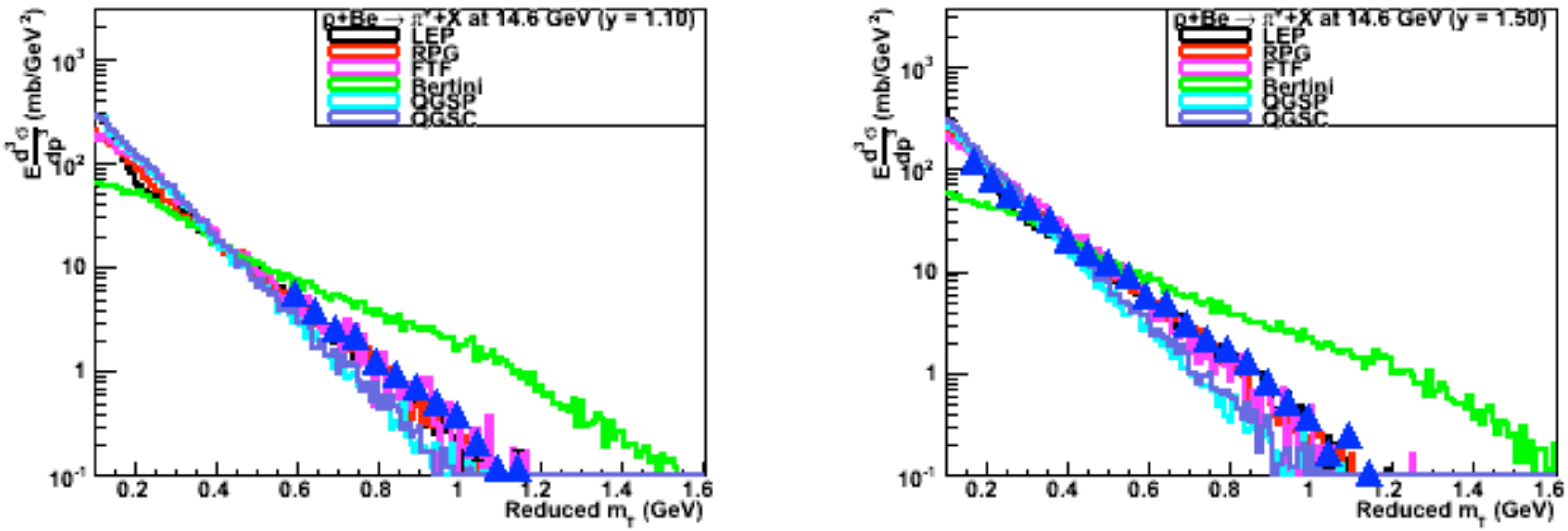
15 years' activity

Validation database at FNAL (http://g4validation.fnal.gov:8080/G4ValidationWebApp/index.jsp), LCG Simulation Validation Project, Geant4 Collaboration's Validation Task Force…

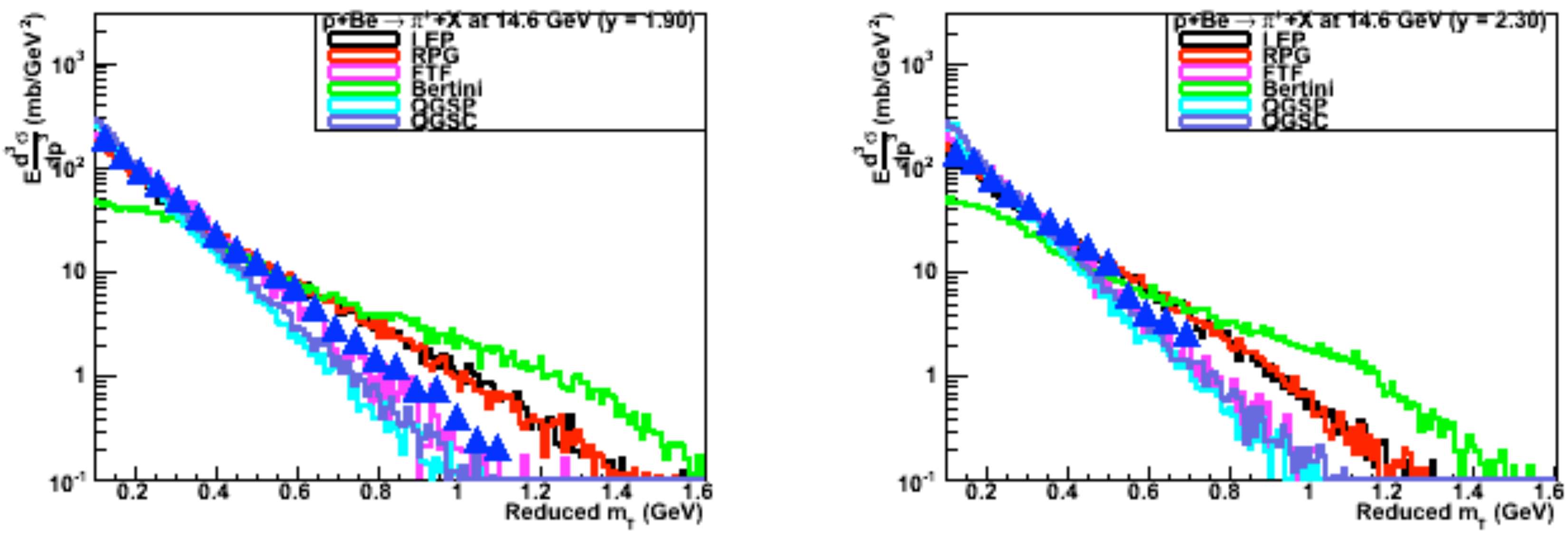
List of Tests		
Name	**Description**	**Working Group**
ATLAS	shower characteristics of ATLAS Calorimeters	LHC-feedback
CMS	shower characteristics of CMS Calorimeters	LHC-feedback
HadrIon	Test of Physics Lists (thick targets, ion beams)	hadronic
HadrXS	Test of Physics Lists (cross sections)	hadronic
Hadrcap	is an analogous to Hadr00, with advanced features.	hadronic
IAEA	IAEA Benchmark of Nuclear Spallation Models	hadronic
Ndata	Test concerning developments of new nXS, it is calling HP XS as well as HPW XS.	hadronic
Testfragm	Test of hadronic generators (thin targets, ion beams)	hadronic
atlasbar	Test of ALTAS barrel type em calorimeter, determines response, resolution, and CPU performance	electromagnetic
placeholder	Dummy testdes	hadronic
simplifiedCalo	Test of Shower shapes using selected simplified calorimeter setups.	hadronic
test19	High energy test, provides comparison with NA61 (31 GeV/c proton beam) and NA49 (158 GeV/c proton beam) data sets.	hadronic
test22	Testing of the FTF model and comparison with experimental data for a wide energy region	hadronic
test30	Test of hadronic generators of inelastic processes	hadronic
test35	Test of hadronic generators of inelastic processes, based on results of HARP collaboration, Experiment PS214 at CERN.	hadronic
test37	Test against Sandia data, electron beam in semi-infinite media.	electromagnetic
test41	Comparison with MUSCAT experiment for multiple scattering validation	electromagnetic
test45	Test of hadronic generators of inelastic processes on thick targets.	hadronic
test47	Intermediate energy validation is done by comparing Monte Carlo predictions vs experimental data.	hadronic
test48	Stopping particle test Monte Carlo predictions are compared to experimental data.	hadronic
test75	Test of gamma-nuclear interactions	hadronic

A sample of results, impossible to show all!

Inclusive pi+ production in 14.6 GeV/c p-Be interactions

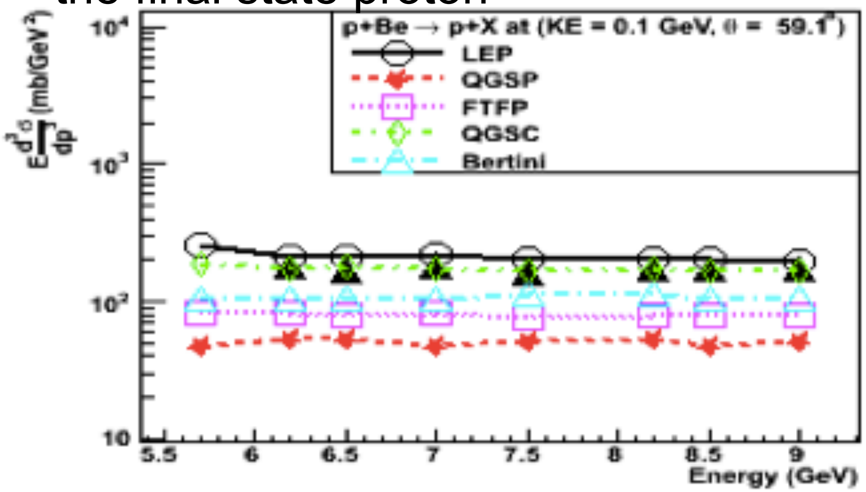


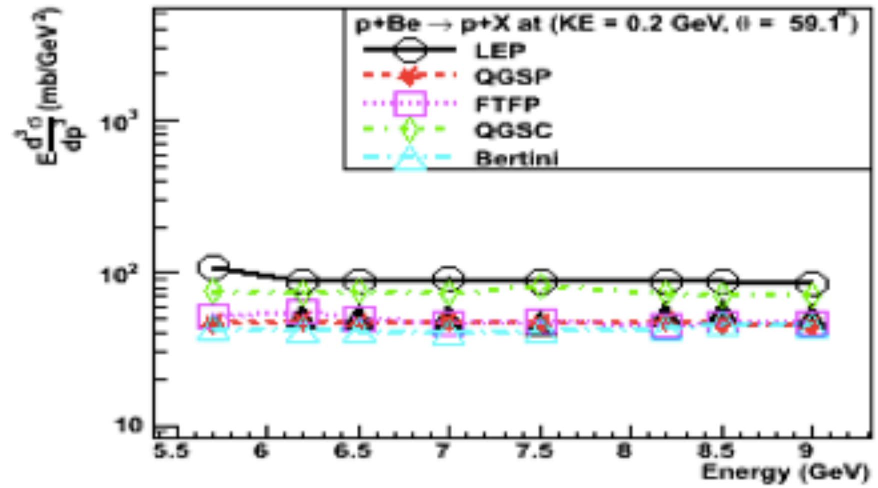
http://geant4.cern.ch/results/validation_plots/thin_target/hadronic/medium_energy/test_bnl_802/bnl_data.shtml



