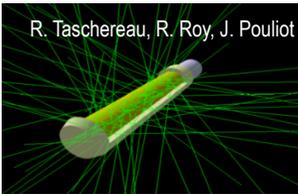
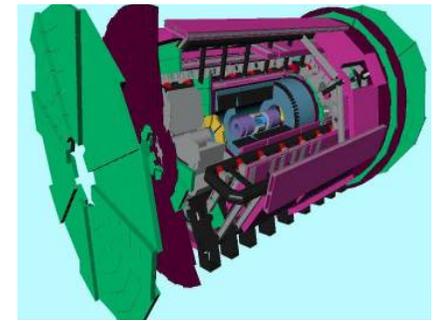


Courtesy T. Ersmark, KTH Stockholm



R. Taschereau, R. Roy, J. Pouliot



Courtesy of ATLAS Collaboration

Geant 4

Refresher Course

(mostly about Geant4 physics)

Maria Grazia Pia

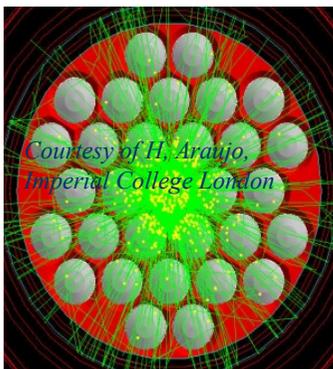
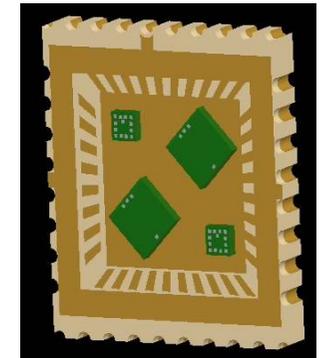
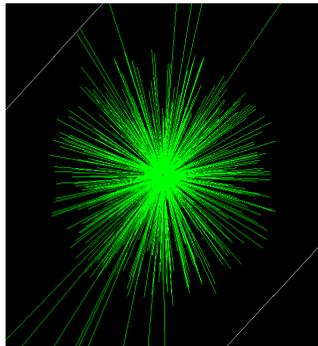
INFN Genova, Italy

For early risers at IEEE NSS-MIC 2011

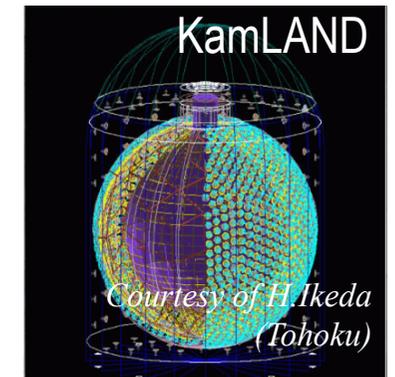
Wednesday, 26 October 2011, 7.30 am

Valencia, Spain

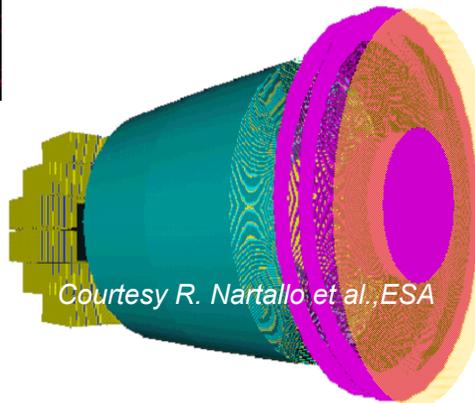
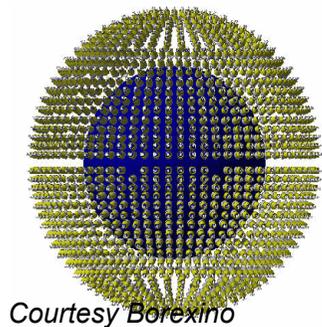
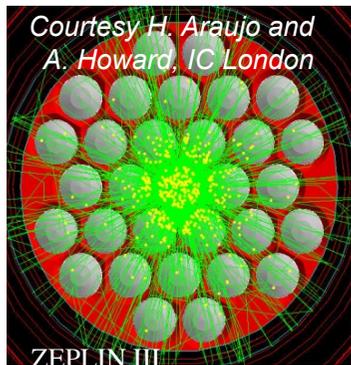
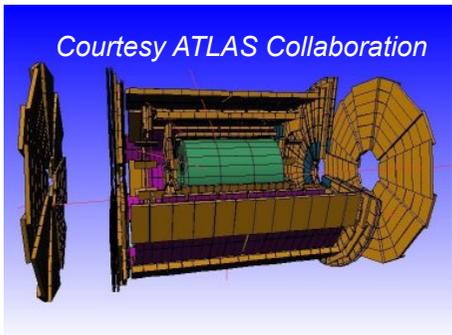
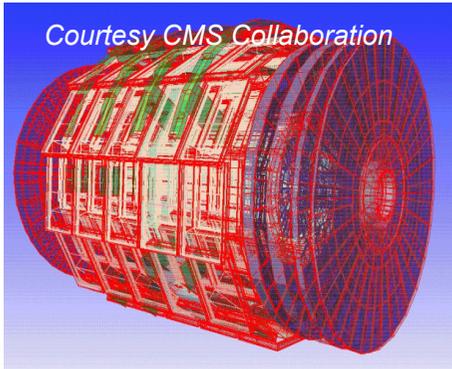
<http://cern.ch/geant4>



Courtesy of H. Araujo,
Imperial College London



KamLAND
Courtesy of H. Ikeda
(Tohoku)

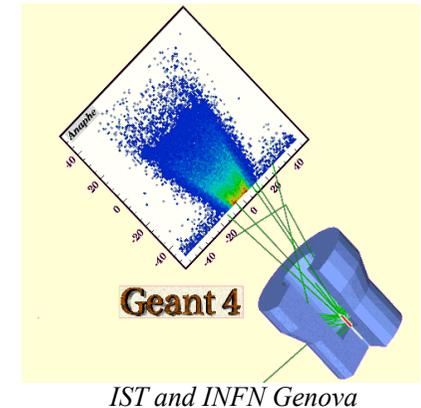
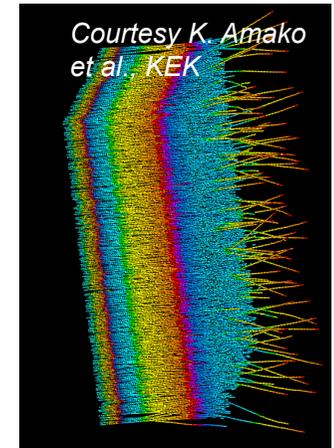


Geant 4

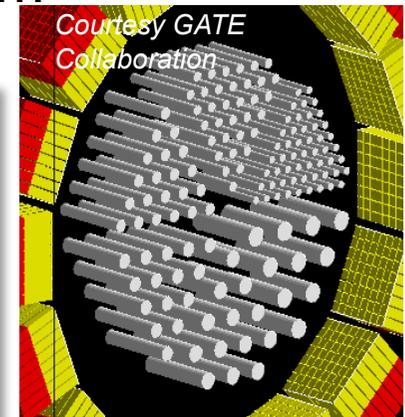
Born from the requirements of large scale HEP experiments

Widely used also 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...



Most cited
“Nuclear Science and Technology” publication
 Thomson-Reuters, ISI Web of Science, 1970-October 2011



Outline

Geant4 in one hour...

- **A little bit of software**

- Basic concepts of Geant4 use: application, PhysicsList

- **Overview of Geant4 physics functionality**

- Electromagnetic and hadronic physics

- **Validation**

- Concepts and a few results

- **Outlook**

Geant4 users

- What is the difference between Standard and low energy?
- What is the difference between Geant4 and MCNP? (*Geant4 and EGS, Geant4 and FLUKA...*)
- Which PhysicsList should I use?

TNS editor

- Could you please document the validation of your simulation?
- Could you please quantify the accuracy of your simulation?
- Why did you use model X in your simulation?

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

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

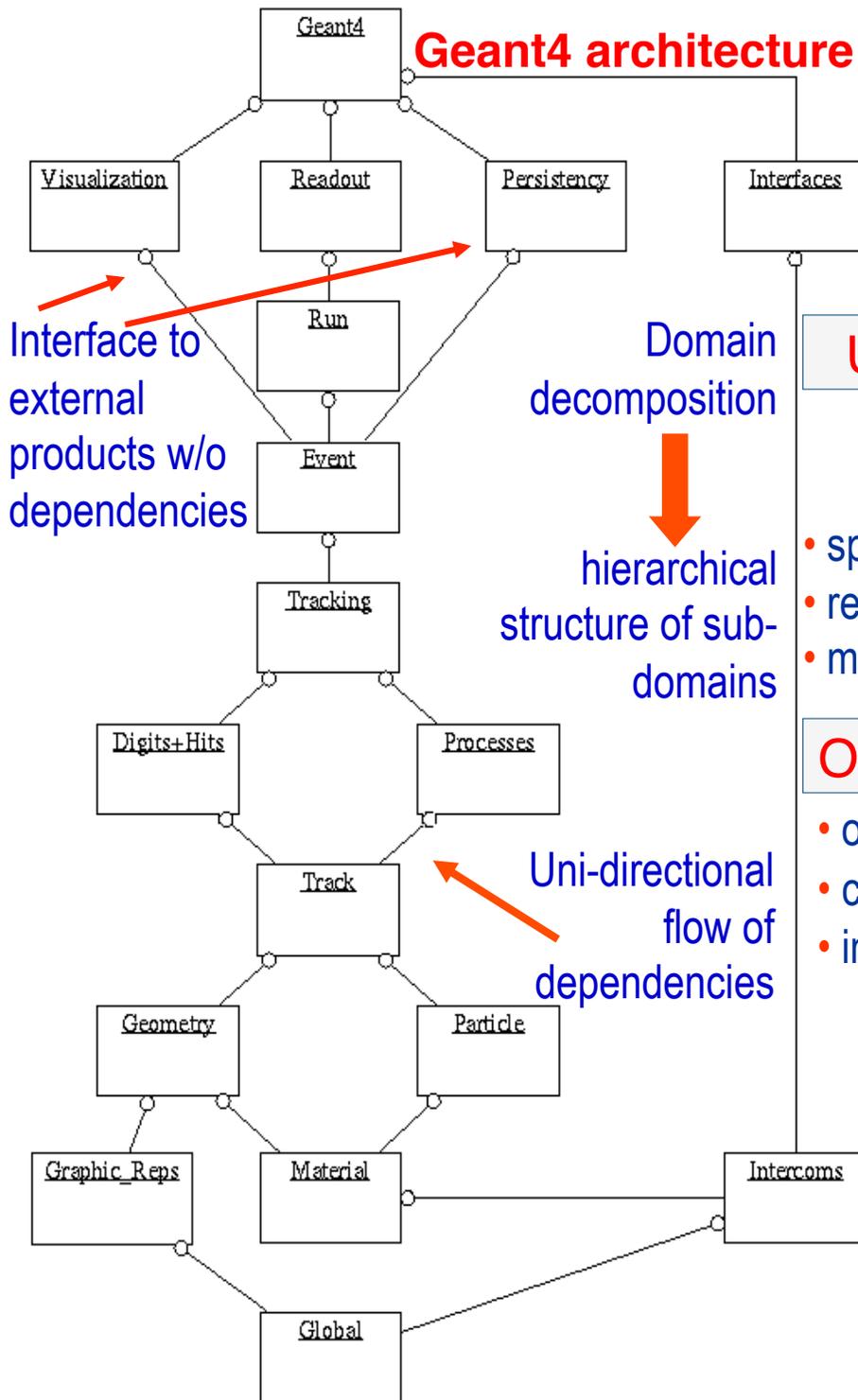
Toolkit

A set of **compatible components**

- each component is **specialised** for 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

Software Engineering

plays a fundamental role in Geant4



Geant4 architecture

Interface to external products w/o dependencies

Domain decomposition
↓
hierarchical structure of sub-domains

Uni-directional flow of dependencies

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 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**

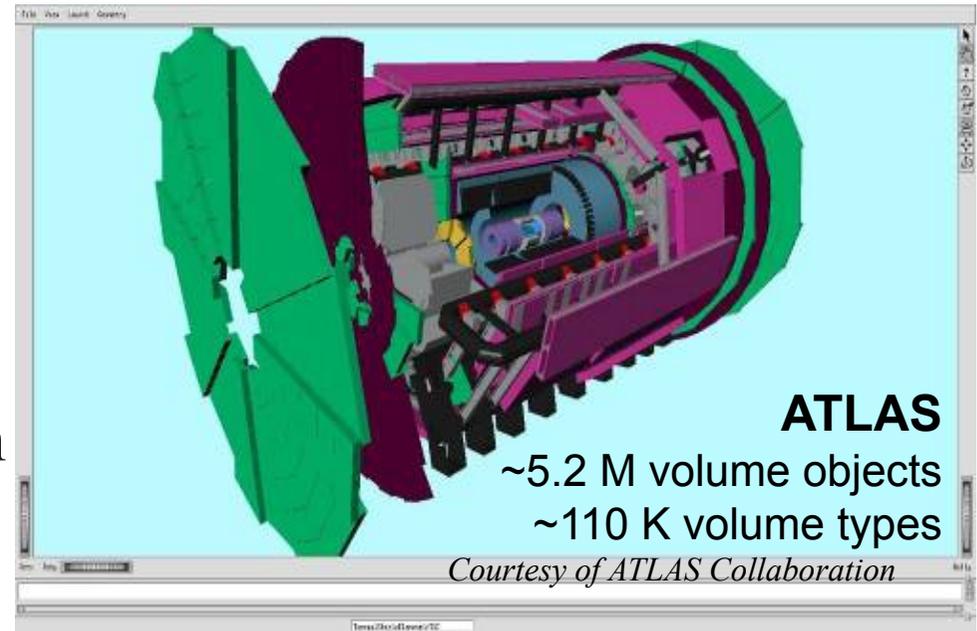
- Decoupled from physics
 - all processes handled through the same abstract interface
- Independent from particle type
- New physics processes can be added to the toolkit without affecting tracking
- Geant4 has only **secondary production thresholds, no tracking cuts**
 - all particles are tracked down to zero range
 - energy, TOF ... cuts can be defined by the user

Materials

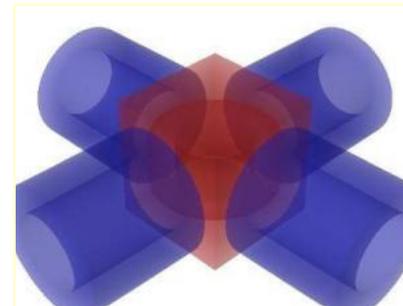
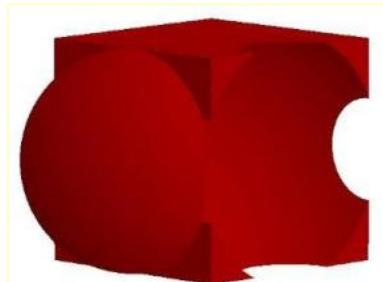
- Different kinds of materials can be defined
 - **isotopes**  G4Isotope
 - **elements**  G4Element
 - **molecules**  G4Material
 - **compounds and mixtures**  G4Material
- Associated attributes:
 - temperature
 - pressure
 - state
 - density

Geometry

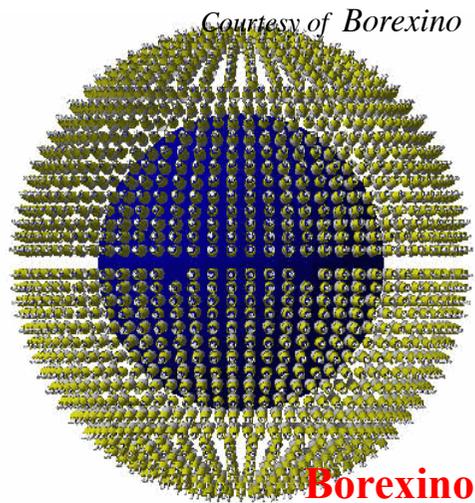
- Role
 - detailed detector description
 - efficient navigation
- Three conceptual layers
 - **Solid**: shape, size
 - **LogicalVolume**: material, sensitivity, daughter volumes, etc.
 - **PhysicalVolume**: position, rotation
- One can do fancy things with geometry...