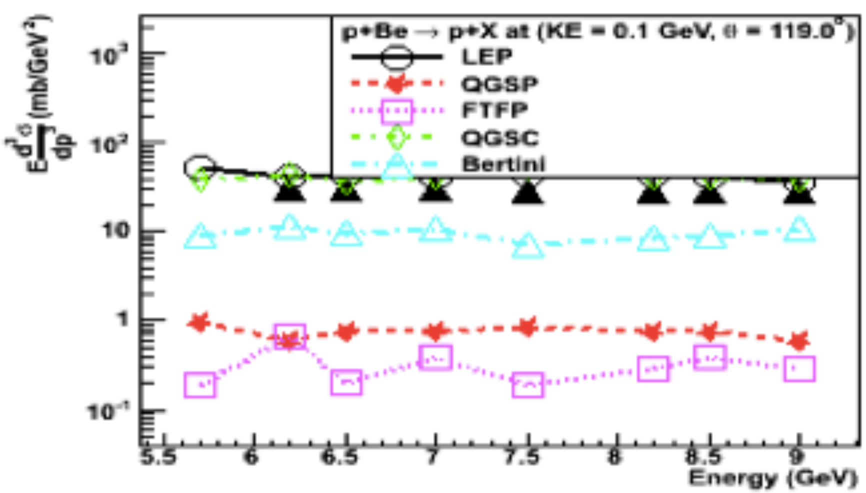
Inclusive proton production

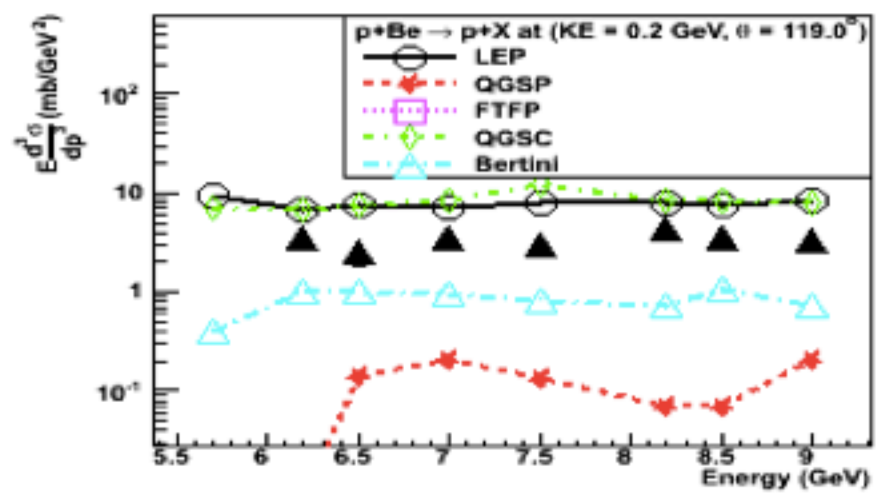
Differential cross-section of the inclusive proton production in proton-Be interactions as a function of beam energy, in 2 kinetic energy bins and for 2 different angles of the final state proton





Geant4 9.0.p01

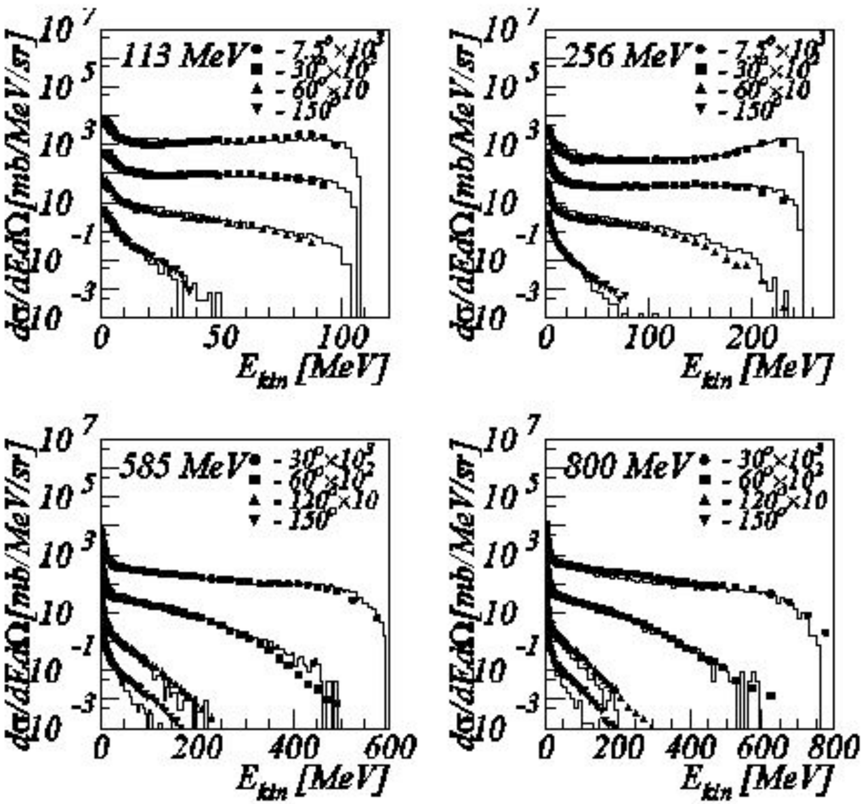




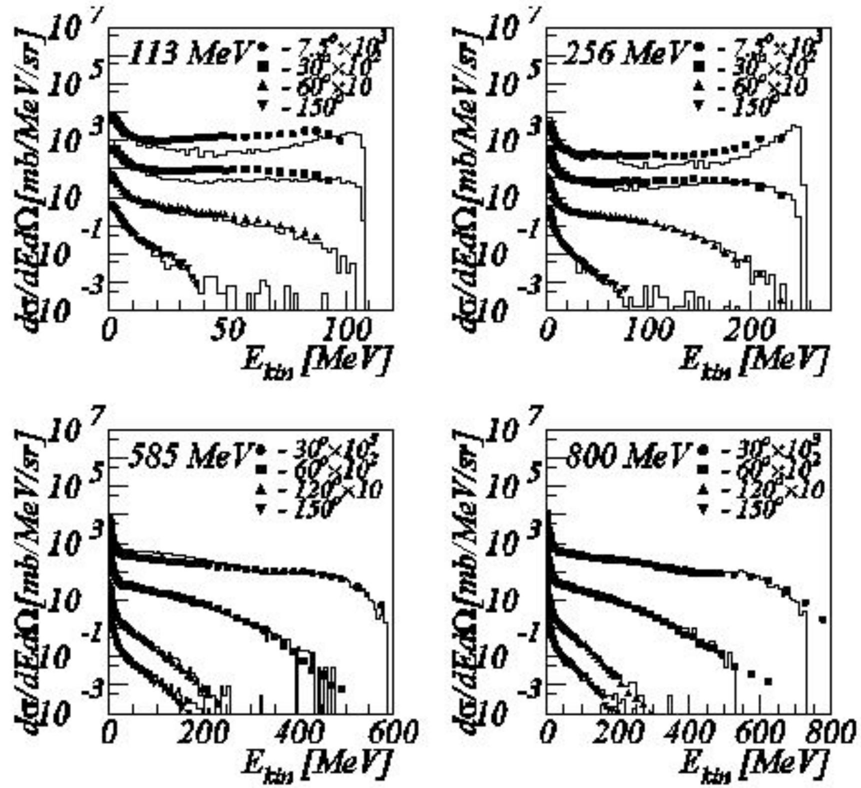
A sample of results

Impossible to show all!

Al(p,n) Binary cascade



Al(p,n) Bertini cascade

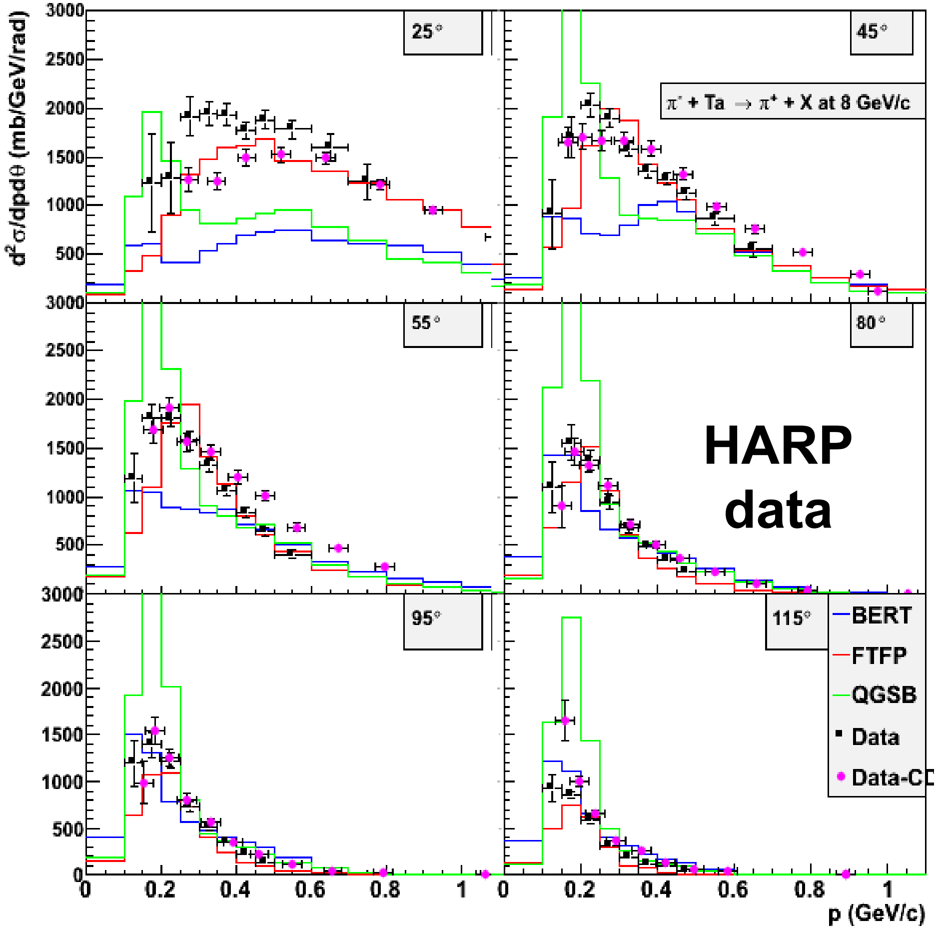


What does one evince from these plots?

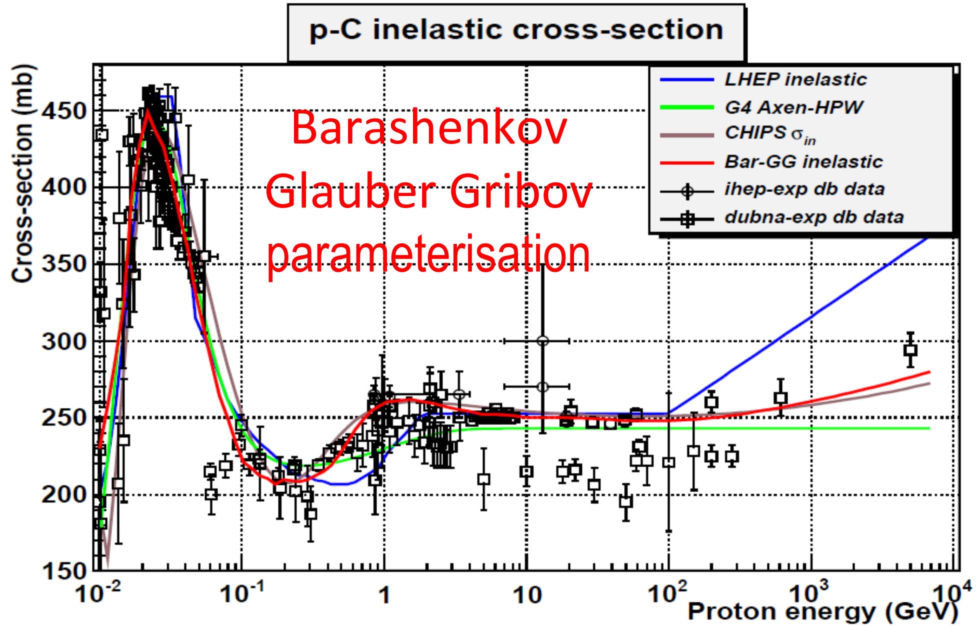
Quantification? Meta-analysis? Changes in the code?

Recent developments

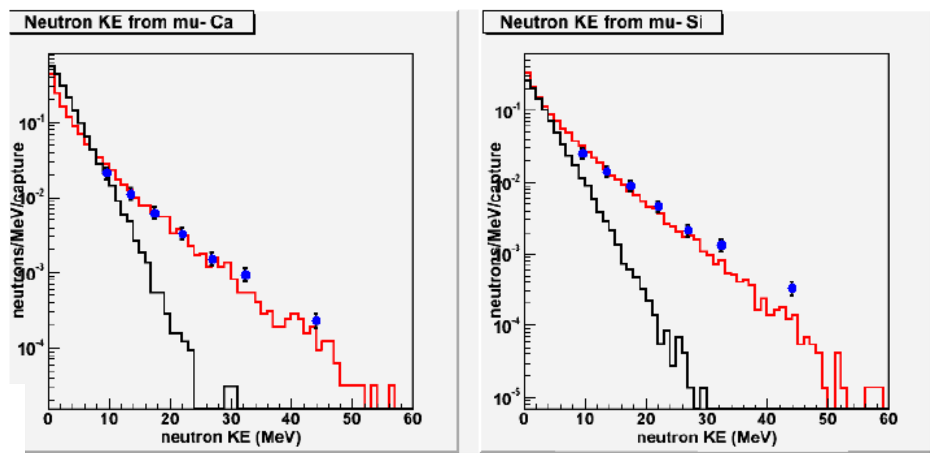
G. Folger et al.,
IEEE NSS 2013



Evolutions in Bertini cascade



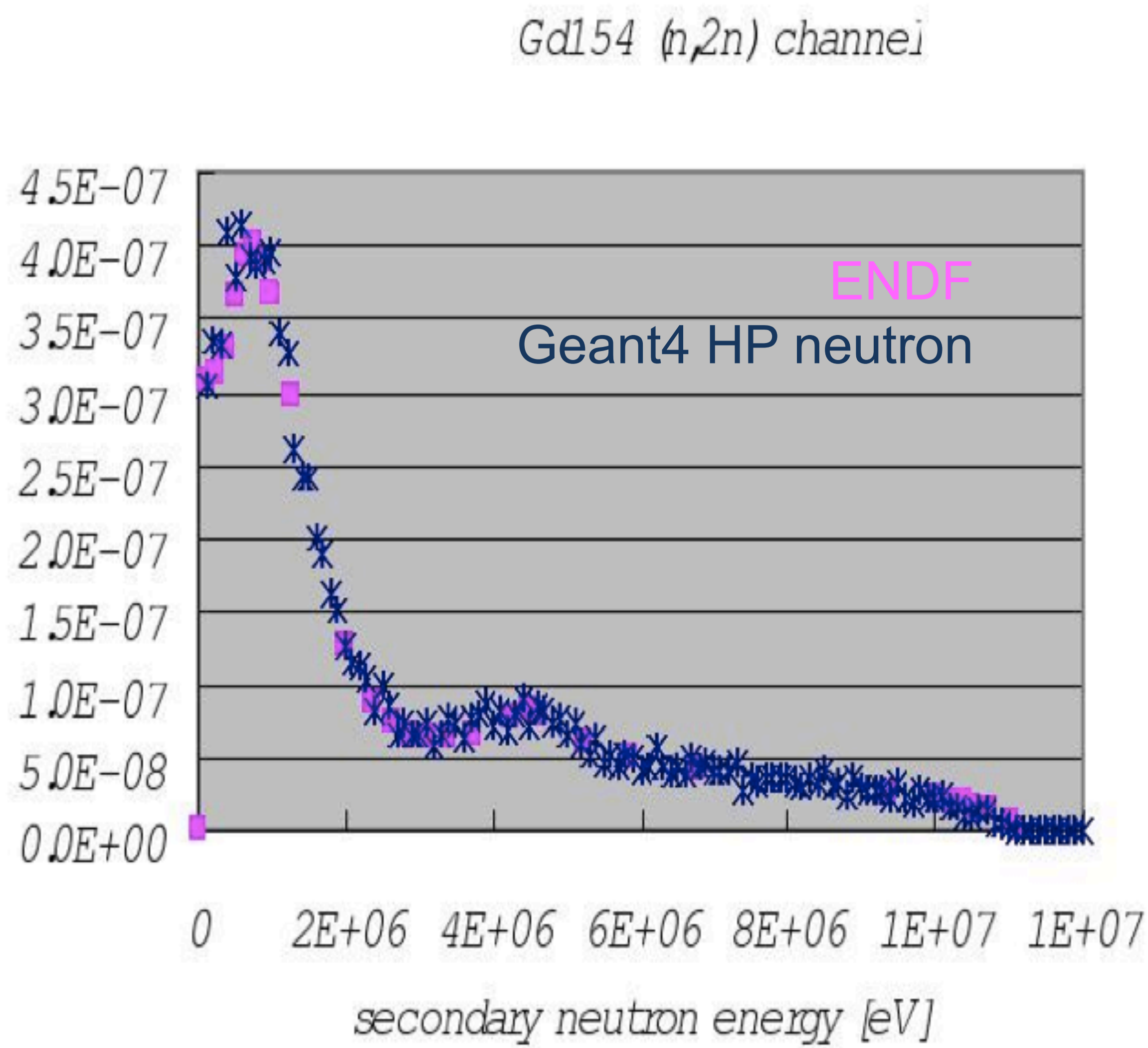
Evolutions in cross sections



HP neutrons

Reference: ENDF/B-VI Release 8, Tape162

Geant4 version: 8.1



Data-driven model

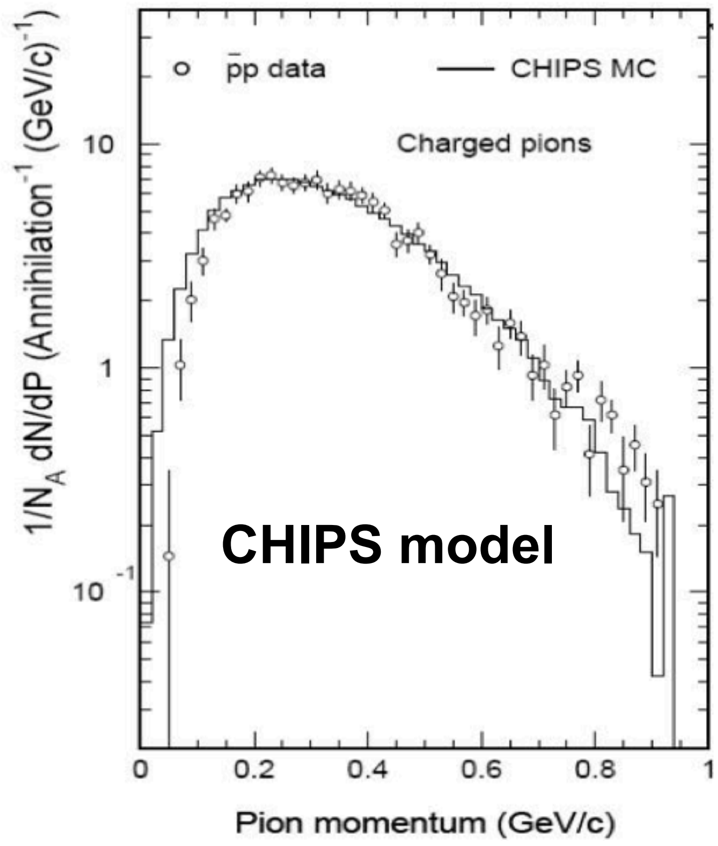
The model is as good as the data on which it is based

Systematics of evaluated data compilations

Stopped particles

antiprotons stopping in H: **charged pion production**

Geant4 **CHIPS model** deleted in Geant4 10.0 version



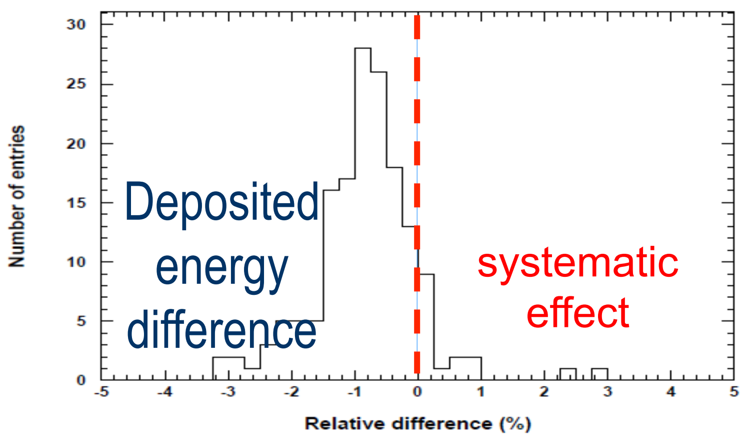
Can we quantify our ignorance?