Boolean
operations

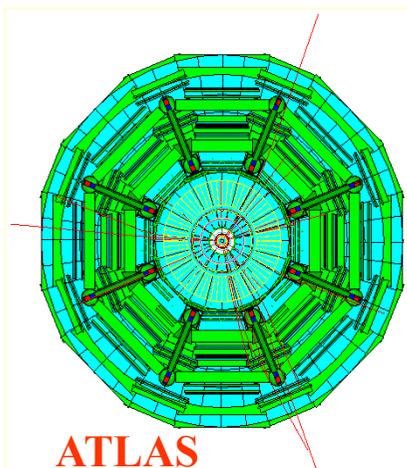
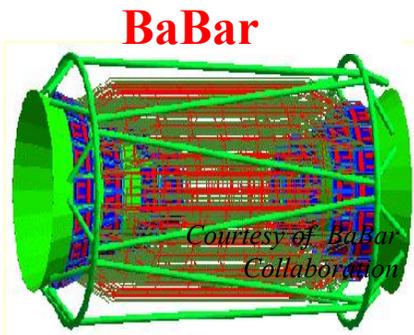
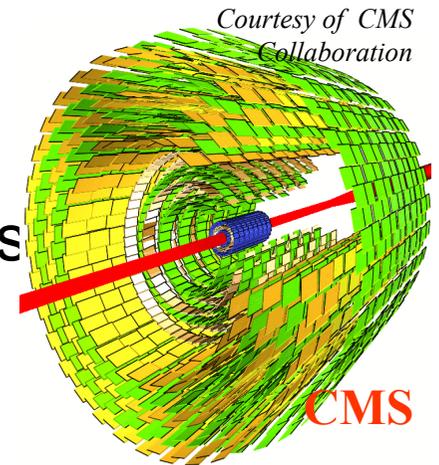
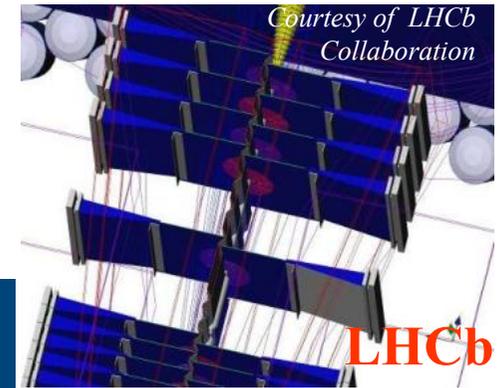


Transparent
solids



Solids

Multiple representations
Same abstract interface



CSG (Constructed Solid Geometries)

- simple solids

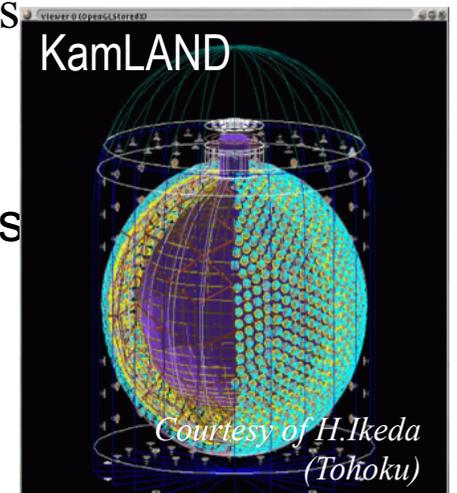
STEP extensions

- polyhedra, spheres, cylinders, cones, toroids etc.

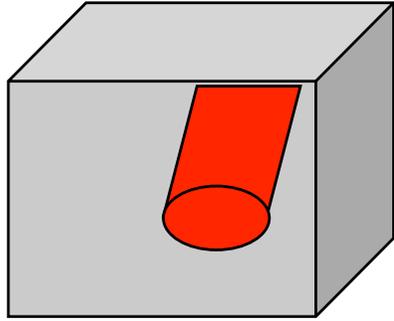
BREPS (Boundary REPresented Solids)

- volumes defined by boundary surfaces

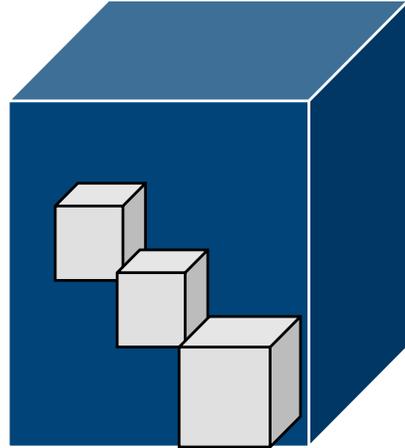
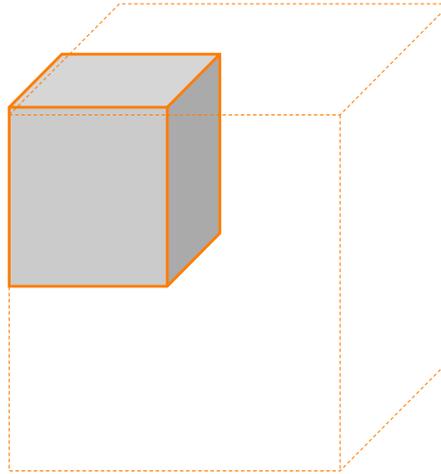
CAD exchange



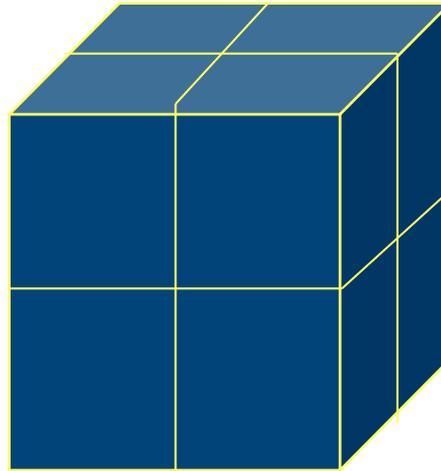
Physical Volumes



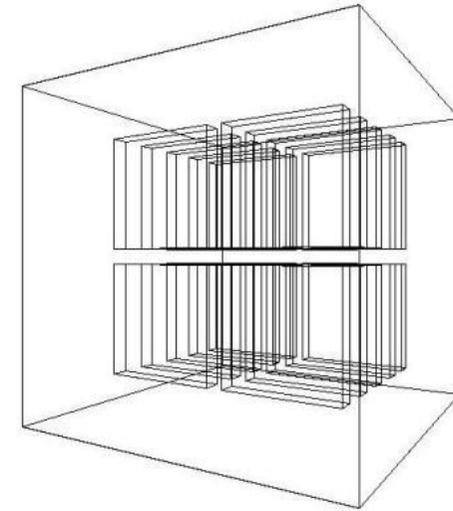
placement



parameterised

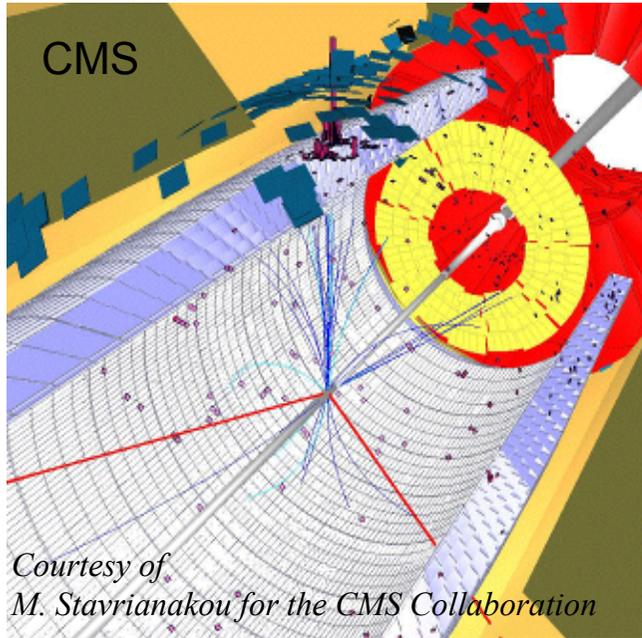


replica



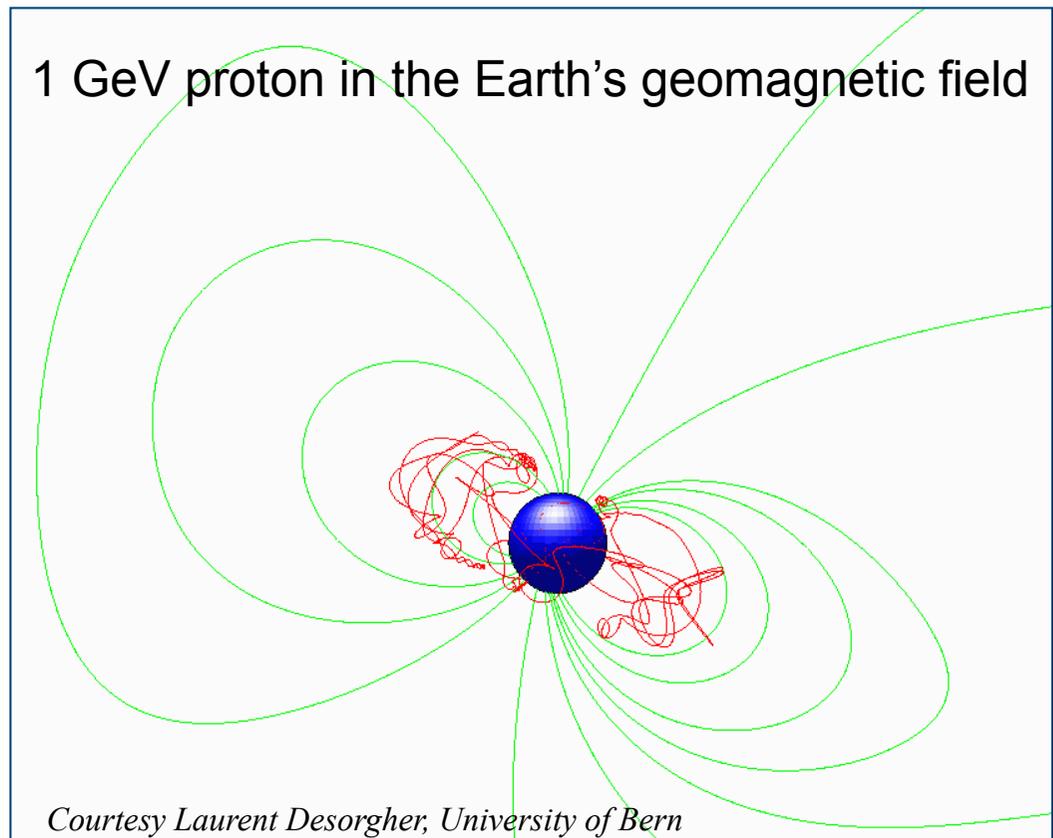
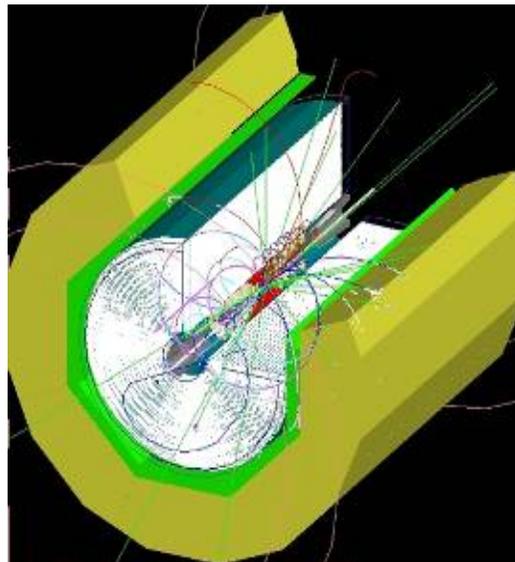
assembled

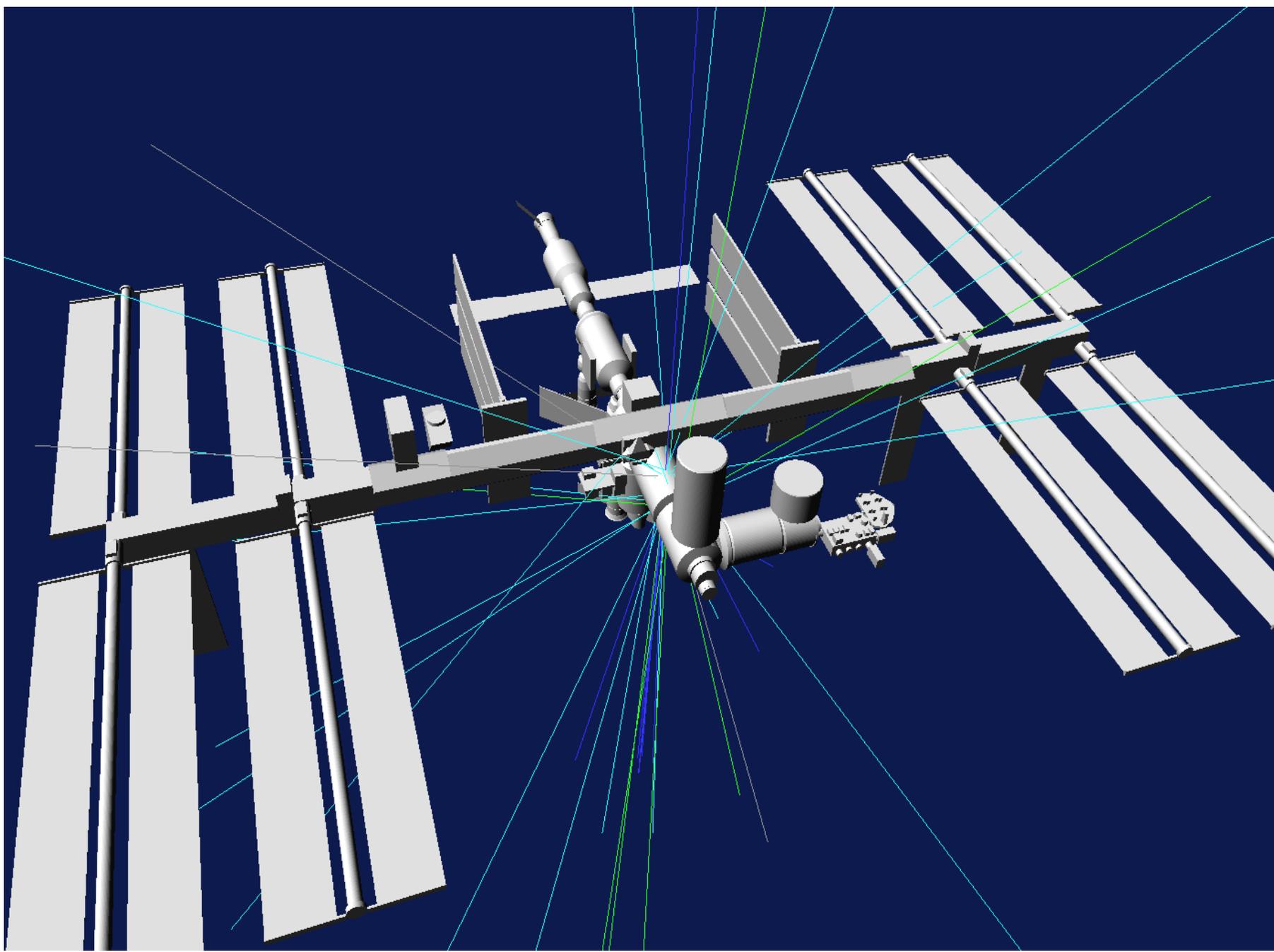
Electric and magnetic fields



of variable non-uniformity
and differentiability

MOKKA
Linear Collider
Detector

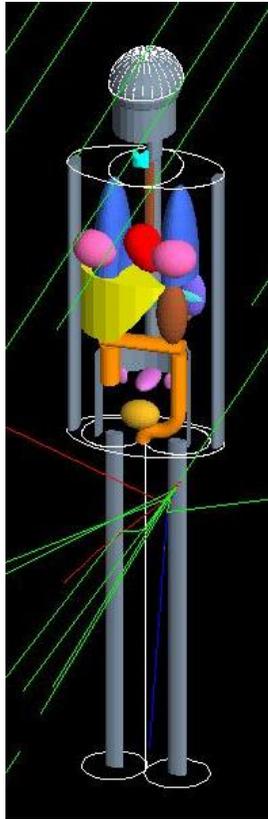




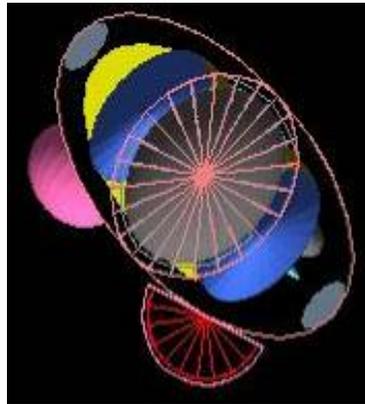
Courtesy T. Ersmark, KTH Stockholm

Not only large scale, complex detectors...