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

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



Geant4 Precompound model activated through **Binary Cascade** w.r.t. standalone Precompound model

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

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

No generally accepted method of measuring epistemic uncertainties

Interval analysis

Dempster-Shafer theory of evidence

Data for software validation

Passive observations of physical events *(e.g. supernovae explosions or the weather)*
Experiments designed to elucidate a general physics principle or law *(e.g. typical HEP experiments)*
Experiments designed to certify a detector *(e.g. test beams)*
Experiments **specifically designed** to **validate a software** system/component

We need a paradigm shift…

- Scientists and funding agencies understand the value of experiments designed
  - to **explore new scientific phenomena**
  - to **test theories**
  - to **examine the performance of design components**
- Few appreciate the value of experiments explicitly conducted for **software validation**
- Gain of consciousness in some fields *(e.g. NASA, military projects)*

Things change…

In 1998, when it was first developed, Geant4 low energy package based on EADL-EEDL-EPDL was an advanced simulation tool

When it was first re-engineered into Geant4, Penelope adopted a different modeling approach w.r.t. using EEDL/EPDL

15 years later…

The state-of-the-art has evolved

Rethink Geant4 low energy electromagnetic domain

geant4/electromagnetic/pii/

Electromagnetic physics revisited

- Wide scope project to assess **quantitatively** the **state-of-the-art** of electromagnetic physics modeling for Monte Carlo particle transport
  - Implementation and evaluation of many physics modeling methods
  - Extension of current Geant4 low energy coverage
  - Comparisons with large experimental data samples of various origin
  - Statistical data analysis

Current status

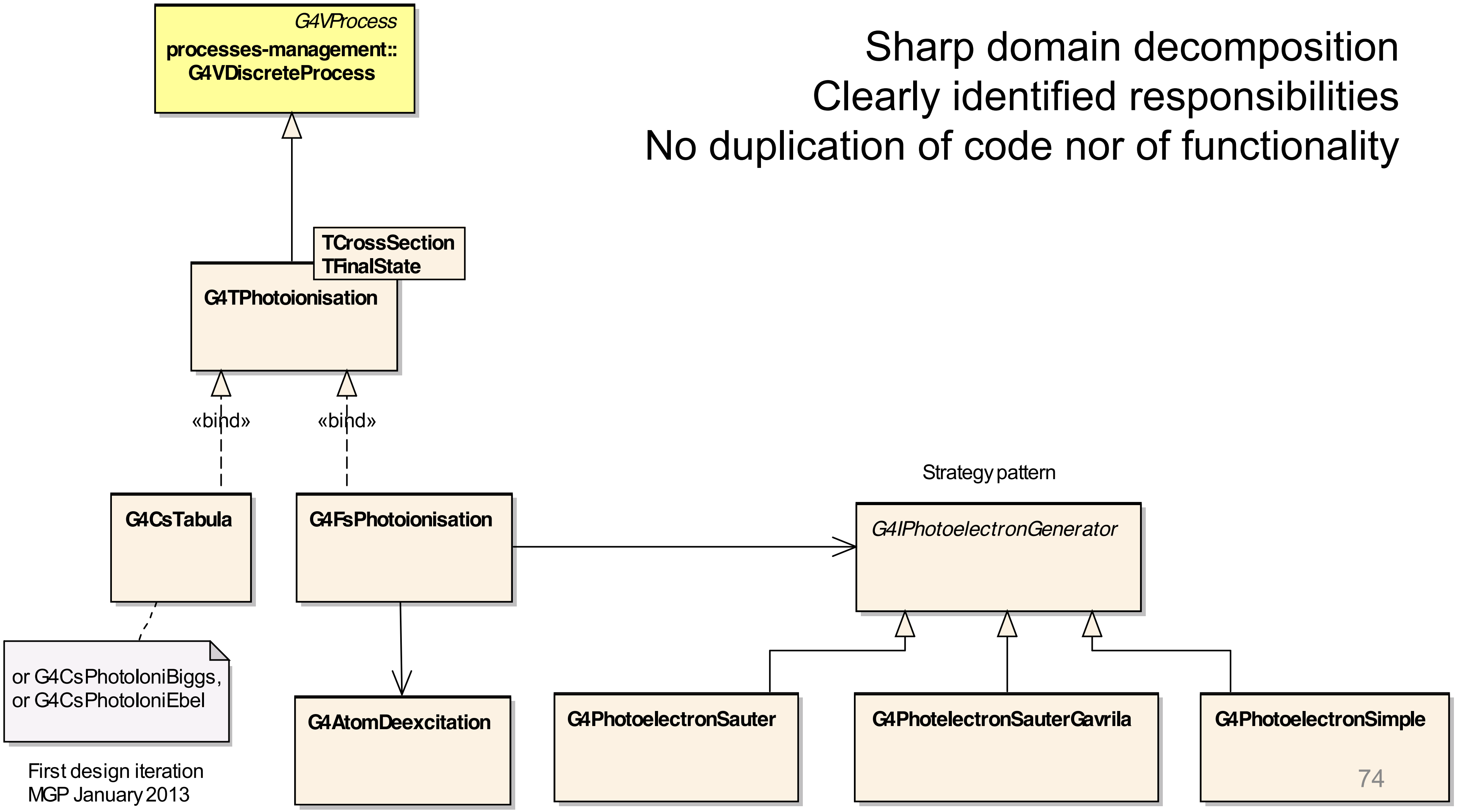
- **Photons**
  - **Elastic scattering**: published
  - **Compton scattering**, **photoionisation**: in progress
  - **Pair production**: early stage
- **Electrons**
  - **Ionisation** at low energies (challenge IPA and isolated atom assumption)
- **Protons**
  - **Ionisation** cross sections, PIXE

…more to come

Sound software process

Streamlined software design consistent with Geant4 kernel

Sharp domain decomposition
Clearly identified responsibilities
No duplication of code nor of functionality

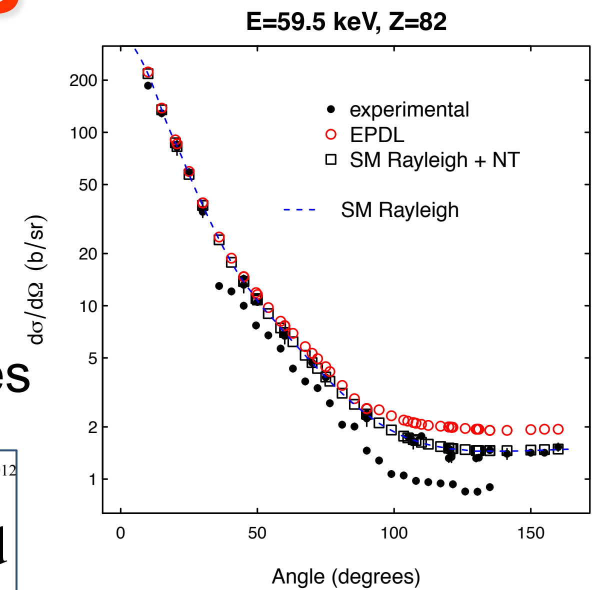


First design iteration
MGP January 2013

Photon elastic scattering

Form factor approximation:
non relativistic, relativistic,
modified + anomalous scattering factors

2nd order S-matrix calculations
recent calculations, not yet used in Monte Carlo codes



1636 IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 59, NO. 4, AUGUST 2012

Photon Elastic Scattering Simulation: Validation and Improvements to Geant4

Matej Batič, Gabriela Hoff, Maria Grazia Pia, and Paolo Saracco

Differential cross sections

	Penelope 2001	Penelope 2008	EPDL	Relativ. FF	Non-Rel. FF	Modified FF	MFF ASF	RFF ASF	SM NT
ε	0.27	0.38	**0.38**	0.25	0.35	0.49	0.52	0.48	**0.77**
error	±0.05	±0.06	±0.06	±0.05	±0.06	±0.06	±0.06	±0.06	±0.05

ε = fraction of test cases compatible with experiment, 0.01 significance

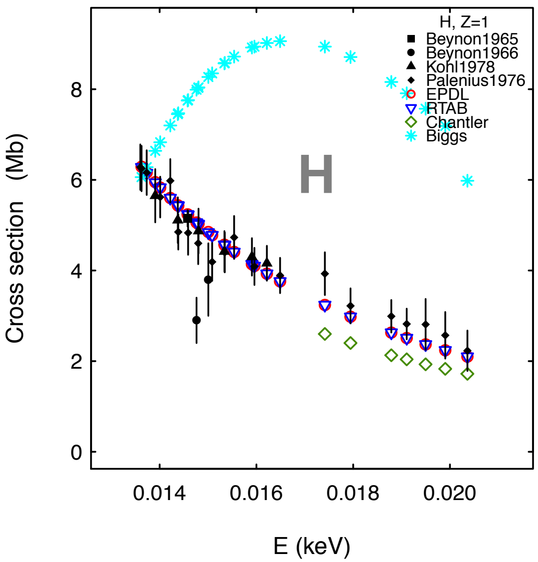
Photoionisation total cross sections

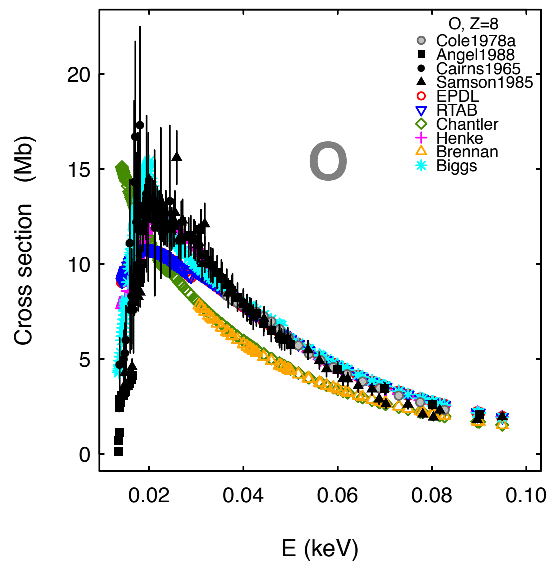
Year	Compilation	Energy	Z	(sub)Shell	Method
1967-1988	**Biggs-Lighthill**	10 eV – 100 GeV	1-100	-	parameterised
1992	**Brennan-Cowan**	30 eV – 700 keV	3-92	-	tabulated
2000	**Chantler**	10 eV – 433 keV	1-92	K	tabulated
2003	**Ebel**	1 keV – 300 keV	1-92	all	parameterised
2002	**Elam**	100 eV – 1 MeV	1-98	-	tabulated
1997	**EPDL97** *(Scofield)*	10 eV – 100 GeV	1-100	all	tabulated
1982-1993	**Henke**	10 eV – 30 keV	1-92	-	tabulated
1970-2006	**McMaster/Shaltout**	1 keV – 700 keV	1-94	-	tabulated
1989	**PHOTX** *(Scofield)*	1 keV – 100 MeV	1-100		tabulated
2001	**RTAB**	10 eV – 30 keV	1-99	all	tabulated
1973	**Scofield**	1 keV – 1.5 MeV	1-100	all	tabulated
1970	**Storm-Israel**	1 keV – 100 GeV	1-100	-	tabulated
1973	**Veigele**	100 eV – 100 MeV	1-94	-	tabulated
1987-2010	**XCOM** *(Scofield)*	1 keV – 100 GeV	1-100	-	tabulated

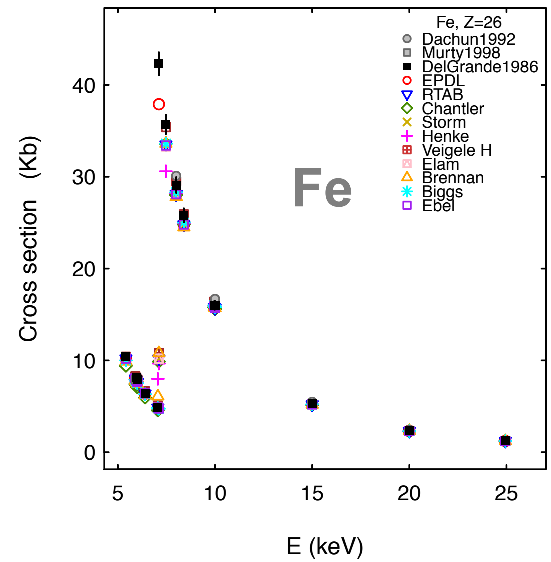
Different methods and calculations

e.g. Chantler's exchange potential in his DHF calculation is different from Scofield's

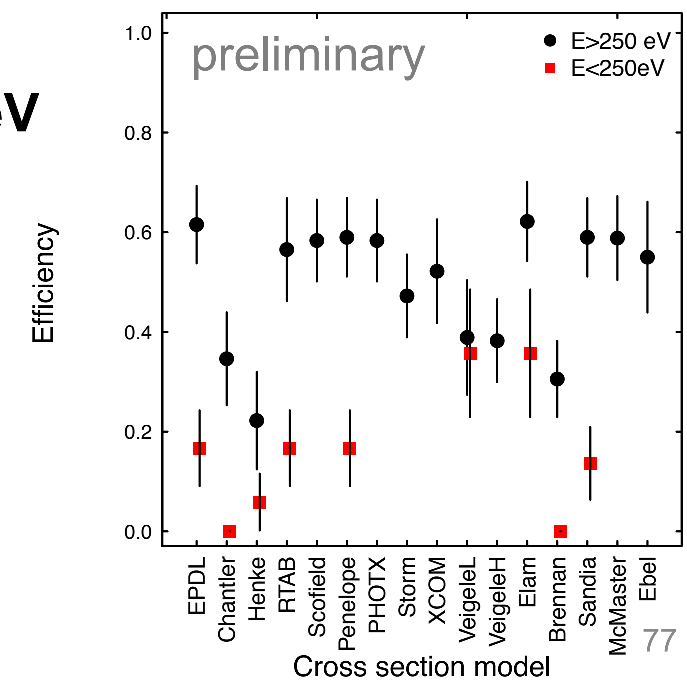
Total photoionisation cross sections







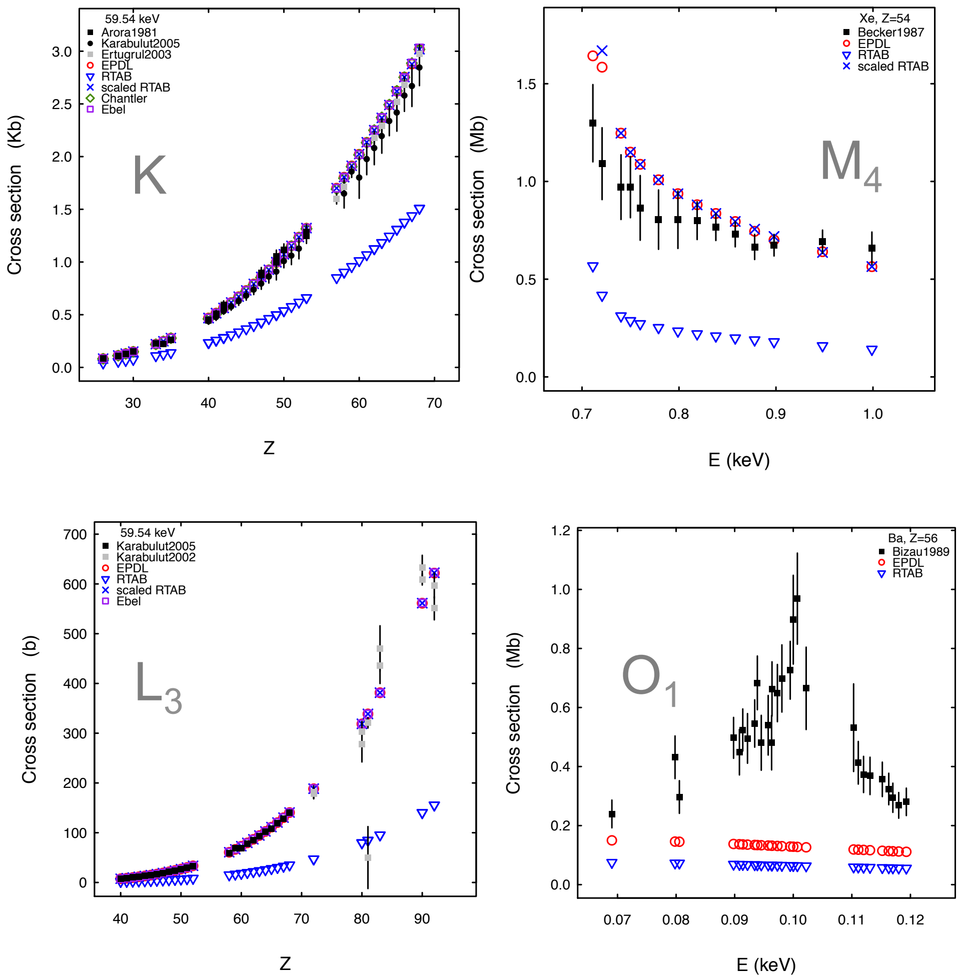
- Most calculation methods exhibit similar compatibility with experiment for **E >250 eV**
  - *Chantler, Brennan-Cowan look worse*
- Degraded accuracy below ~250 eV



Analysis of contingency tables

	EPDL Chantler	EPDL Brennan-Cowan
Fisher	0.044	0.011
Pearson χ^2	0.033	0.007
Barnard	0.035	0.007

Shell cross sections



Calculated **inner shell** cross sections compatible with experiment

Outer shell cross sections inconsistent with experimental data

Beware: small data sample, limited experimental sources

p-value χ^2 test

shell	EPDL	Chantler	RTAB	scRTAB	Ebel
K	0.209	0.350	<0.001	0.315	<0.001
L1	0.075		<0.001	0.069	0.964
L2	0.339		<0.001	0.299	0.154
L3	1		<0.001	1	1
M1	<0.001		<0.001	<0.001	
M4	0.031		<0.001	<0.001	
M5	<0.001		<0.001	<0.001	
N1	<0.001		<0.001	<0.001	
N6	<0.001		<0.001	<0.001	<0.001
N7	<0.001		<0.001	<0.001	<0.001
O1	<0.001		<0.001	<0.001	<0.001
O2	<0.001		<0.001	<0.001	<0.001
O3	<0.001		<0.001	<0.001	<0.001
P1	<0.001		<0.001	<0.001	<0.001

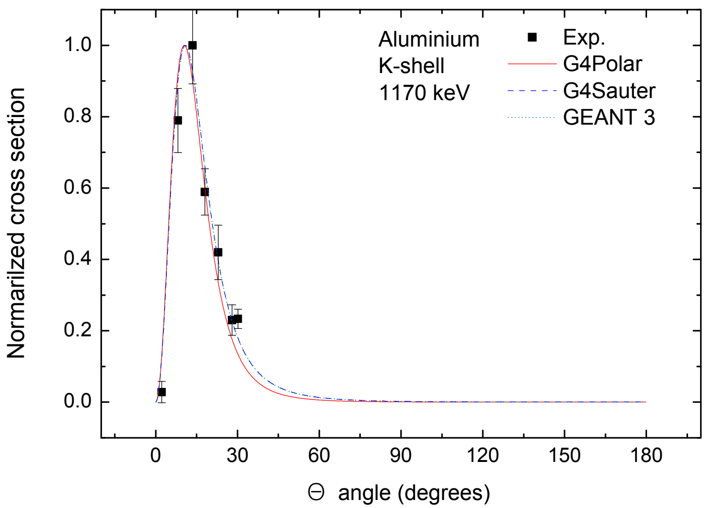
Systematic effect observed with RTAB shell cross sections

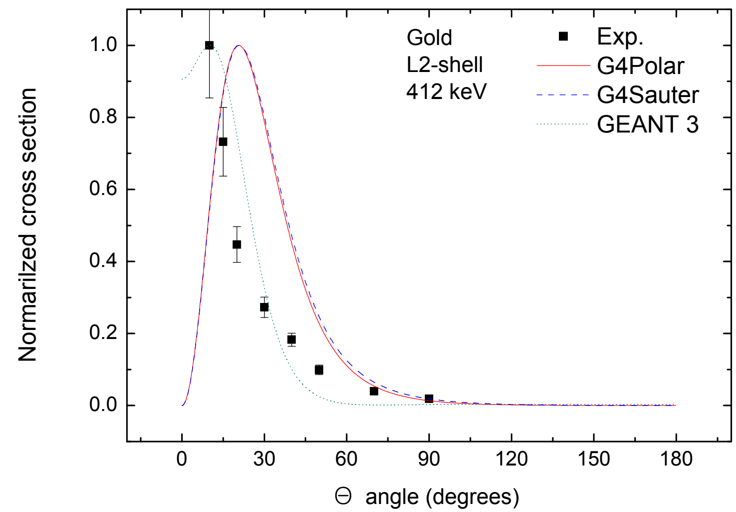
(presumably a missing factor in the calculation)