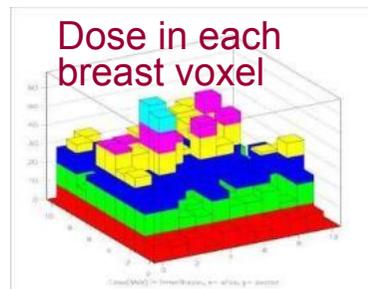
Geant 4



Analytical
breast

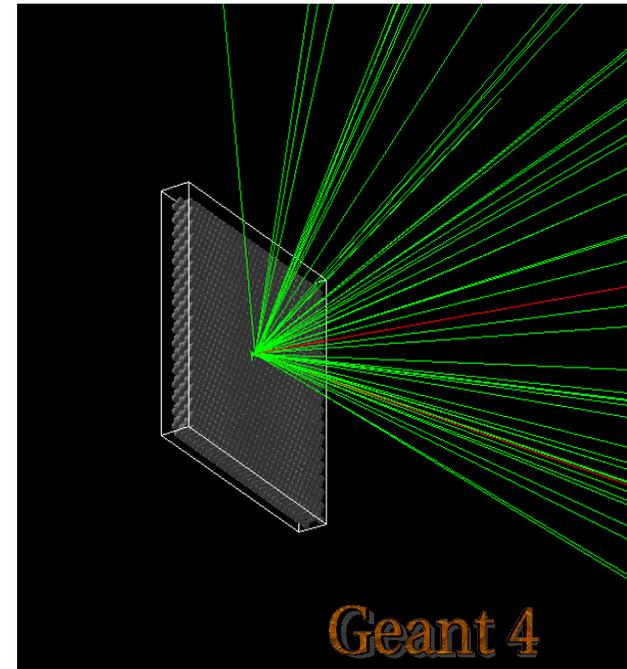


Voxel breast



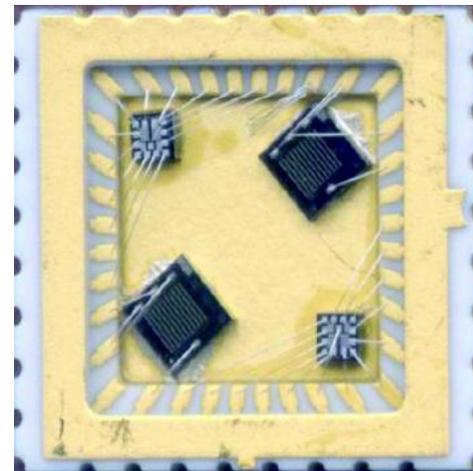
Geant4 anthropomorphic phantoms

Maria Grazia Pia, INFN Genova

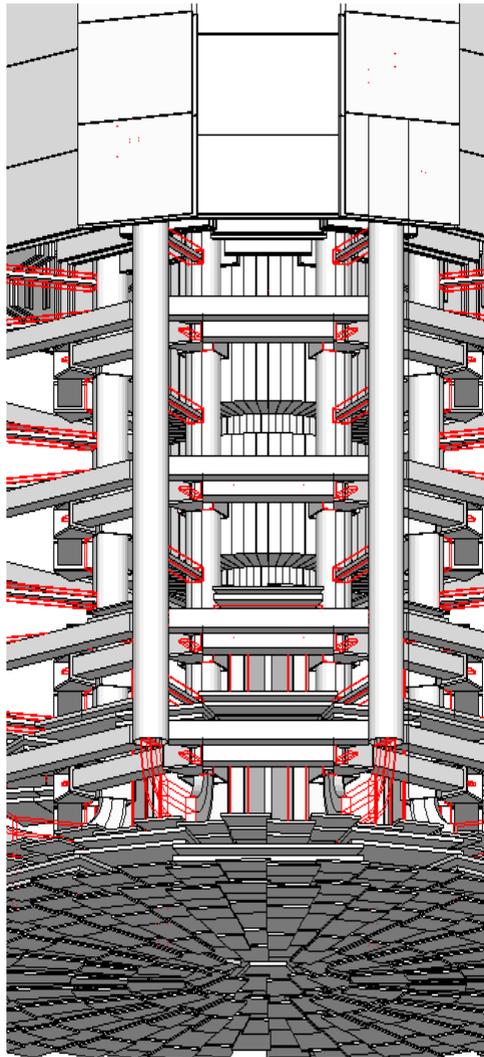


simple geometries

small scale components

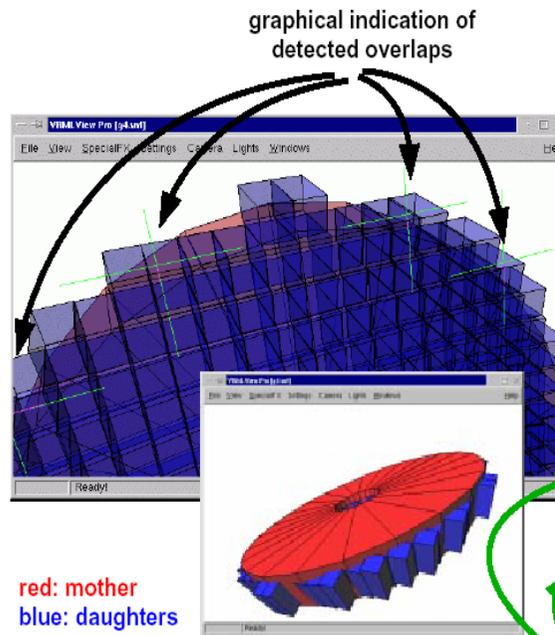


One may also do it wrong...



DAVID

Tools to detect badly defined geometries



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)

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

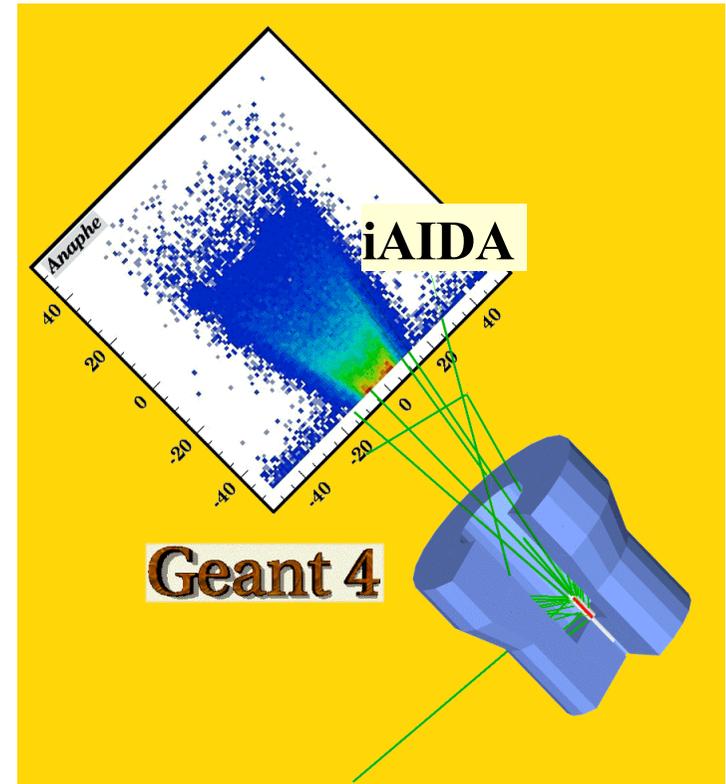
Interface to external tools

through abstract interfaces

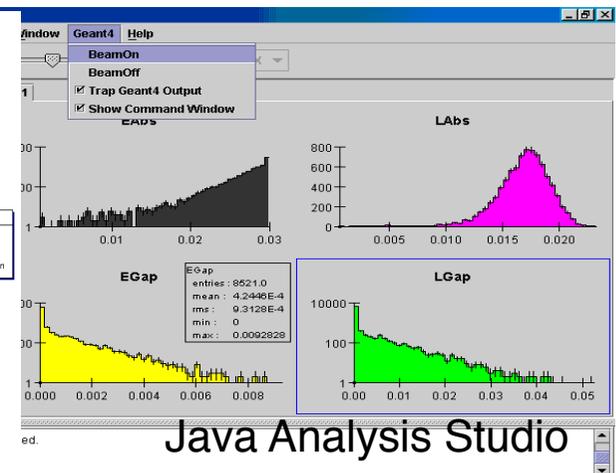
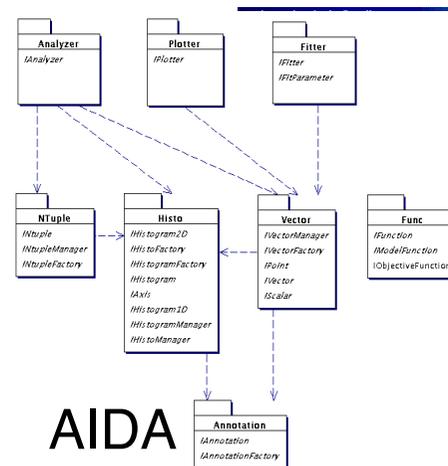
no dependency
minimize coupling of components

Similar approach

- Visualisation
- (G)UI
- Persistency
- Analysis



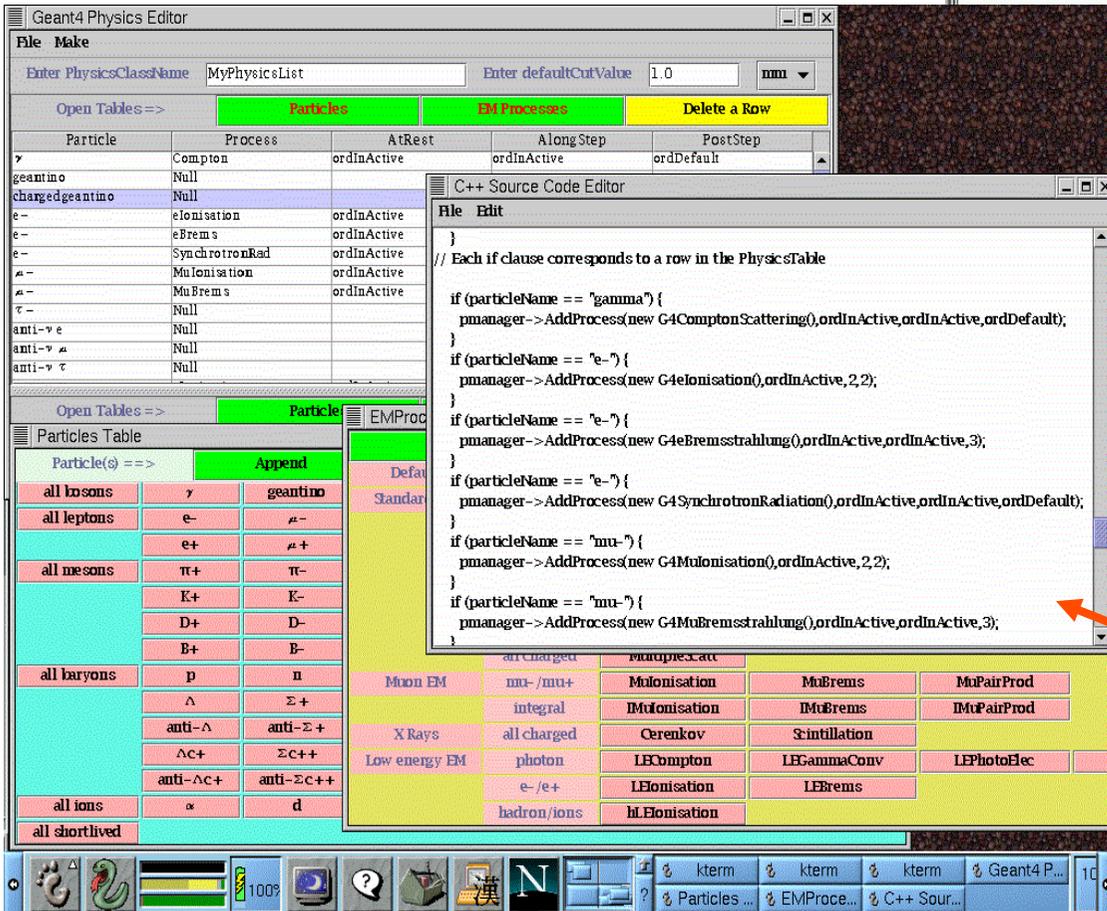
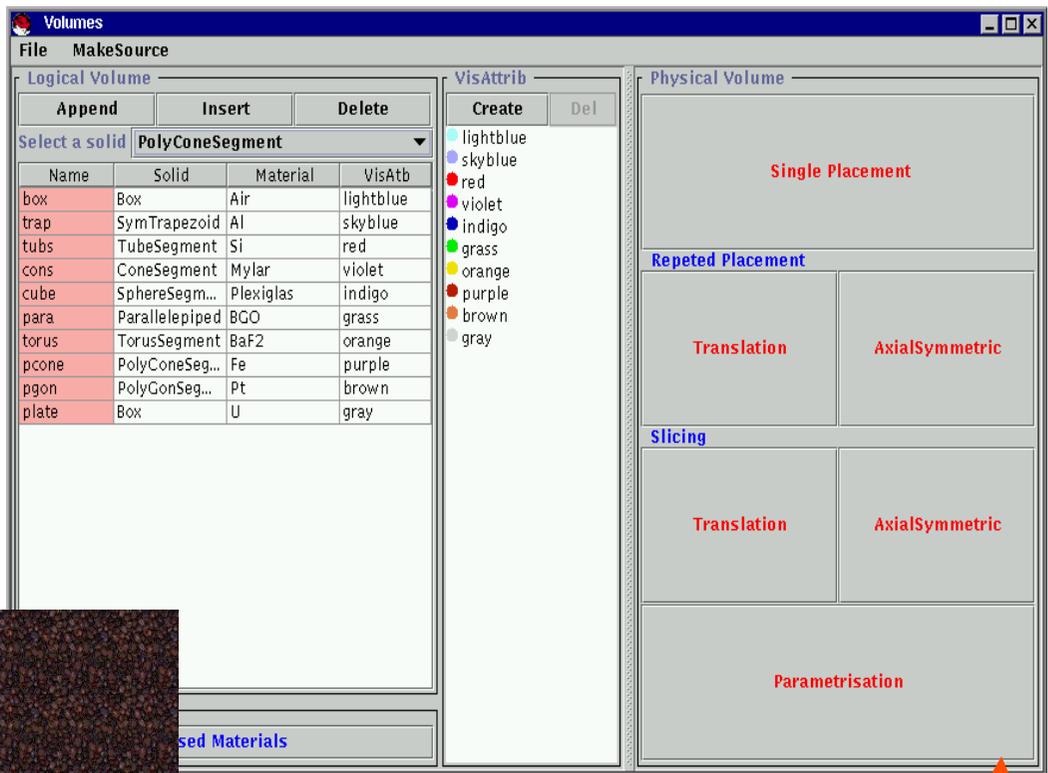
The user is free to choose the concrete system he/she prefers for each component



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

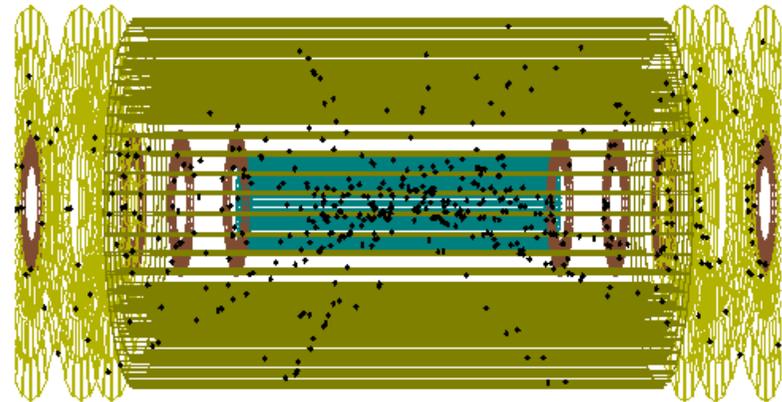
GGE (Geant4 Geometry Editor)

GPE (Geant4 Physics Editor)

Visualisation

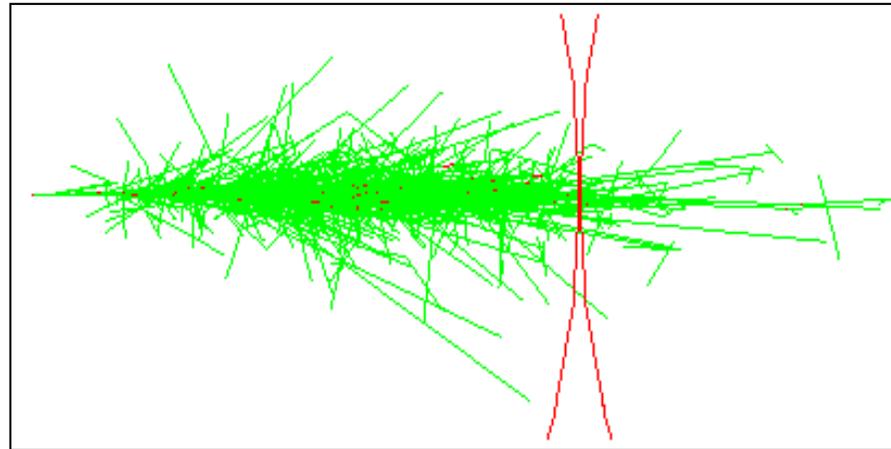
- Control of several kinds of visualisation

- detector geometry
- particle trajectories
- hits in detectors



- Various **drivers**

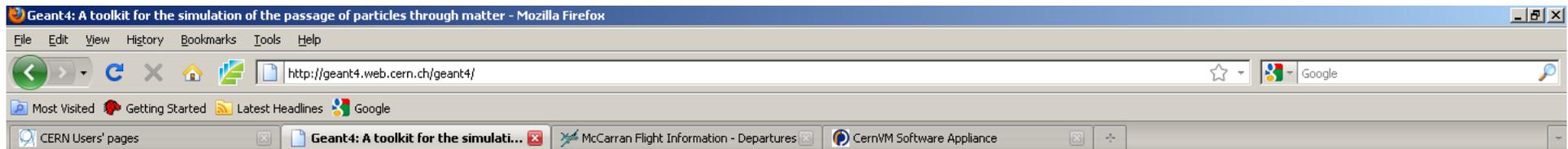
- OpenGL
- OpenInventor
- X11
- Postscript
- DAWN
- OPACS
- HepRep
- VRML...