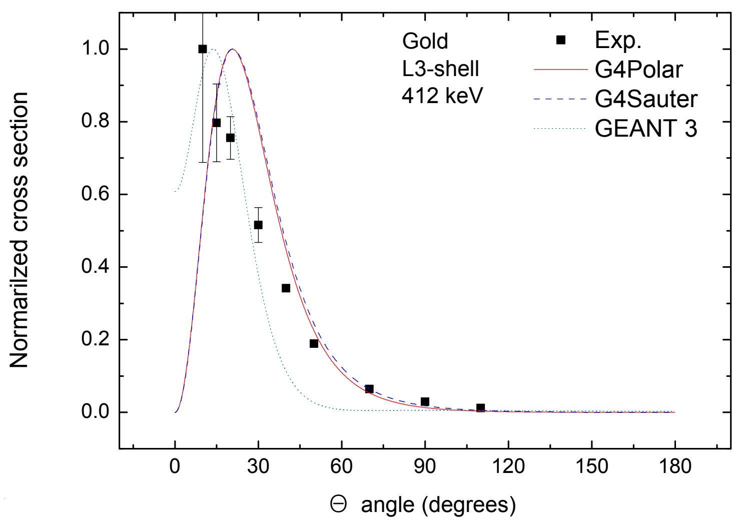
Photoelectron angular distribution

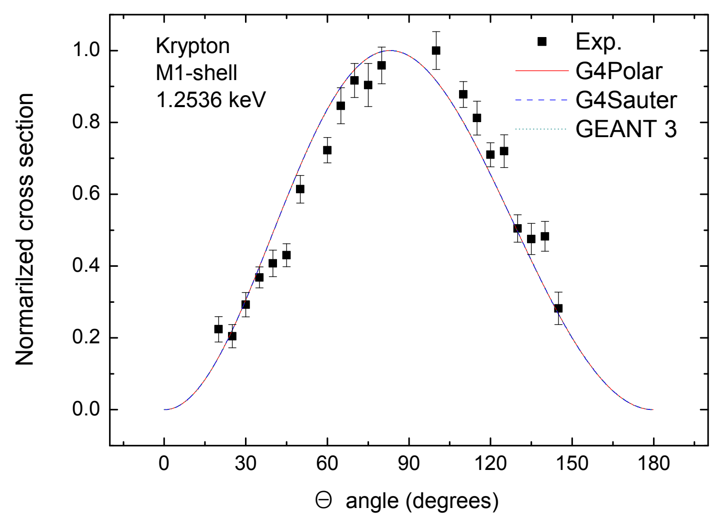
Qualitative appraisal
Limited experimental sample
Experimental systematic effects
(corrected/uncorrected data)

Option à la **GEANT 3** (Sauter) evaluated along with other Geant4 options









Differential Compton scattering cross section

$$\left[\frac{d\sigma}{d\Omega}\right]_{inc} = \left[\frac{d\sigma}{d\Omega}\right]_{KN} S(x, Z)$$

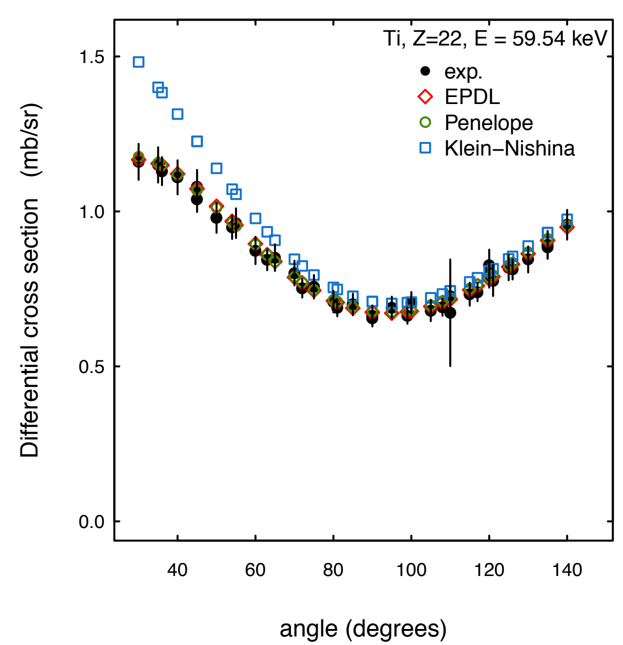
>2300 experimental data

Work in progress!

Scattering functions	Efficiency	Error
EPDL	0.82	0.02
Penelope	0.82	0.02
Klein-Nishina	0.54	0.03
Brusa	0.84	0.02
BrusaF	0.84	0.02
PenBrusa	0.84	0.02
PenBrusaF	0.84	0.02
Biggs	0.84	0.02
BiggsF	0.85	0.02
Hubbell	0.82	0.02
Kahane	0.72	0.02

Geant4 lowenergy

Geant4 standard



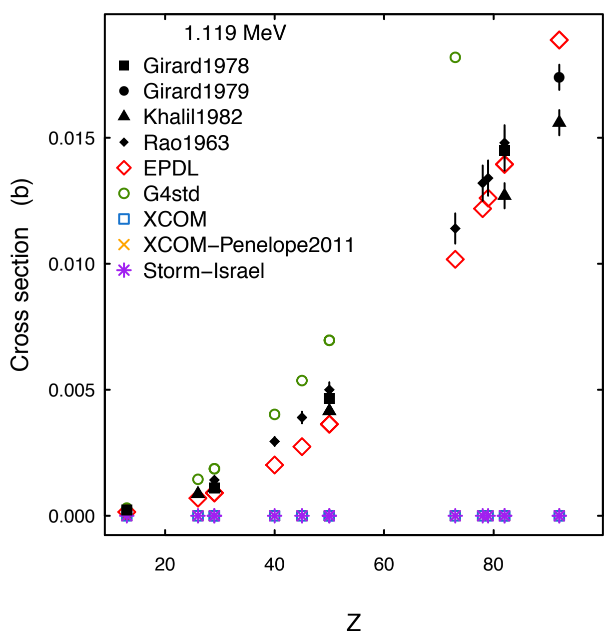
e^+e^- pair production

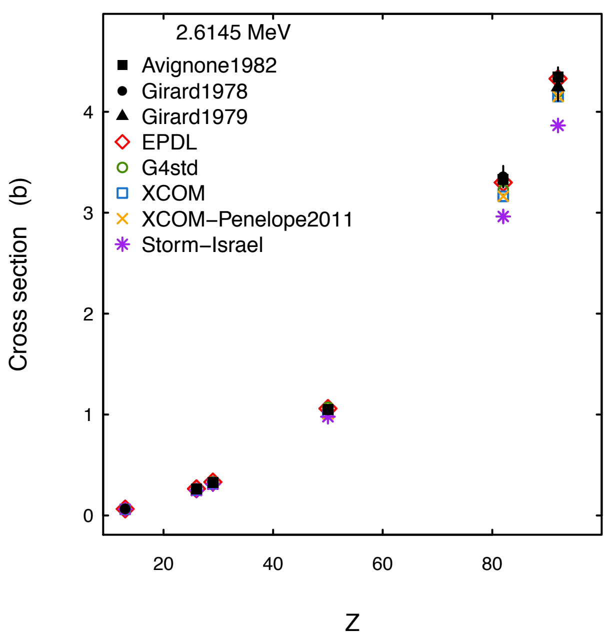
Work in progress!

- Total cross section: Bethe-Heitler with corrections *(Hubbell, Gimm, Overbo)*
- First tests near threshold

	Geant4 standard	EPDL	XCOM
p-value	<0.001	0.982	<0.001

E>1.119 MeV





Validation at high energy in progress

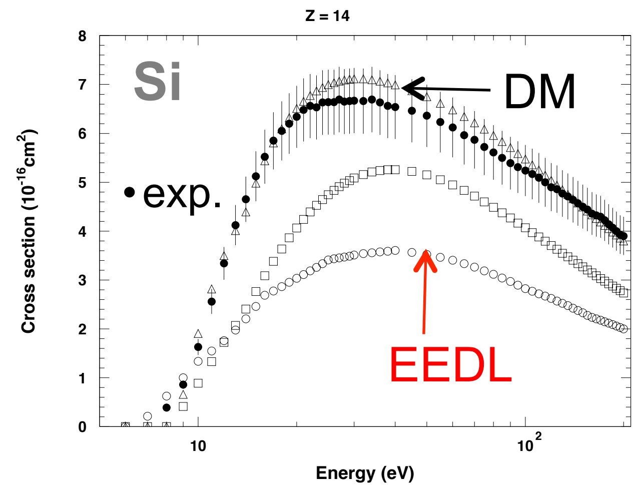
Electron impact ionisation

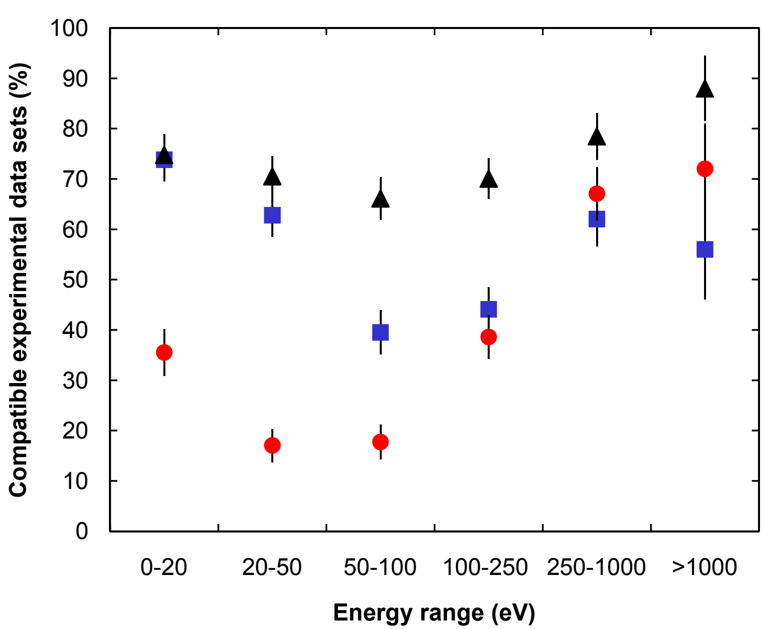
Best Student Award
Monte Carlo 2010

Extension down to ~tens eV for **atoms**
(BEB also applicable to molecules)
Validated over 181 experimental data samples, 57 elements

- **EEDL** *currently in Geant4 low energy package*
- Binary-Encounter-Bethe **BEB**
- Deutsch-Märk **DM**

} **new models**






IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 58, NO. 6, DECEMBER 2011 3219

Ionization Cross Sections for Low Energy Electron Transport

Hee Seo, Maria Grazia Pia, Paolo Saracco, and Chan Hyeong Kim

2013: inner shell ionisation cross sections
New models + validation
Paper in preparation

Proton impact ionisation

K, L, M shells

36 pages

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

PIXE Simulation With Geant4

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

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 58, NO. 6, DECEMBER 2011

Validation of Proton Ionization Cross Section Generators for Monte Carlo Particle Transport

Matej Batič, Maria Grazia Pia, and Paolo Saracco

SUMMARY OF χ^2 TEST RESULTS OF L SUBSHELL IONIZATION CROSS SECTIONS BY PROTON IMPACT

		ISICS 2011 ECPSSR	ISICS 2011 ECPSSR-UA	ERCS08 Default	LIO Default
L_1	Elements	28	28	28	28
	Pass	19	19	18	19
	Fail	9	9	10	9
	Efficiency	0.53±0.09	0.53±0.09	0.48±0.09	0.50±0.09
L_2	Elements	28	28	28	28
	Pass	19	22	20	18
	Fail	9	6	8	10
	Efficiency	0.68±0.09	0.79±0.08	0.71±0.09	0.64±0.09
L_3	Elements	28	28	28	28
	Pass	25	25	26	21
	Fail	3	3	2	7
	Efficiency	0.89±0.06	0.89±0.06	0.93±0.05	0.75±0.08
L	Elements	84	84	84	84
	Pass	63	66	64	58
	Fail	21	18	20	26
	Efficiency	0.75±0.05	0.79±0.04	0.76±0.59	0.69±0.05

Theoretical and **empirical** models for proton ionisation cross sections

PWBA, **ECPSSR** (in various flavours), **Paul-Sacher**, **Kahoul**, **Miyagawa**, **Orlic**, **Sow**

SUMMARY OF THE χ^2 TEST RESULTS OF K SHELL IONIZATION CROSS SECTIONS BY PROTON IMPACT

	ISICS 2011 ECPSSR	ISICS 2011 ECPSSR-HS	ISICS 2011 ECPSSR-UA	ISICS 2011 ECPSSR-HE	ISICS 2011 ECPSSR-HS-UA	ERCS08 Default	KIO Default
Tested elements	66	66	66	66	66	66	66
Pass	44	51	44	46	51	51	47
Fail	22	15	22	20	15	15	19
Efficiency	0.67±0.06	0.77±0.05	0.67±0.06	0.70±0.06	0.77±0.05	0.77±0.05	0.71±0.06

Proton ionisation + Atomic relaxation = PIXE

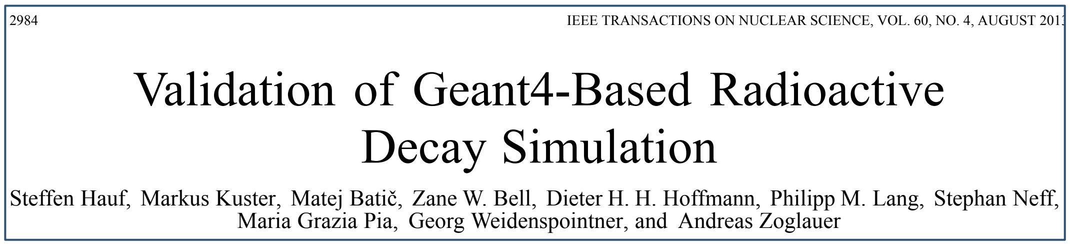
Conceptual challenge for condensed transport!

Radioactive decay


2966 IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 60, NO. 4, AUGUST 2013

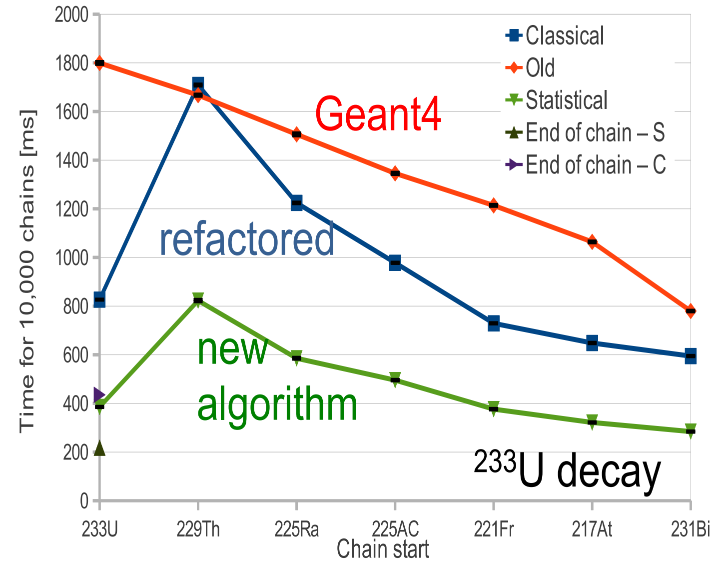
Radioactive Decays in Geant4

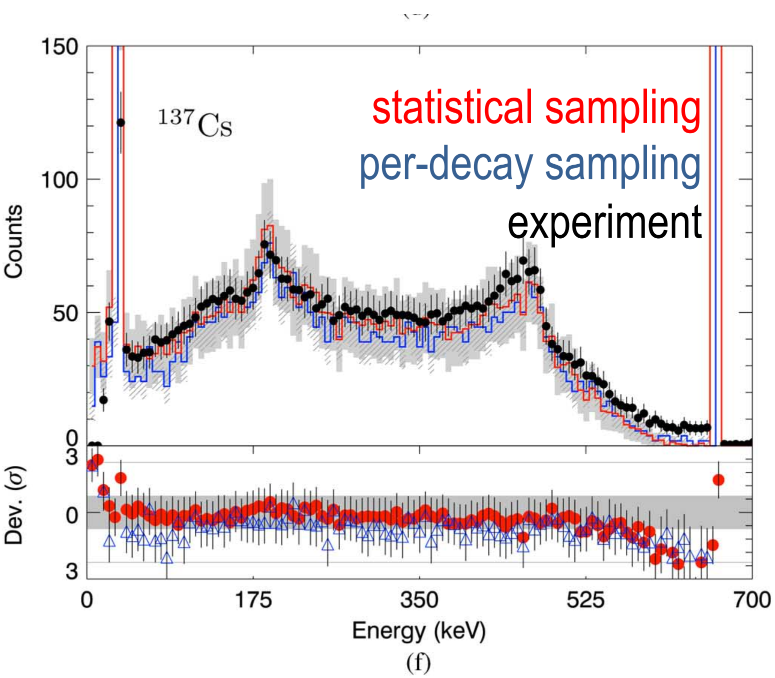
Steffen Hauf, Markus Kuster, Matej Batič, Zane W. Bell, Dieter H. H. Hoffmann, Philipp M. Lang, Stephan Neff, Maria Grazia Pia, Georg Weidenspointner, and Andreas Zoglauer

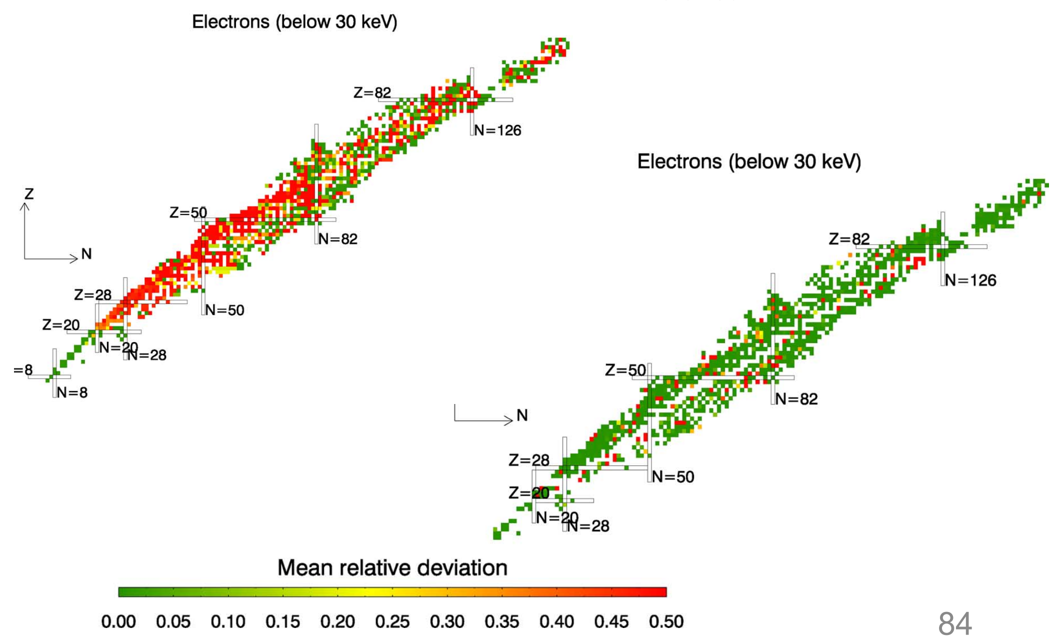

2984 IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 60, NO. 4, AUGUST 201

Validation of Geant4-Based Radioactive Decay Simulation

Steffen Hauf, Markus Kuster, Matej Batič, Zane W. Bell, Dieter H. H. Hoffmann, Philipp M. Lang, Stephan Neff, Maria Grazia Pia, Georg Weidenspointner, and Andreas Zoglauer







This is only the first step…

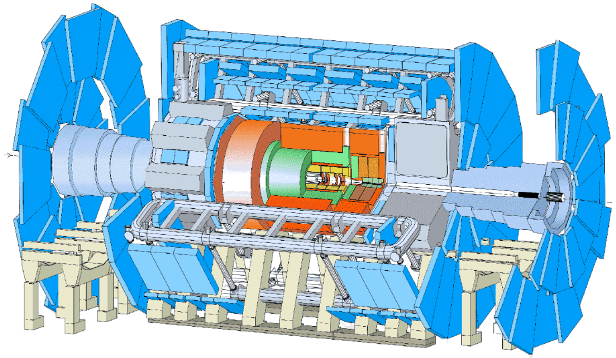
- Deployment: make it usable
  - Integration testing
  - Examples
  - Web documentation
  - etc.
- Lessons learned
  - Interplay with change management
- Make, release and maintain new data libraries

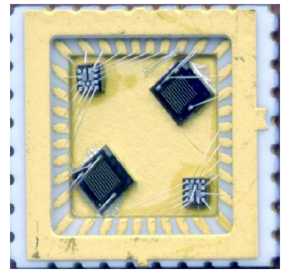
- Charged particles
- Condensed transport

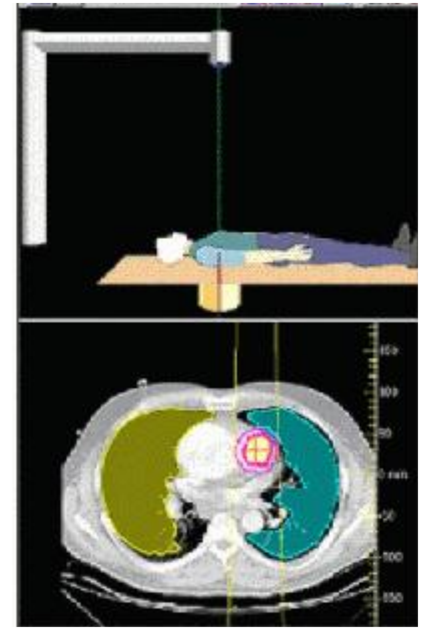
etc.

Challenges

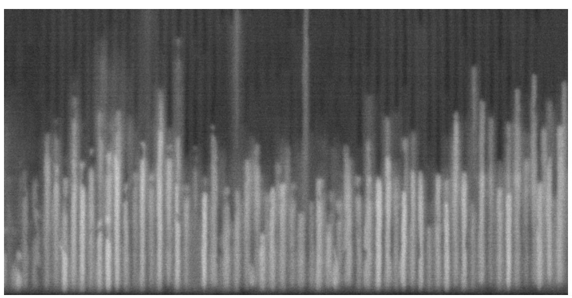
Condensed and discrete transport







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



How does one relate dosimetry to radiation biology?