- all handled through abstract interfaces

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 by the Geant4 collaboration
 - On a best effort basis
 - User Forum: mutual support within the user community



Geant 4

[Download](#) | [User Forum](#) | [Gallery](#)
[Contact Us](#)

Search Geant4

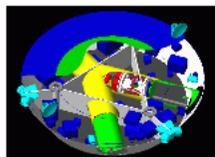
Geant4 is a toolkit for the simulation of the passage of particles through matter. Its areas of application include high energy, nuclear and accelerator physics, as well as studies in medical and space science. The two main reference papers for Geant4 are published in *Nuclear Instruments and Methods in Physics Research A* [506 \(2003\) 250-303](#), and *IEEE Transactions on Nuclear Science* [53 No. 1 \(2006\) 270-278](#).

Applications



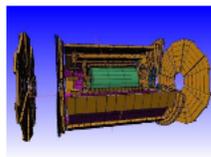
A [sampling of applications](#), technology transfer and other uses of Geant4

User Support



[Getting started](#), [guides](#) and information for users and developers

Results & Publications



[Validation of Geant4](#), results from experiments and publications

Collaboration



[Who we are](#): collaborating institutions, [members](#), organization and legal information

News

- 24 September 2010 - **Patch-02 to release 9.3** is available from the [download](#) area.
- 24 September 2010 - **Patch-04 to release 9.2** is available from the [archive download](#) area.
- 25 June 2010 - **Release 9.4 BETA** is available from the [Beta download](#) area.
- 16 March 2010 - [2010 planned developments](#).

Physics

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

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

Physics: general features

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

Electromagnetic physics

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

- Comparable to GEANT 3 already in α release 1997
- 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 effect
- γ conversion
- e^+e^- pair production
- Synchrotron radiation
- Transition radiation
- Cherenkov
- Refraction
- Reflection
- Absorption
- Scintillation
- Fluorescence
- Auger emission

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

Toolkit + User application



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

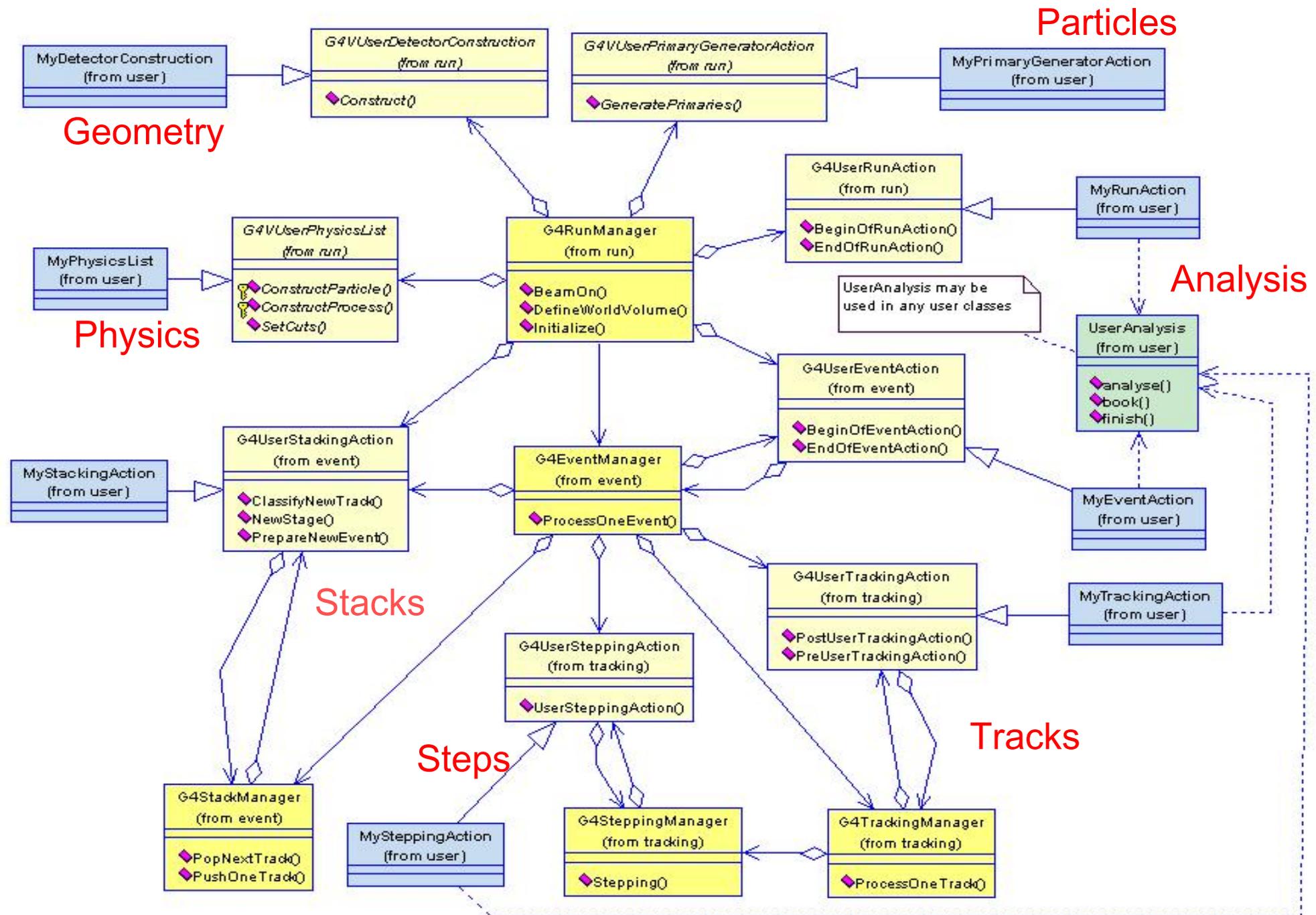
Basic actions

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

Interaction with Geant4 kernel

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

A simple Geant4-based application



User classes

Initialisation classes

Invoked at initialization

- *G4VUserDetectorConstruction*
- *G4VUserPhysicsList*

Action classes

Invoked during the execution

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

Mandatory classes:

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

G4VUserPhysicsList

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

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

Concepts

What is tracked

G4ParticleDefinition
G4DynamicParticle
G4Track

Process interface

G4VProcess
Processes interacting with tracking

Production cuts

Why production cuts are needed
The cuts scheme in Geant4

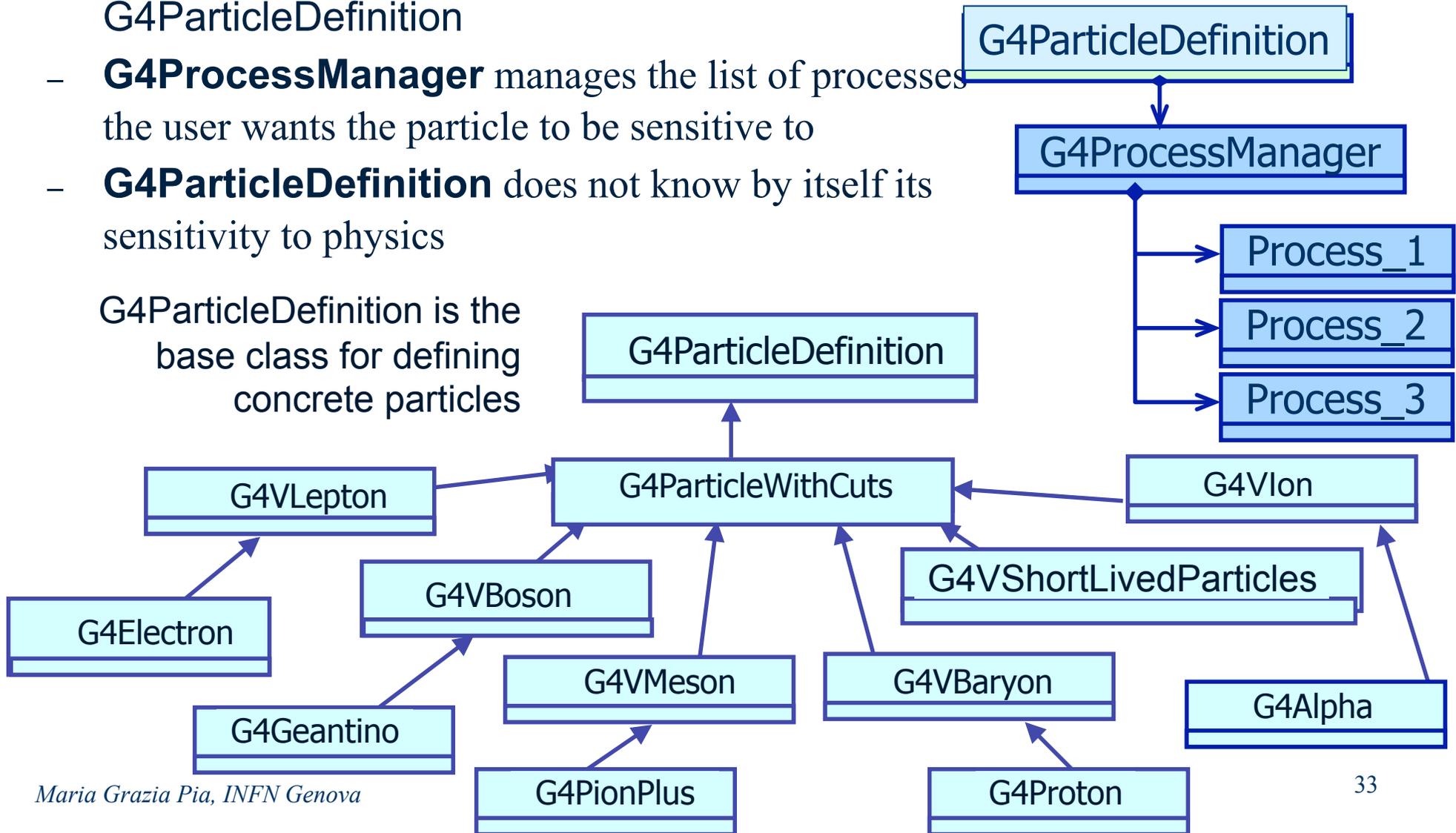
How the user
interacts with
Geant4 kernel

G4VUserPhysicsList
Concrete physics lists

G4ParticleDefinition

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

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



G4ParticleDefinition is the base class for defining concrete particles

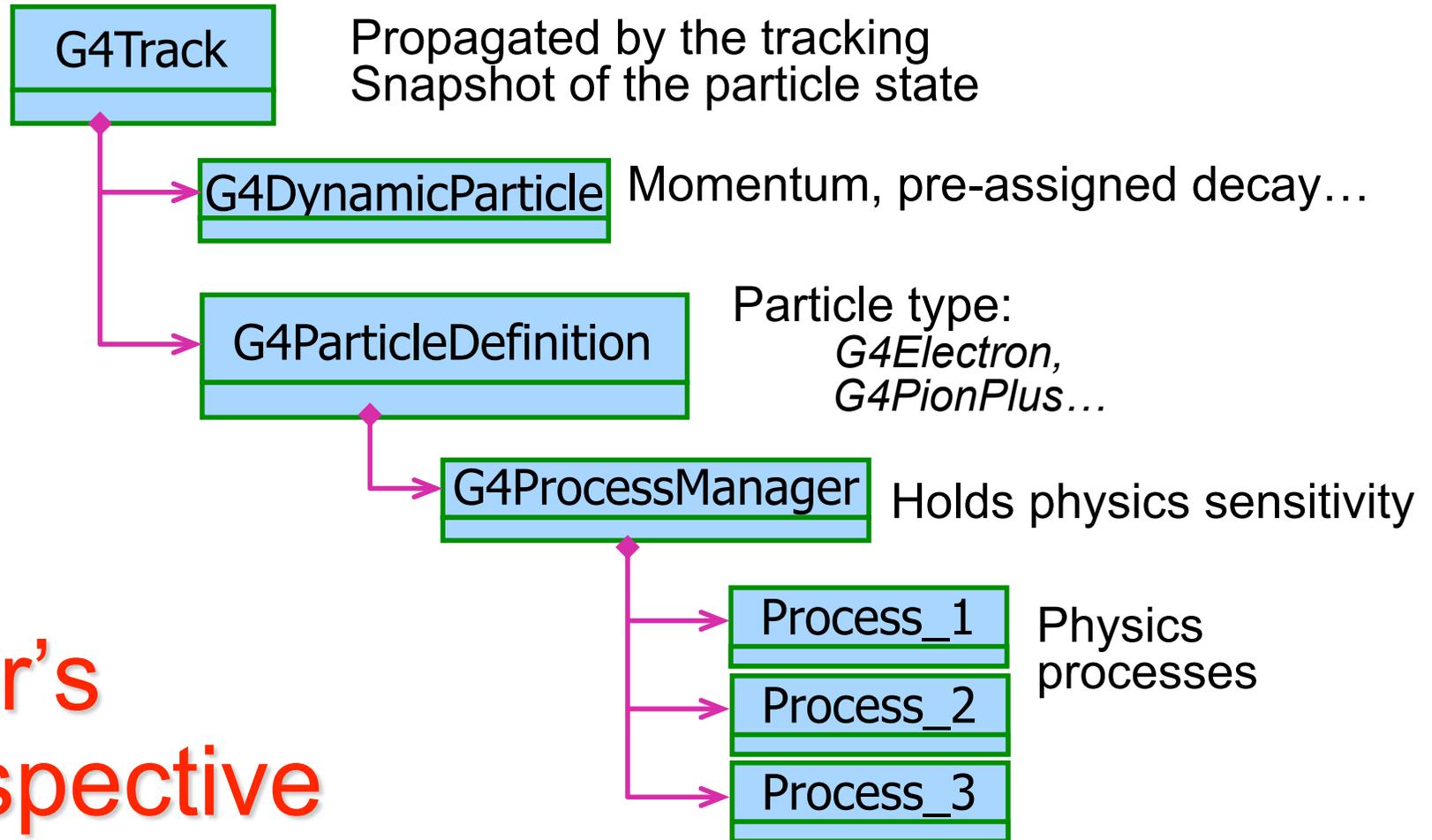
G4DynamicParticle

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

G4Track

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

User's perspective

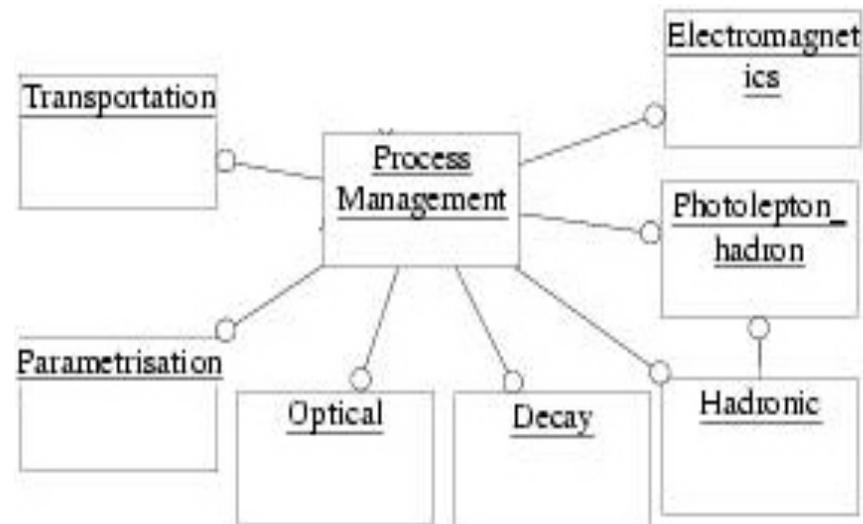


The classes involved in implementing a **PhysicsList** are:

- G4ParticleDefinition concrete classes
- G4ProcessManager
- the processes

Processes

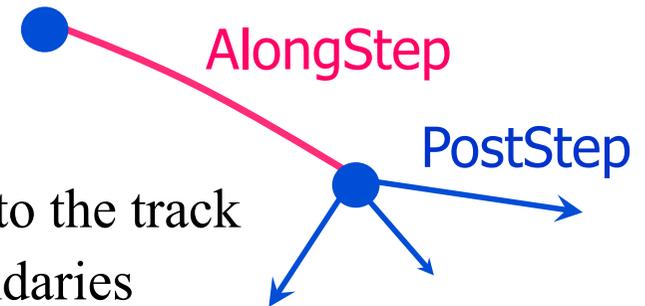
- Processes describe how particles interact with material or with a volume
- Three basic types
 - **At rest** process
(eg. *decay at rest*)
 - **Continuous** process
(eg. *ionisation*)
 - **Discrete** process
(eg. *Compton scattering*)
- **Transportation** is a process
 - interacting with volume boundary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



G4VProcess

Abstract class defining the common interface of all processes in Geant4

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



Cuts in Geant4

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

Why are production cuts needed ?

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

Electromagnetic packages in Geant4

- High energy
- Low energy
- Standard
- Muons
- Optical
- Pii
- Polarisation (*but some polarised processes are elsewhere*)
- X-rays (*but most X-ray physics is elsewhere*)

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

Different modeling approach

Specialized according to particle type, energy scope

Standard electromagnetic physics

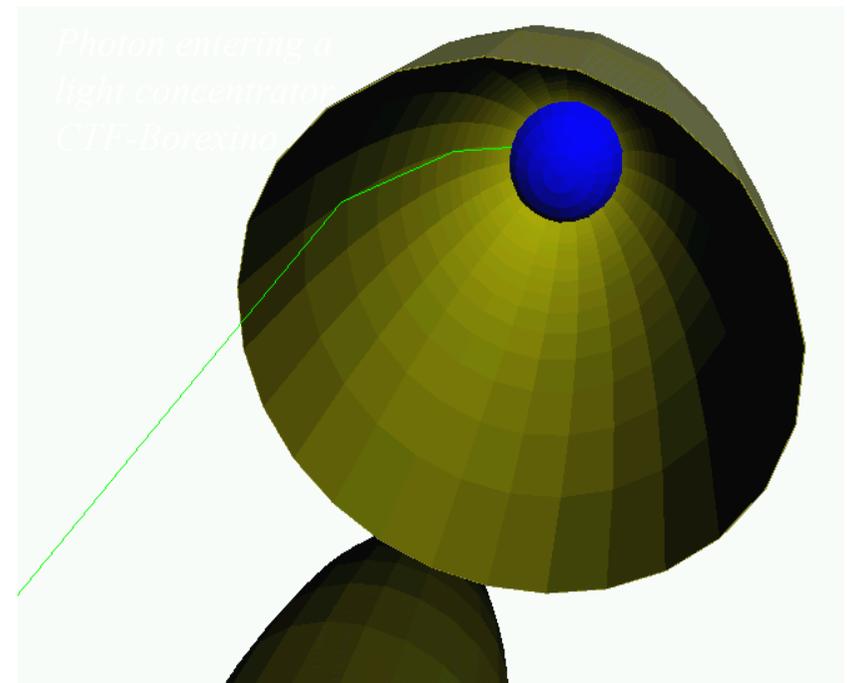
Package	Description
Standard	Gamma, Electrons up to 100 TeV, Hadrons, Ions up to 100 TeV
Muons	Muons up to 1PeV, Energy loss propagator
X-rays	X-ray and optical photon production processes
Optical	Optical photon interactions
High-energy	Processes at high energy ($E > 10$ GeV), Physics for exotic particles
Polarization	Simulation of polarized beams

Optical photons

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

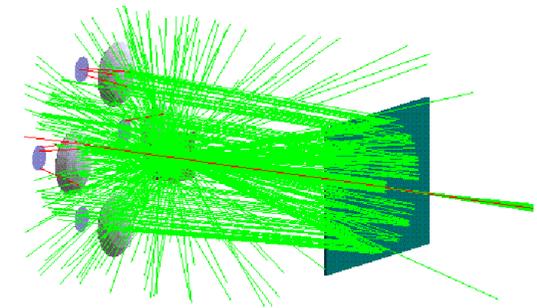
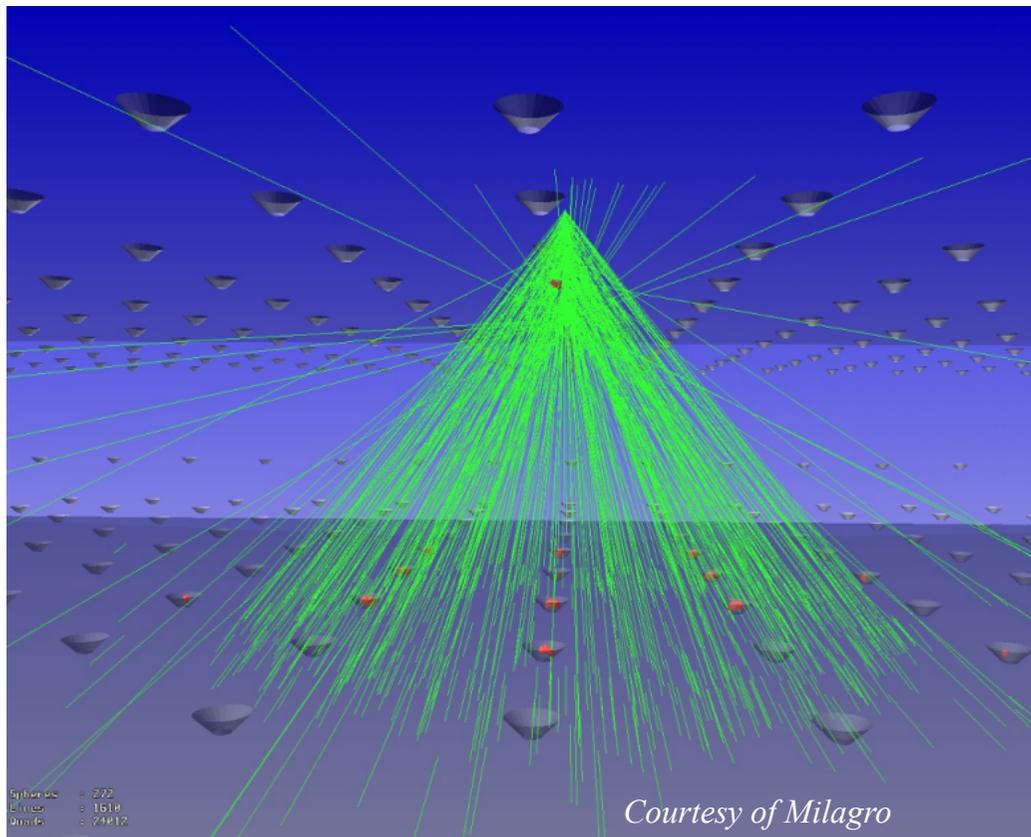
Processes in Geant4:

- 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



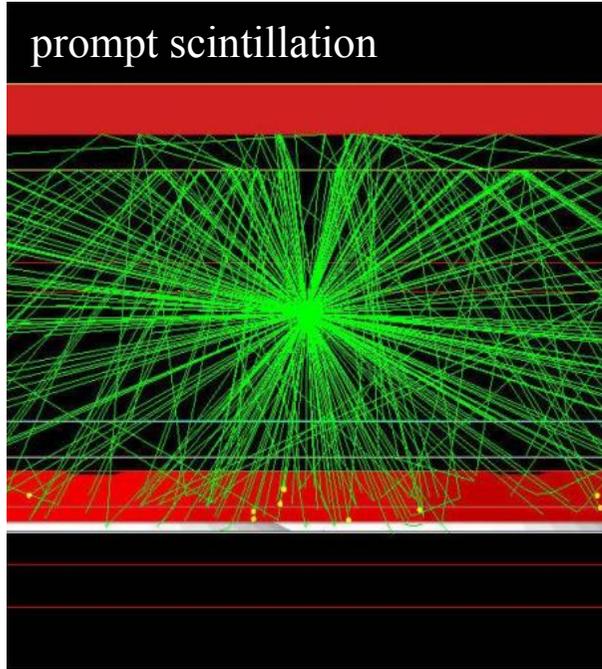
LHCb

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

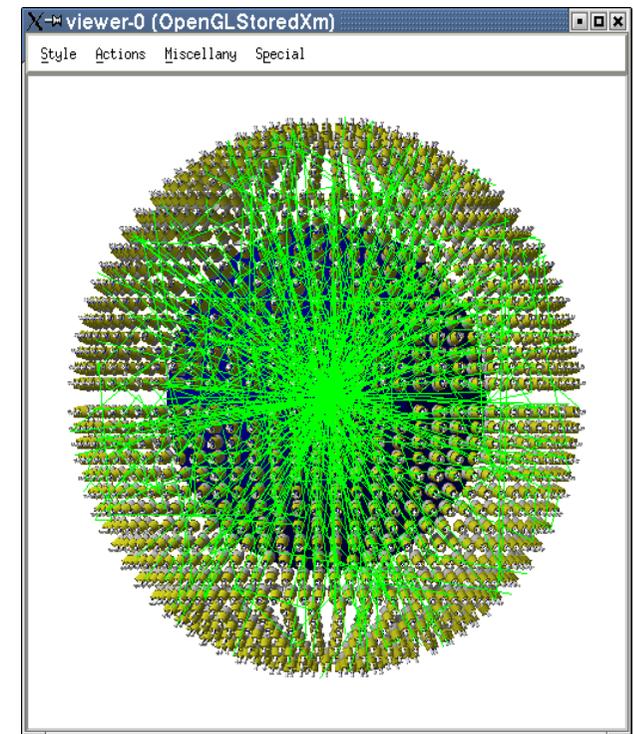
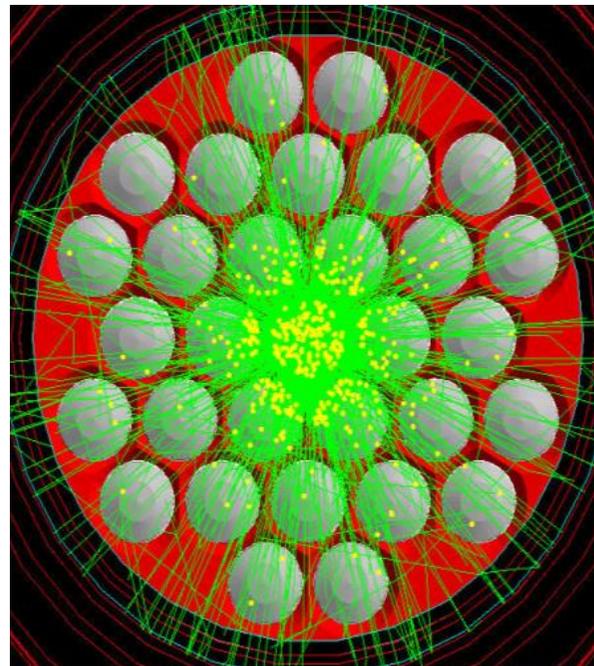
Scintillation

ZEPLIN III
Dark Matter Detector

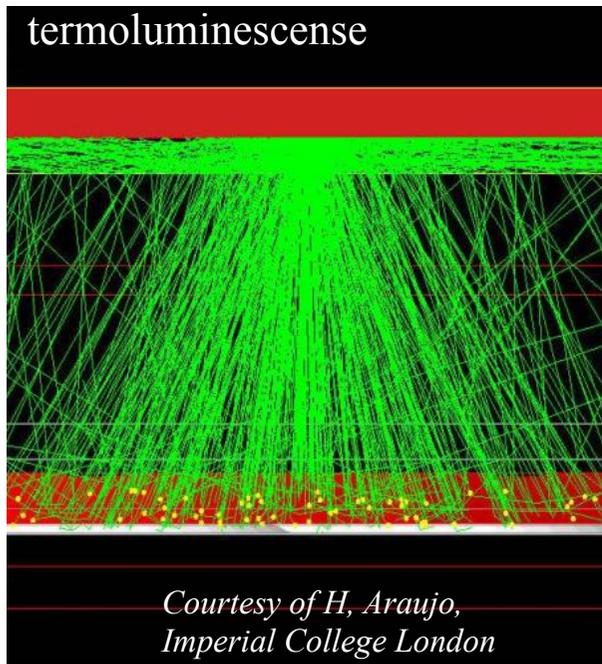
GEANT4 Scintillation Event in
BOREXINO,
INFN Gran Sasso
National Laboratory



signal in PMT



Courtesy of Borexino



*Courtesy of H, Araujo,
Imperial College London*

Muons

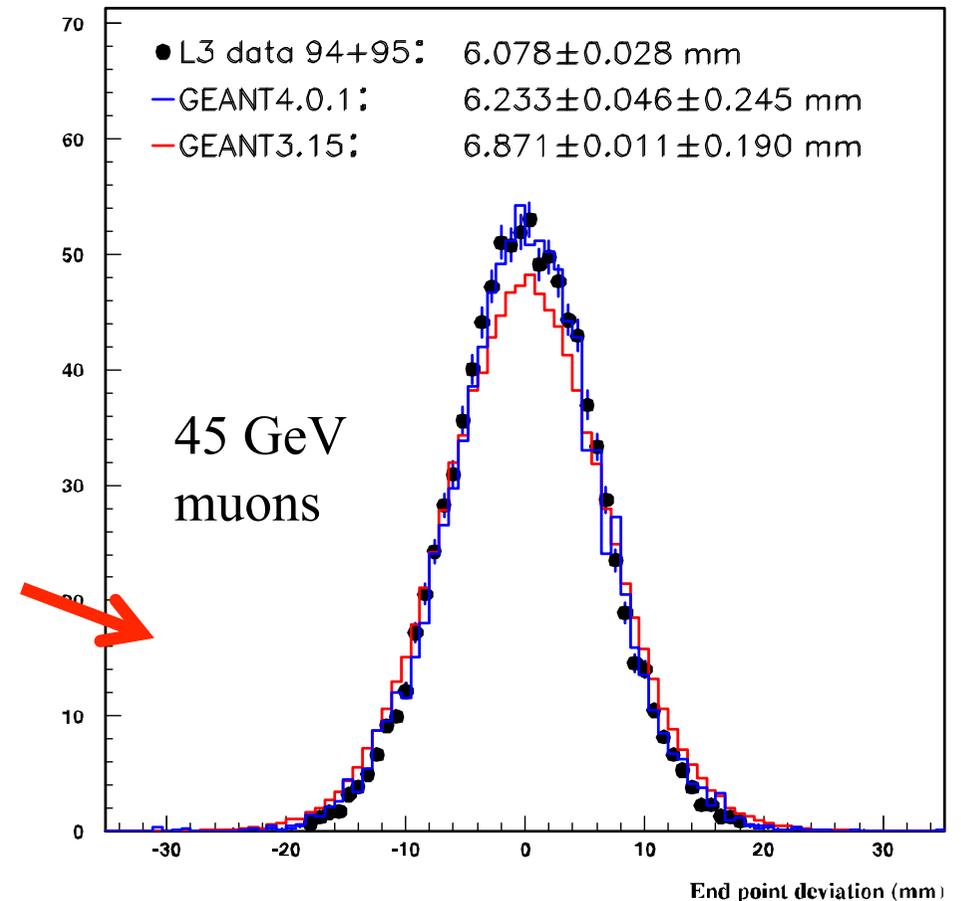
- *simulation of ultra-high energy and cosmic ray physics*
- High energy extensions based on theoretical models

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

Deviation of 45 GeV muons in L3



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

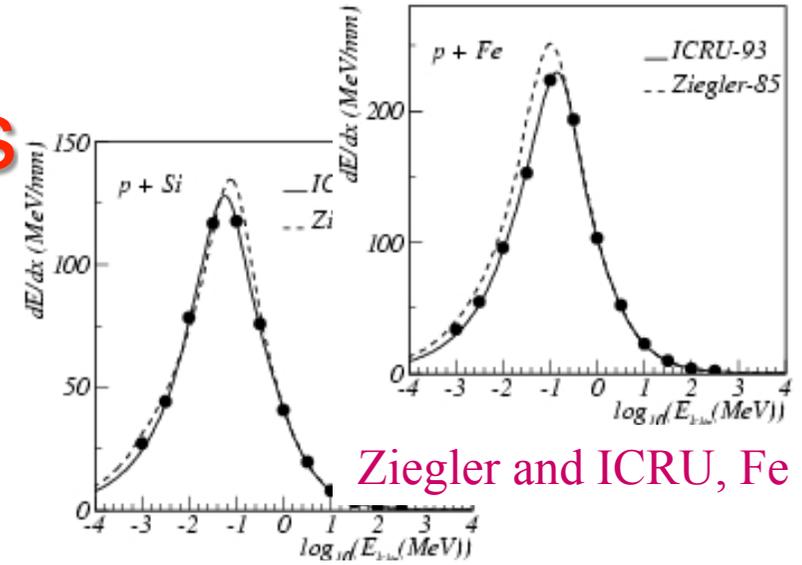
 - Bremsstrahlung
 - Ionisation

 - Polarised Compton

 - + atomic relaxation
 - fluorescence
 - Auger effect
- following processes leaving a vacancy in an atom*

Positive charged hadrons

- Bethe-Bloch model of energy loss, $E > 2 \text{ MeV}$
- 5 parameterisation models, $E < 2 \text{ MeV}$
 - based on Ziegler and ICRU reviews
- 3 models of energy loss fluctuations
 - Density correction for high energy
 - Shell correction term for intermediate energy