And what about nanotechnology-based detectors for HEP?

And tracking in a gaseous detector?
And plasma facing material in a fusion reactor?

IPA and IA assumption

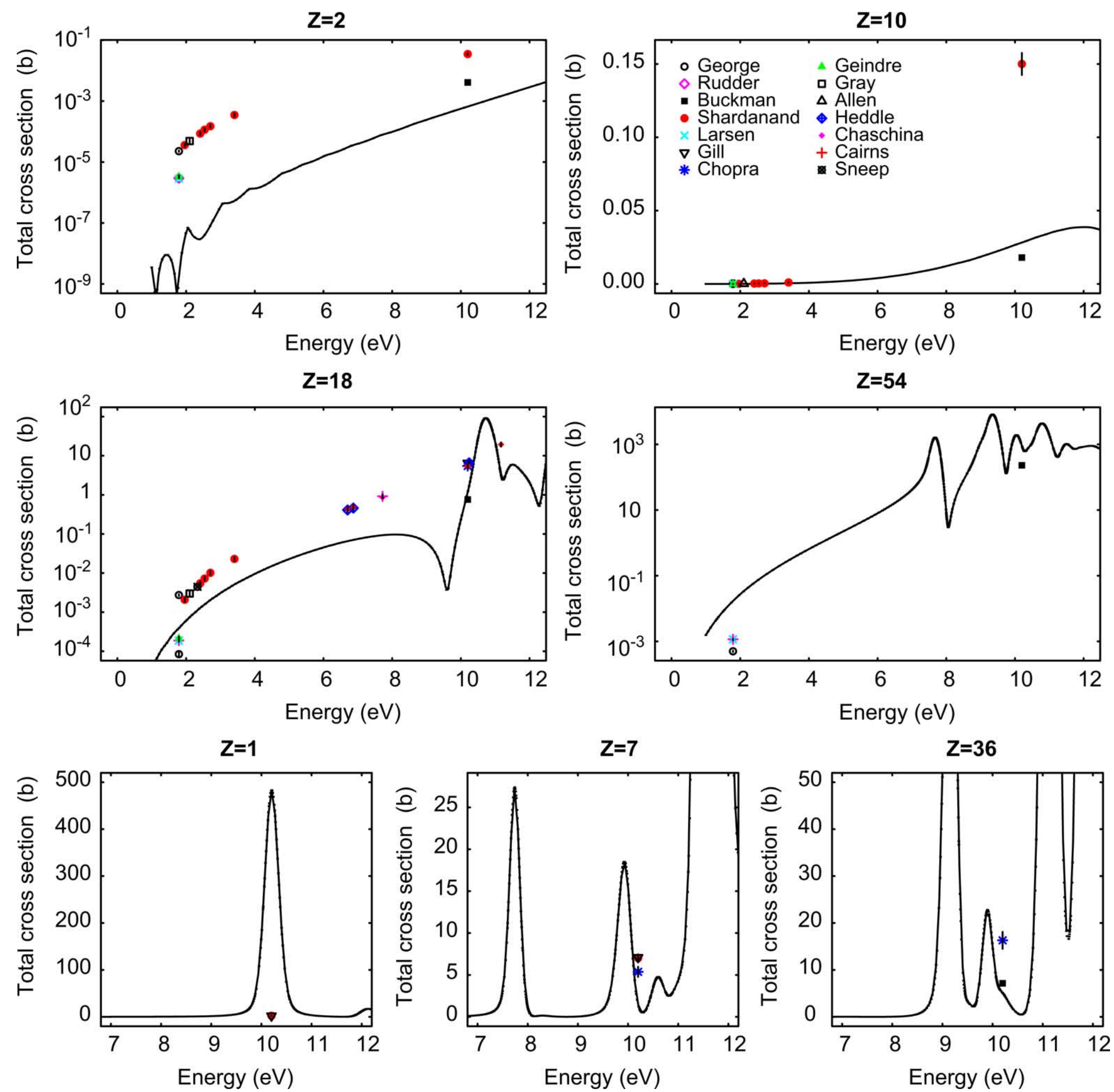
Micro/nano-dosimetry
Radiation effects

IPA (Independent Particle Approximation) and IA (Isolated Atom) assumption are the foundation of all "general purpose" Monte Carlo codes

In what conditions do they break?
Down to what energy are they valid?

Monte Carlo particle transport **beyond IPA and IA?**

Photon elastic scattering



Maria Grazia Pia, INFN Genova

Detectors

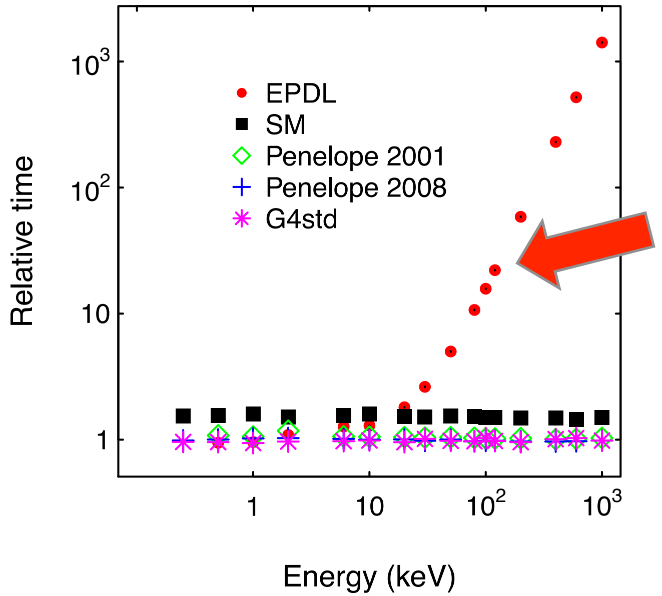
Still the same vision as 40 years ago!

- Detector simulation in Geant4 and other general purpose Monte Carlo codes is limited to phenomena described in IPA and matter treated in IA
- What about interactions with solids?
- Crystals, organic and inorganic scintillators
- Semiconductor detectors
- Nanotechnology-based detectors
- Home-made simulation codes for detector R&D
  - Usually not publicly available
- An environment for these studies in a Monte Carlo toolkit?

Synergy of **complementary competence**
Detector, physics, software

Computational performance

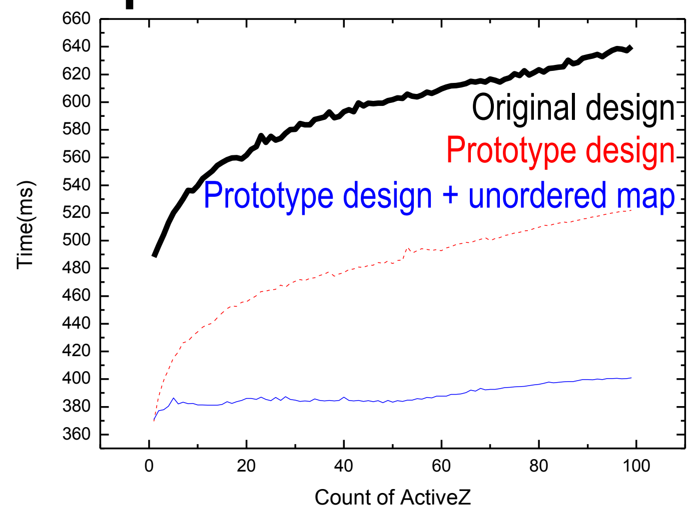
- Not only a matter of fancy techniques
  - Multi-threading, vectorization, GPUs etc.
- Software quality, efficient algorithms, smart ideas
  - …and also user application code!



Photon elastic scattering

Computational performance improvement as a by-product of refactoring/testing

Pair production cross sections



time (ms) to **retrieve** data

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

The fastest algorithm

no algorithm at all

Shift modeling from algorithms to data

Uncertainty quantification

cross sections,
branching ratios,
physics models,
physics parameters..

Input

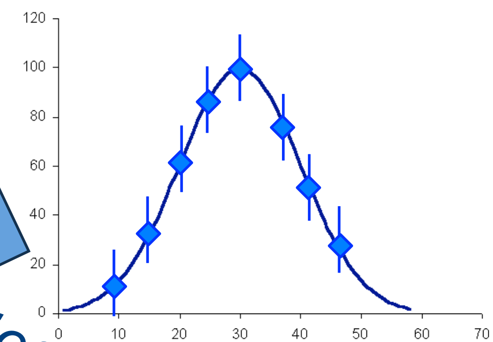
Monte Carlo method

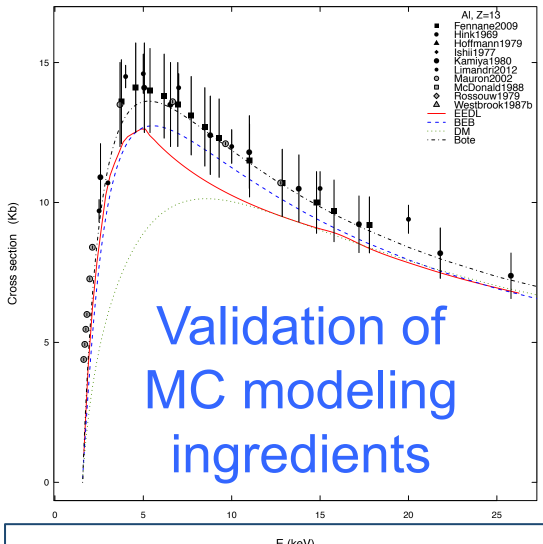
Statistical uncertainty

Geant 4

observable

with uncertainties





Validation of MC modeling ingredients

$$G(x)=\int_{-\infty}^{+\infty} d\Sigma_S f(\Sigma_S)\delta(x-x_0(\Sigma_S)) = \left|\frac{d\Sigma_S(x_0)}{dx_0}\right|_{x_0=x} f(\Sigma_S(x))$$

P. Saracco, M.G. Pia, M. Batic, Theoretical ground for the propagation of uncertainties in Monte Carlo particle transport, TNS Feb. 2014

Uncertainty quantification is the ground for **predictive Monte Carlo simulation**

Meditation

Food for thought

- Geant4 is a rich and powerful tool for experimental research
- **Validation** is ongoing
- Software evolution since RD44

> "The main problem with GEANT 3 was that no documentation on its program design was available. Only, say, ten people in the world knew how it worked."

- Detector R&D
- New application domains
- Computational environment
- Beyond IPA and IA
- Multi-scale simulation
- Uncertainty Quantification

In my end is my beginning.

T. S. Eliot, Four Quartets (East Coker)