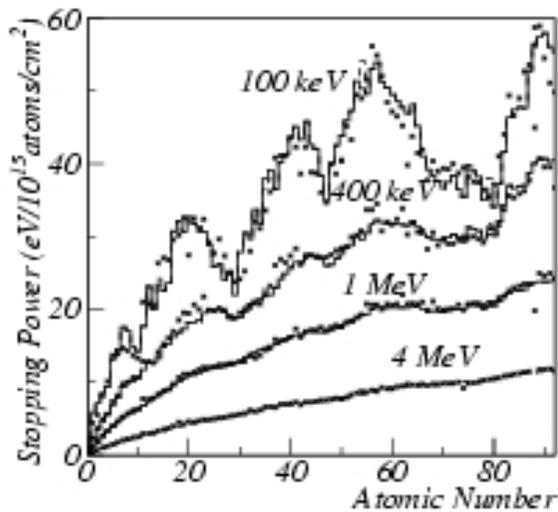


Ziegler and ICRU, Fe

Ziegler and ICRU, Si

- Spin dependent term
- Barkas and Bloch terms

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

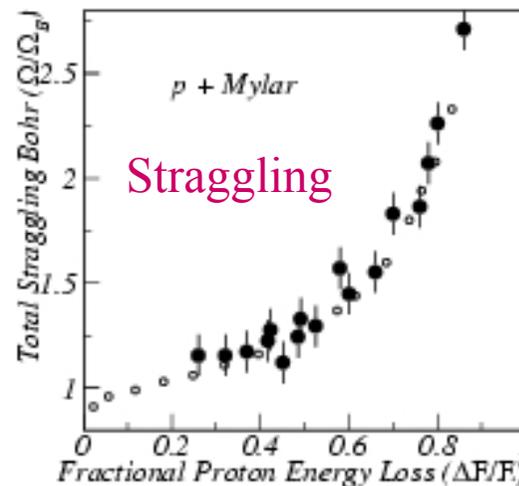


Stopping power

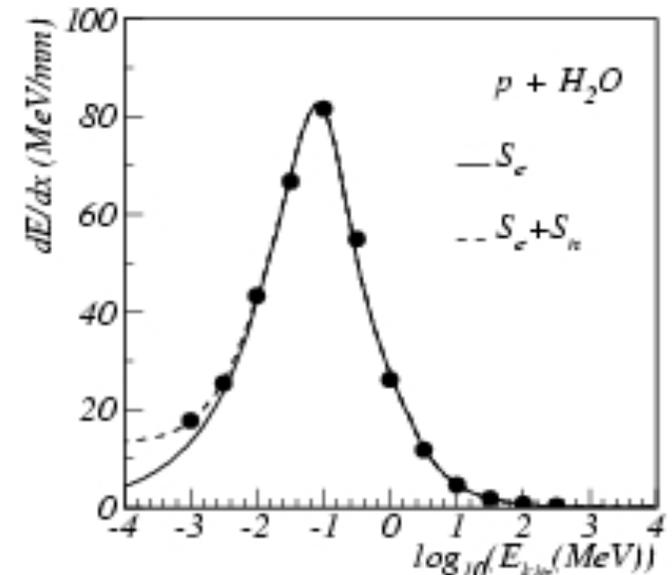
Z dependence for various energies

Maria Grazia Pia, INFN Genova

Ziegler and ICRU models



Straggling



Nuclear stopping power

Positive charged ions

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

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

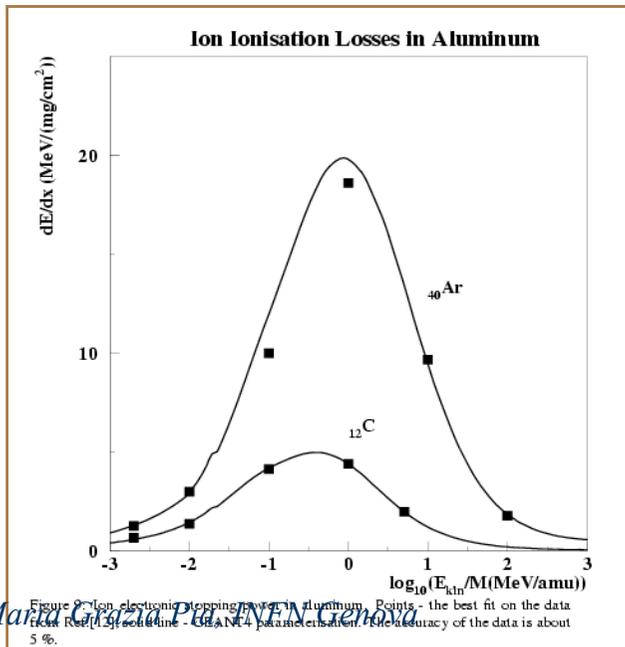
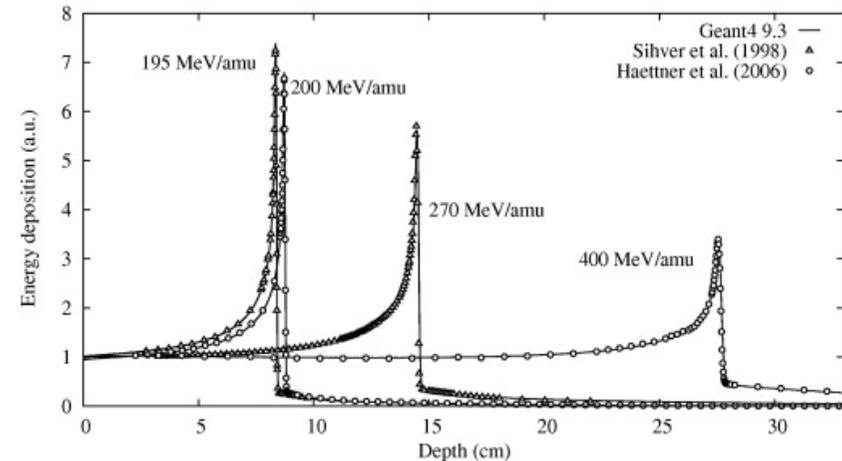
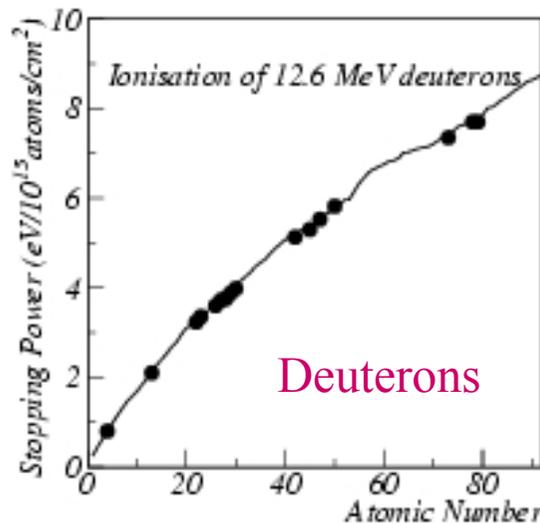


Figure 9 Ion electronic stopping power in aluminum. Points - the best fit on the data from Ref [13]. Ion time - GEA N4 parameterisation. The accuracy of the data is about 5%.



Comparison of simulated and measured ^{12}C depth-dose profiles in water (0.997 g/cm^3). Simulations were performed with Geant4 9.3, using revised ICRU 73 stopping power tables and the QMD nuclear reaction model. Experimental data derive from Sihver et al. (triangles) and Haettner et al. (circles), where profiles of Haettner et al. were shifted to match more precise measurements of the peak position by D. Schardt et al. All experimental data by courtesy of D. Schardt.
A. Lechner et al., NIM B 268-14 (2010) 2343-2354

Models for antiprotons

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

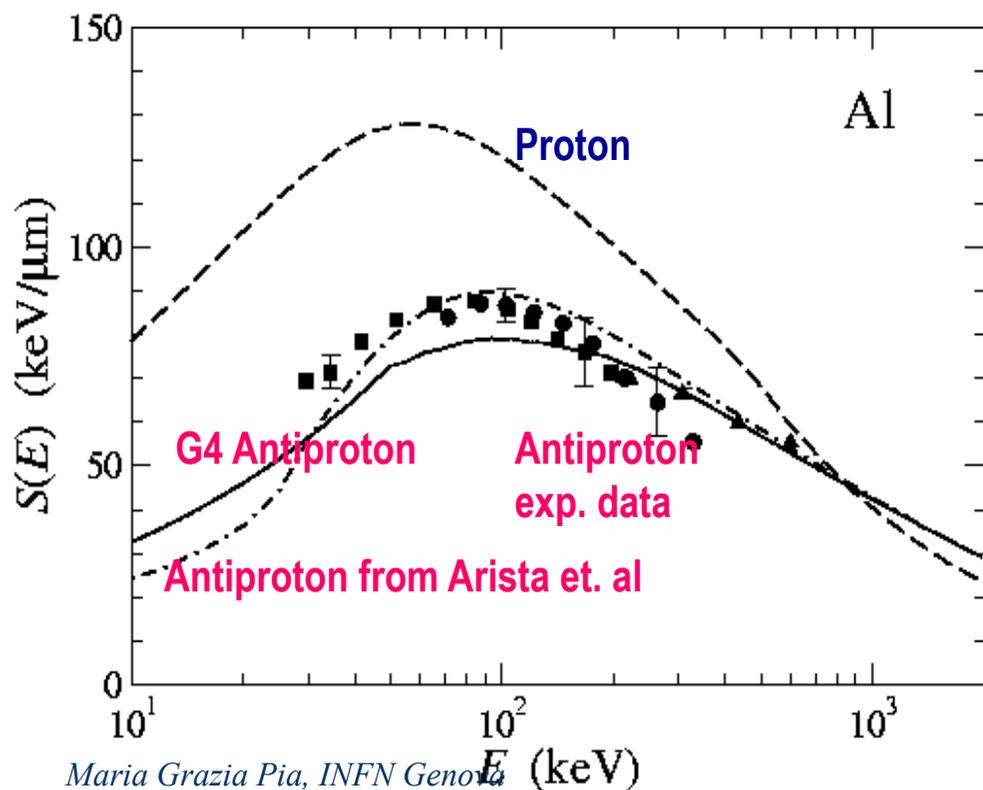
Stéphane Chauvie, Petteri Nieminen, and Maria Grazia Pia

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

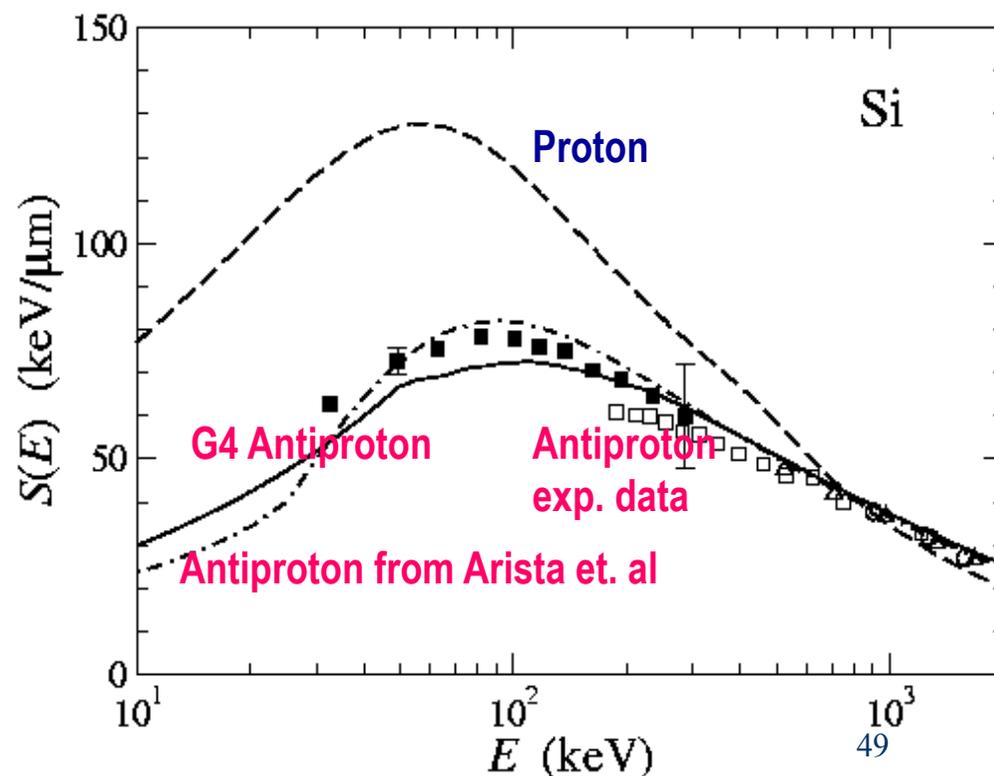
Bethe-Bloch formula

Quantum harmonic oscillator model

Free electron gas mode



Maria Grazia Pia, INFN Genova



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Geant4 Atomic Relaxation **9 pages**

Susanna Guatelli, Alfonso Mantero, Barbara Mascialino, Petteri Nieminen, and Maria Grazia Pia

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

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

Maria Grazia Pia, Paolo Saracco, and Manju Sudhakar

PIXE Simulation With Geant4 **36 pages**

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

PIXE

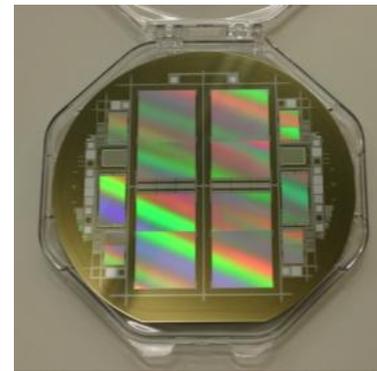
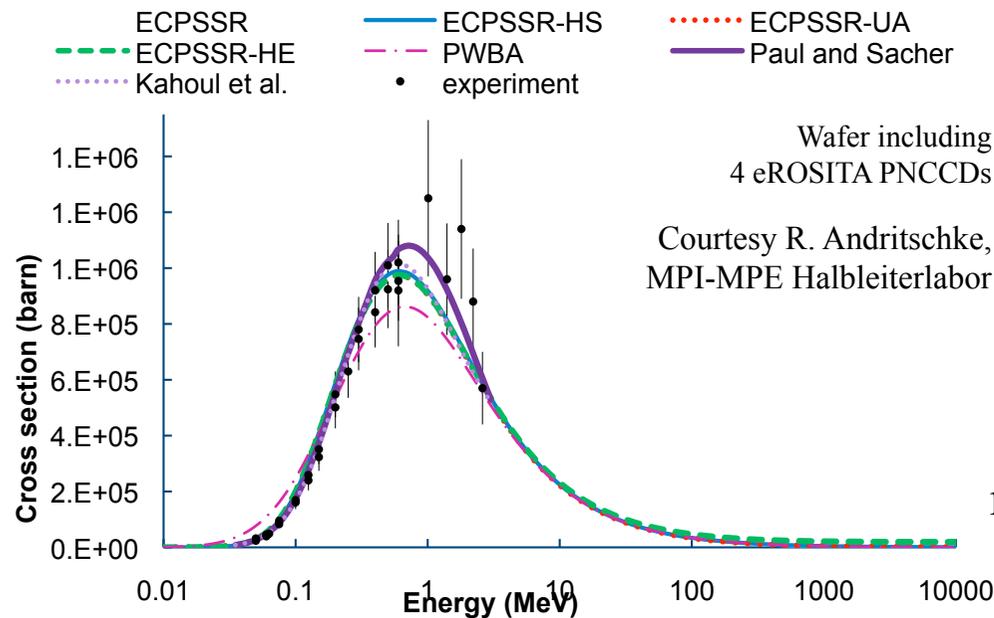
3614

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



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

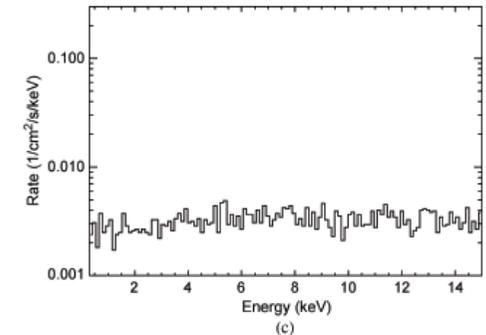
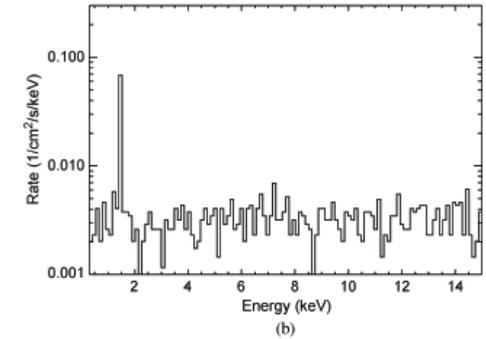
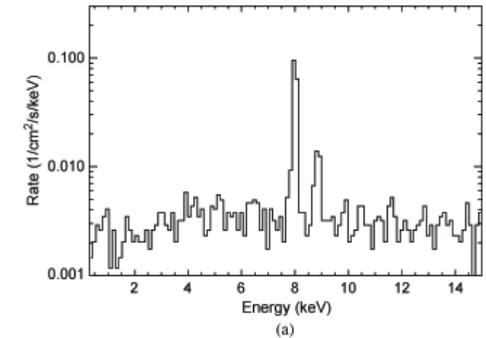
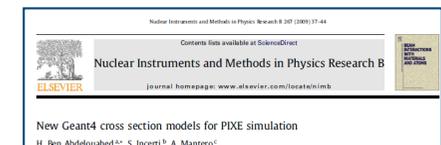


Fig. 12. A comparison of the fluorescence background due to ionization by cosmic-ray protons in an L2 orbit for three different graded Z shield designs for the eROSITA X-ray detectors. (a) Cu shield; (b) Cu-Al shield; (c) Cu - Al - B₄C shield.

Maria Grazia Pia, INFN Genova

Other implementation released
in Geant4 9.2: several flaws



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

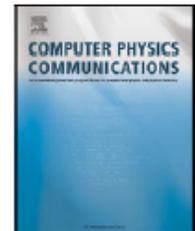
Matej Batič, Maria Grazia Pia, and Paolo Saracco



Contents lists available at SciVerse ScienceDirect

Computer Physics Communications

www.elsevier.com/locate/cpc



ISICSoo: A class for the calculation of ionization cross sections from ECPSSR and PWBA theory [☆]

Matej Batič ^{a,b,*}, Maria Grazia Pia ^a, Sam J. Cipolla ^c

Evaluation of atomic electron binding energies for Monte Carlo particle transport

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

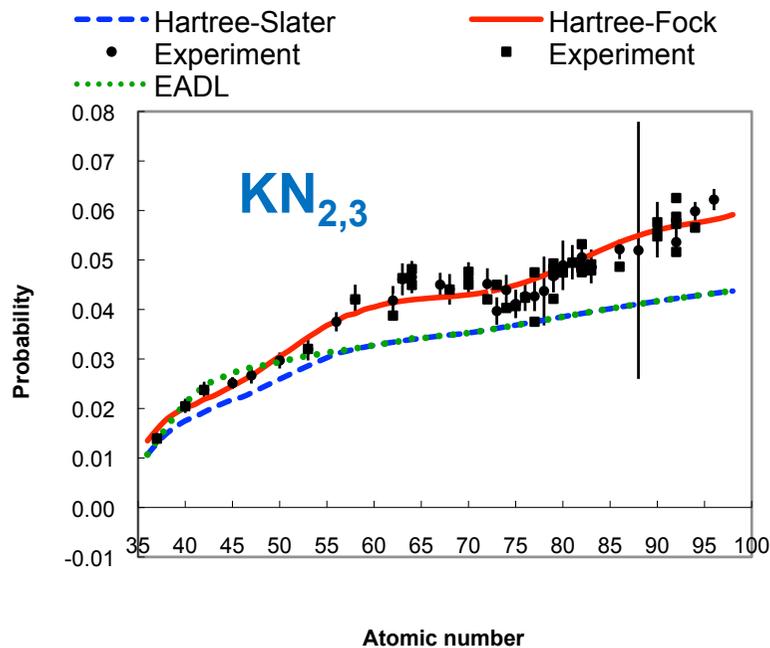
Atomic parameters

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

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

Geant4 X-ray fluorescence simulation is as good as EADL

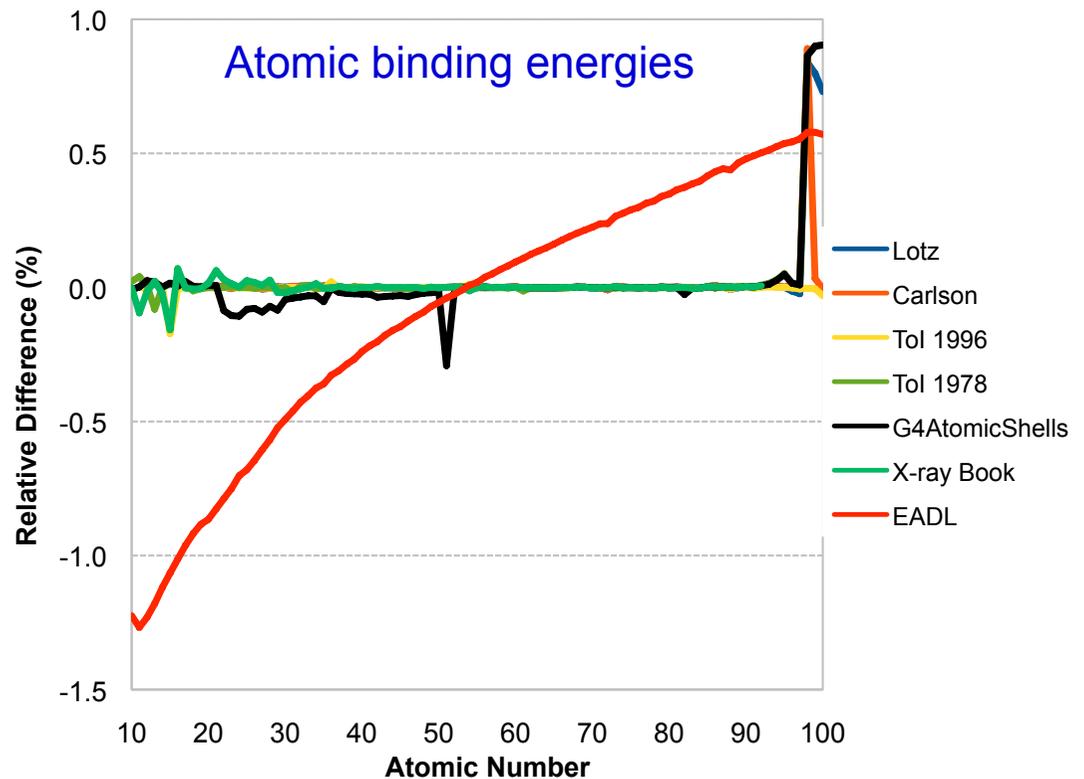
Radiative transition probabilities



Hartree-Slater and Hartree-Fock calculations compared to experiments

Maria Grazia Pia, INFN Genova

Atomic binding energies



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

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. Karamitros¹, A. Mantero², S. Incerti^{1*}, G. Baldacchino³, P. Barberet¹, M. Bernal^{4,5}, R. Capra⁶, C. Champion⁷, Z. El Bitar⁸,
Z. Francis⁹, W. Friedland¹⁰, P. Guèye¹¹, A. Ivanchenko¹, V. Ivanchenko^{7,12}, H. Kurashige¹³, B. Mascialino¹⁴, P. Moretto¹,
P. Nieminen¹⁵, G. Santin¹⁵, H. Seznec¹, H. N. Tran¹, C. Villagrasa⁹ and C. Zacharatou¹⁶

Still consistent with transport assumptions?

Ionisation models for nano-scale simulation

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

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

Hee SEO¹, Maria Grazia PIA^{2*}, Paolo SARACCO², Chan-Hyeung KIM¹

¹ *Hanyang University, 133-791 Seoul, Korea*
² *INFN Sezione di Genova, 16146 Genova, Italy*

Best Student Award Monte Carlo 2010

IEEE TRANSACTIONS ON NUCLEAR SCIENCE

Ionization cross sections for low energy electron transport

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

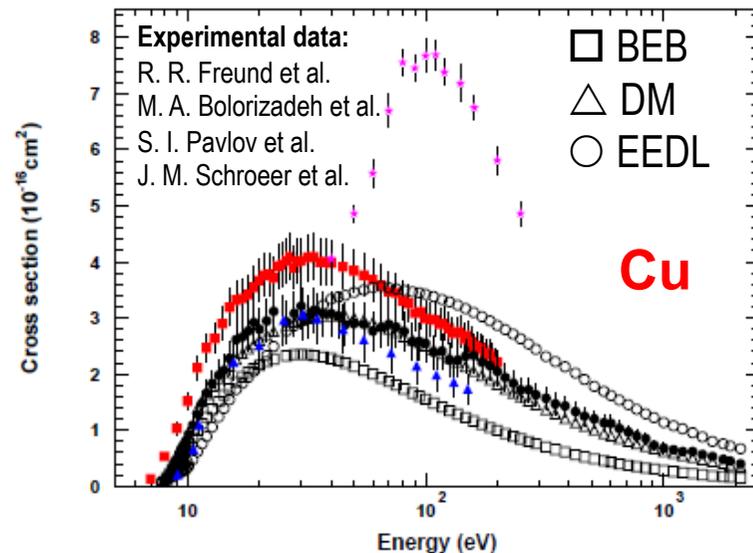
IEEE Trans. Nucl. Sci., vol. 58, no. 6, December 2011

Cross section models

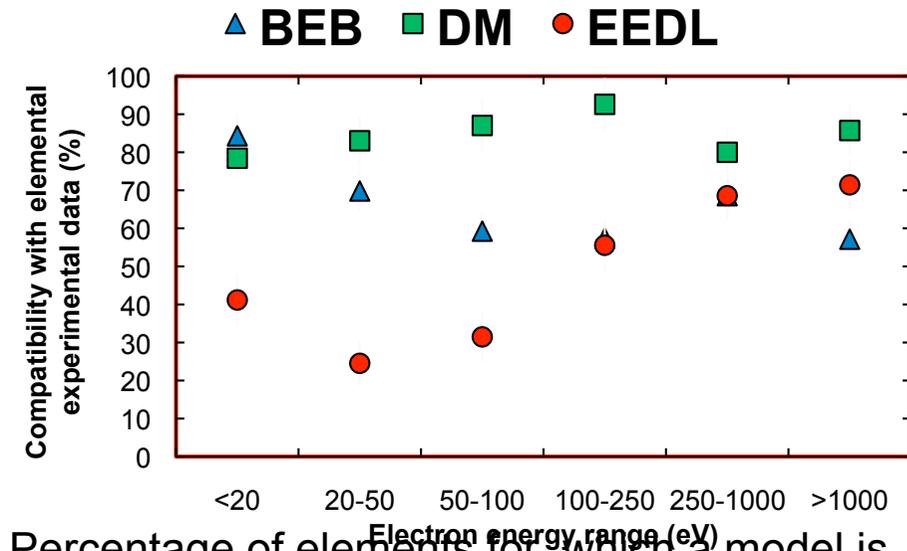
- Binary-Encounter-Bethe (**BEB**)
- Deutsch-Märk (**DM**)
- **EEDL** (*Geant4 Low Energy*)

Validation

- 57 elements
- 181 experimental data sets



Maria Grazia Pia, INFN Genova



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

Hadronic physics challenge

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

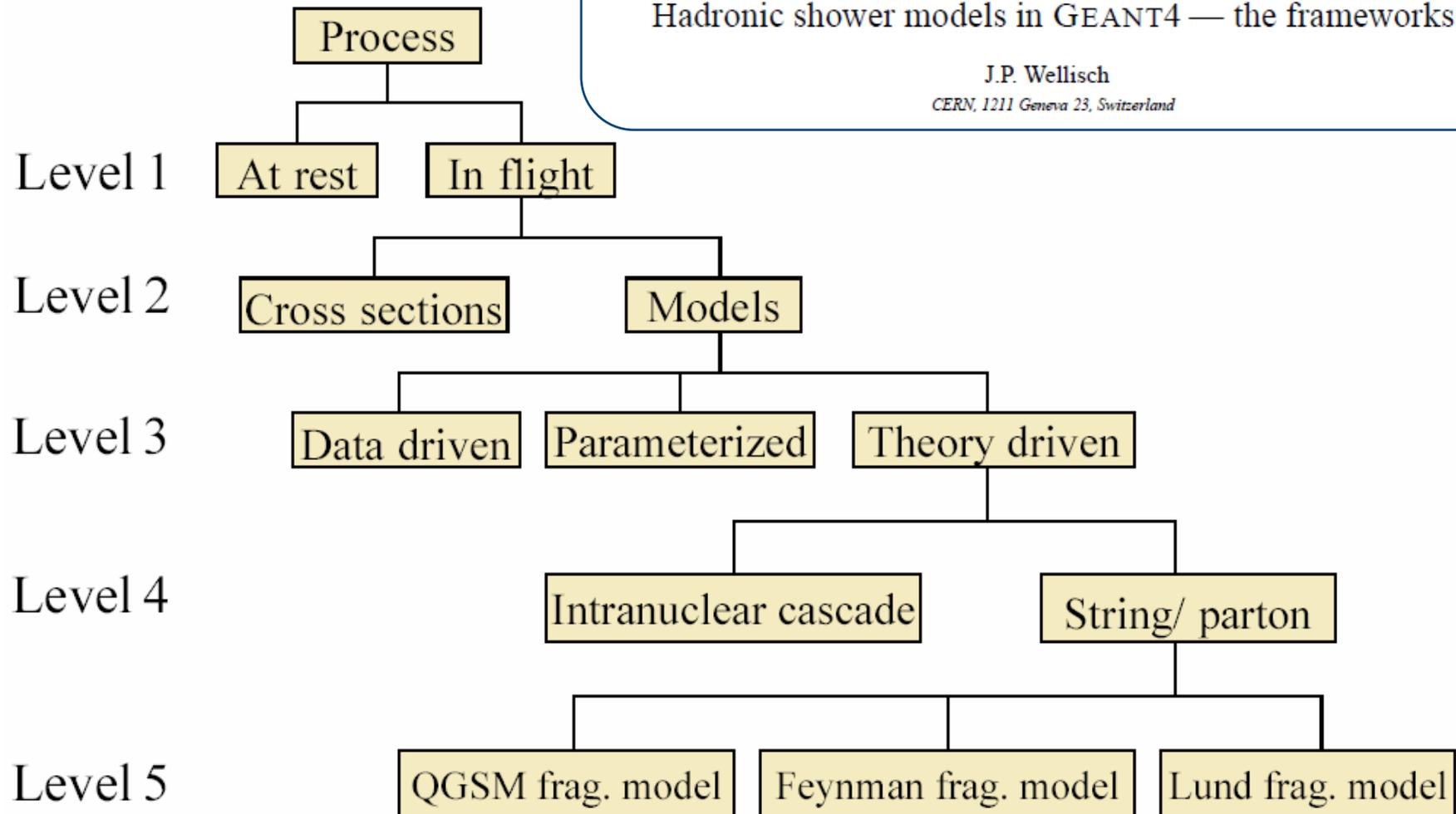
Hadronic framework



Hadronic shower models in GEANT4 — the frameworks

J.P. Wellisch

CERN, 1211 Geneva 23, Switzerland



Hadronic process

- **At rest**

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

- **Elastic**

- Multiple models available

- **Inelastic**

- Different processes for each hadron (with multiple models)
- Photo-nuclear, electro-nuclear, μ -nuclear

- **Capture**

- Pion- and kaon- in flight, neutron

- **Fission**

Cross sections

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

Alternative cross sections

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

Nuclear elastic scattering

G4HadronElasticProcess

G4HadronElasticDataSet

G4LElastic

G4ElasticCascadeInterface

*Not to be confused with
G4CascadeElasticInterface*

G4UHadronElasticProcess

G4HadronElastic

G4WHadronElasticProcess

*Meant to treat elastic models similarly to
inelastic ones*

G4DiffuseElastic

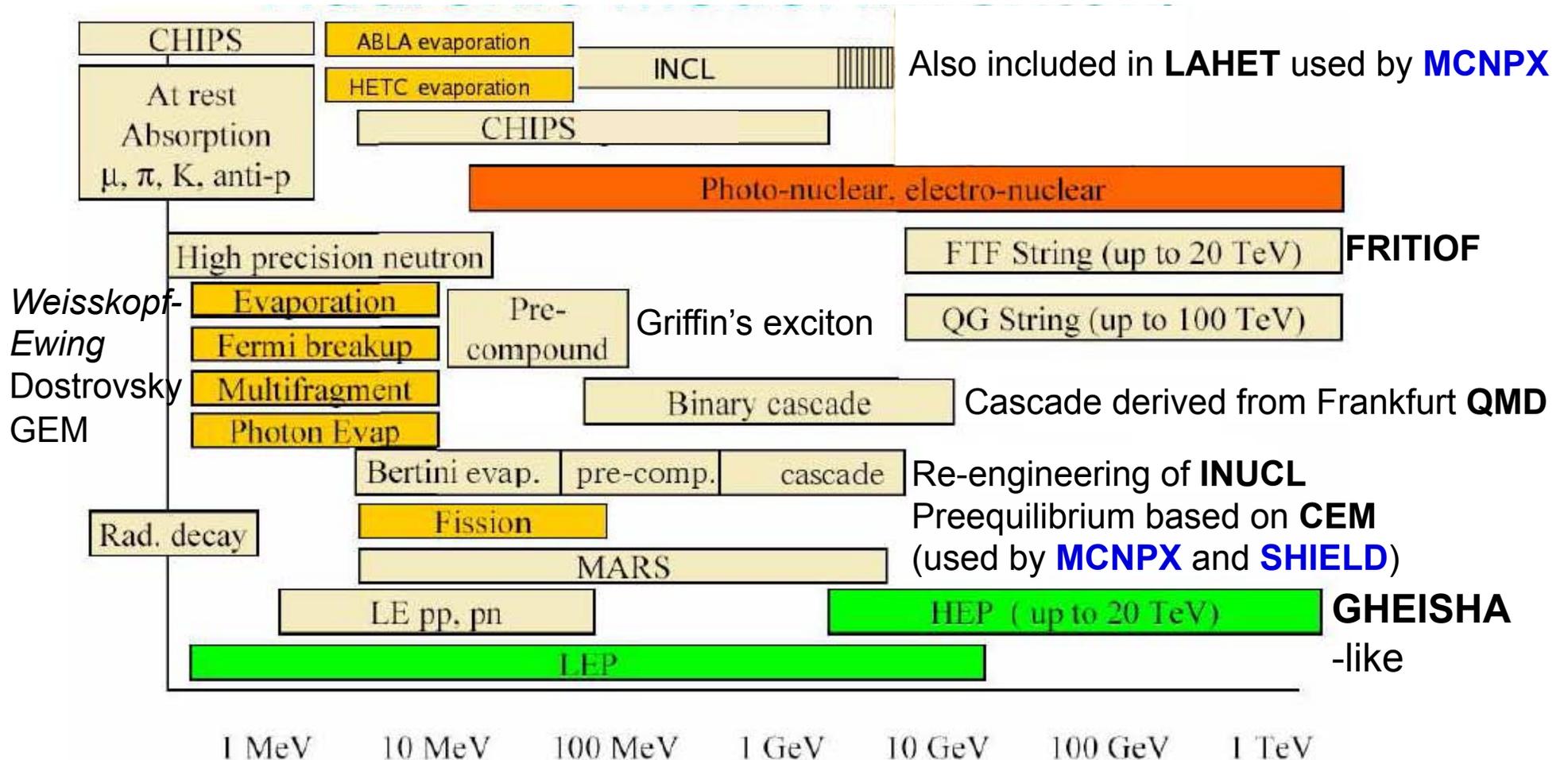
V. Grichine, "GEANT4 hadron elastic diffuse model,"
Comp. Phys. Comm., vol. 181, pp. 921–927, 2010

G4QElasticProcess
AKA "CHIPS elastic"

G4QElasticCrossSection

Hadronic inelastic model inventory

- Data-driven
- Parameterised
- Theory-driven models



Parameterised and data-driven hadronic models

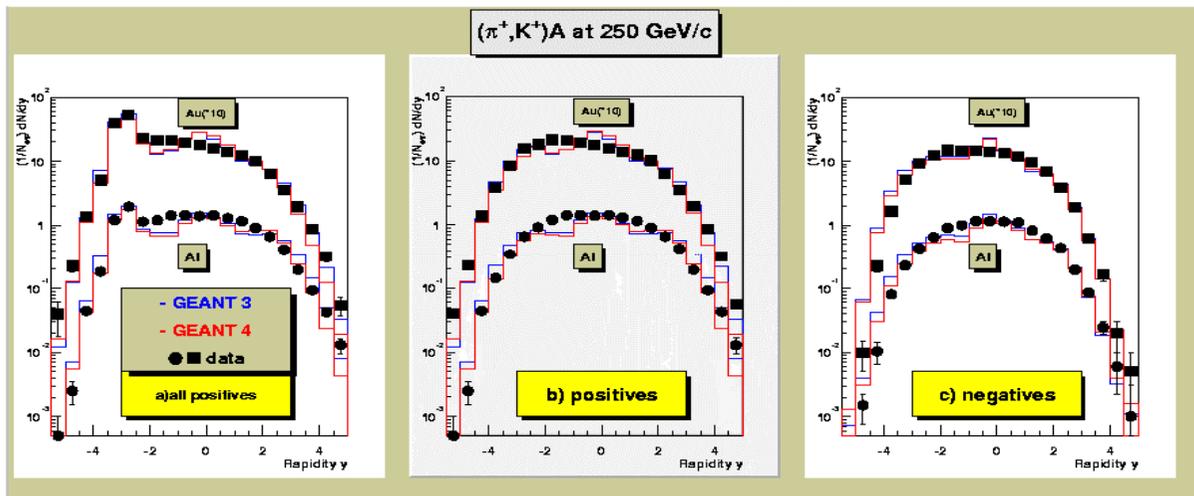
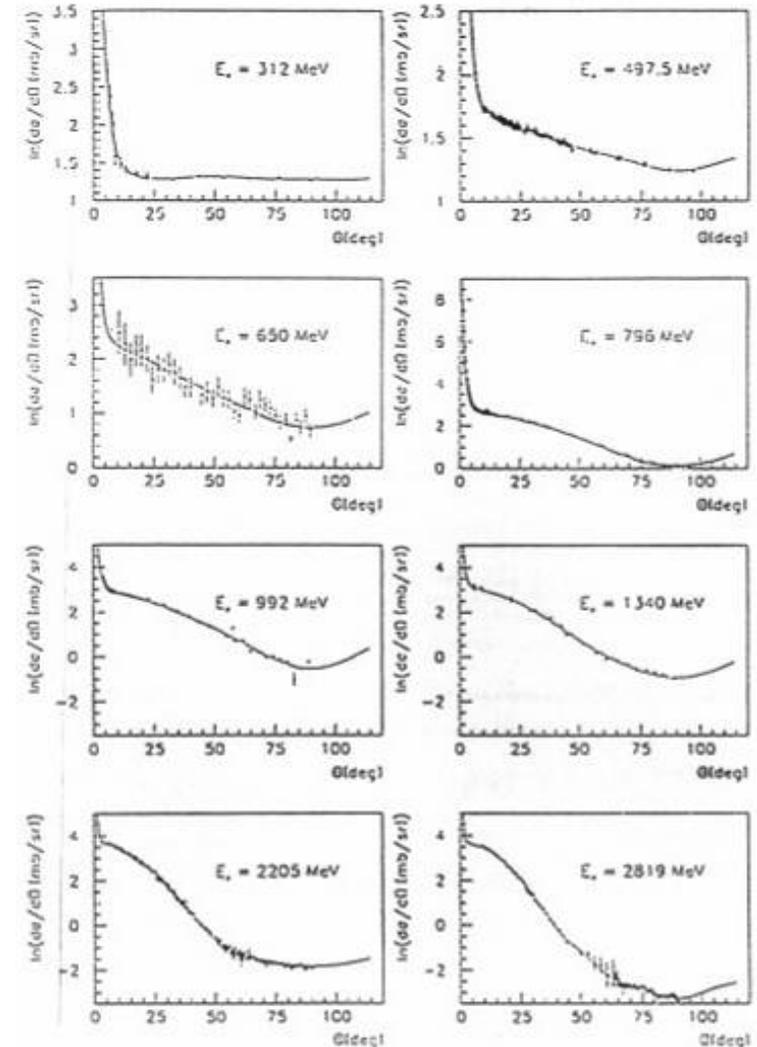
Based on experimental data

- 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
- π N, total cross section
- π N, coherent elastic scattering

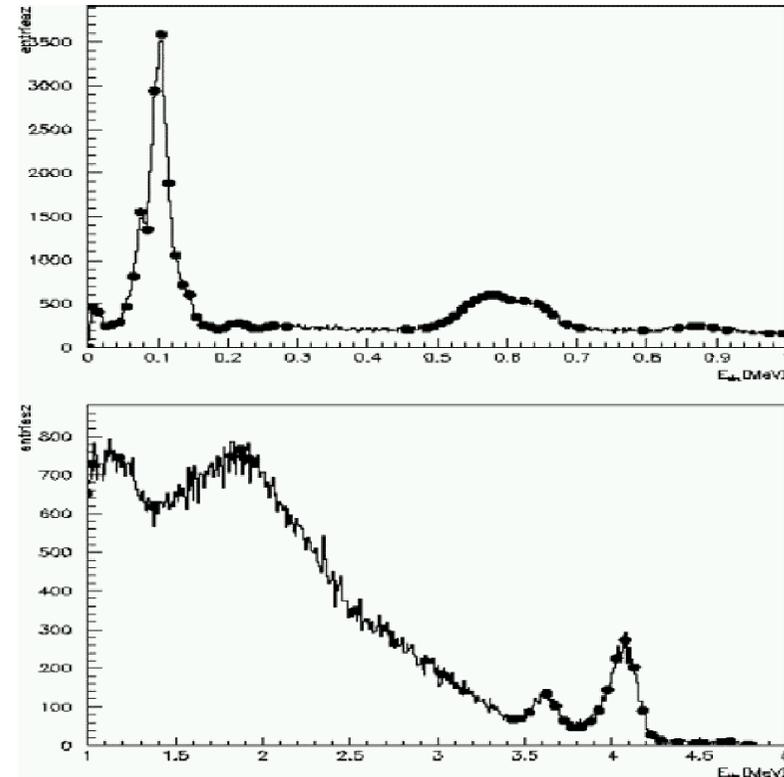


Theory-driven hadronic non-elastic models

- 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**

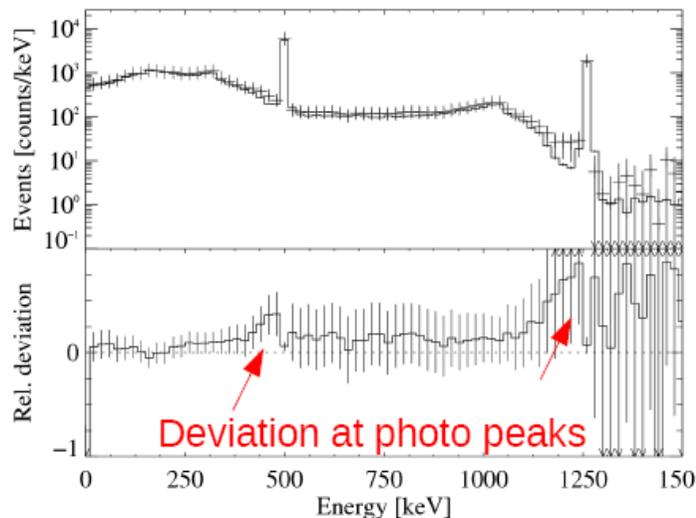
Transport of low-energy neutrons

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

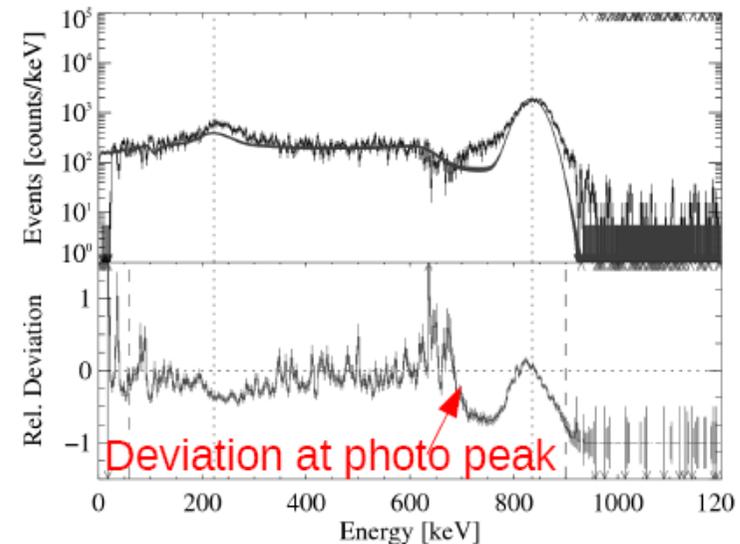
Radioactive decay

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

HPGe measurement and simulation of ^{22}Na



NaI measurement and simulation of ^{54}Mn



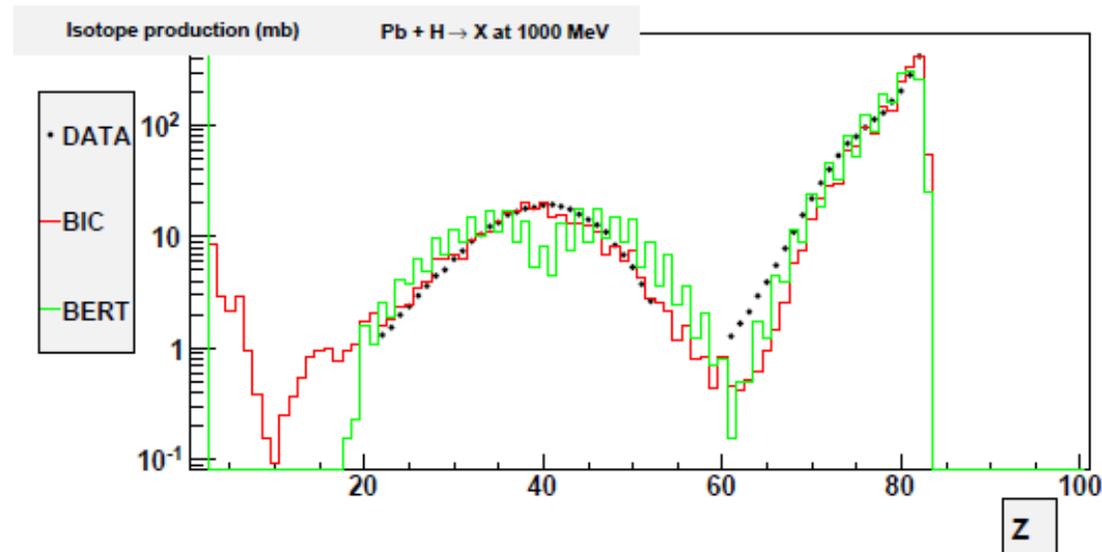
Validation in progress (S. Hauf et al.), experimental data: Z.W. Bell, ORNL

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**



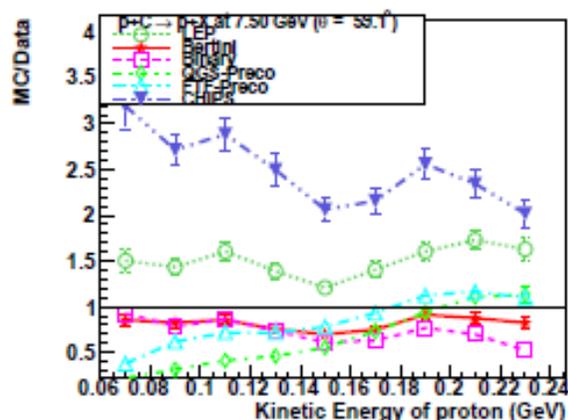
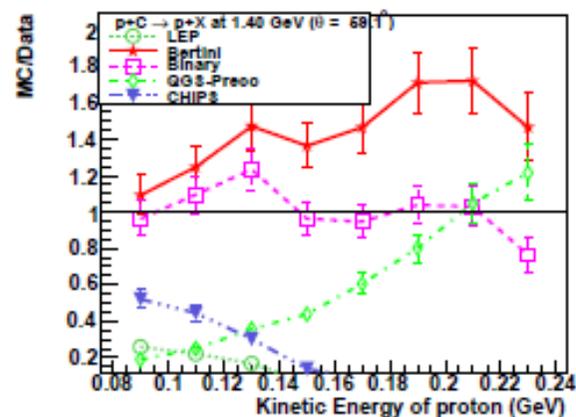
Calibration or validation?

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

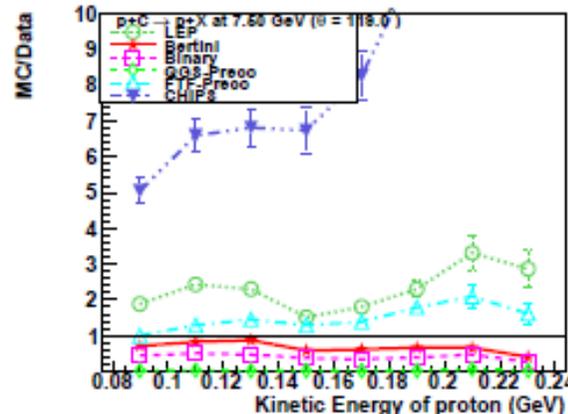
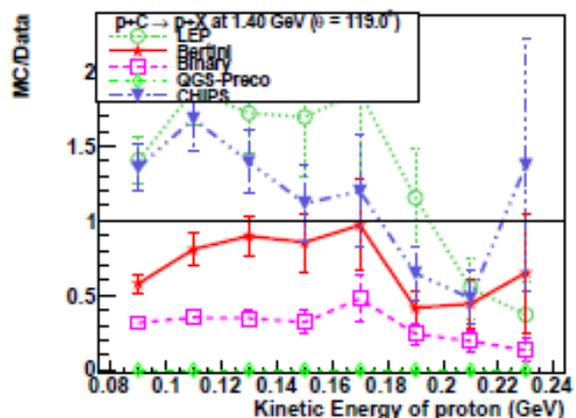
Recent Developments In Pre-Equilibrium And De-Excitation Models In Geant4

José Manuel QUESADA^{1,*}, Vladimir IVANCHENKO^{2,3,4}, Anton IVANCHENKO^{2,5},
Miguel Antonio CORTÉS-GIRALDO¹, Gunter FOLGER², Alex HOWARD⁶, Dennis WRIGHT⁷
on behalf of the Geant4 Hadronic Working Group

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

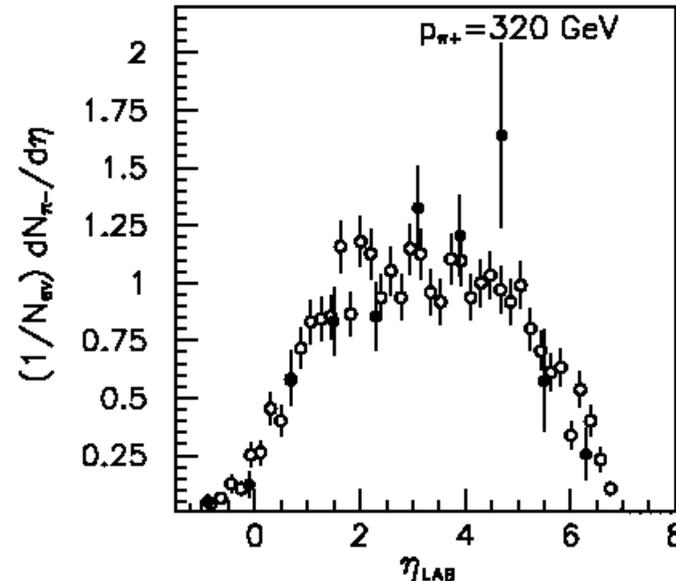
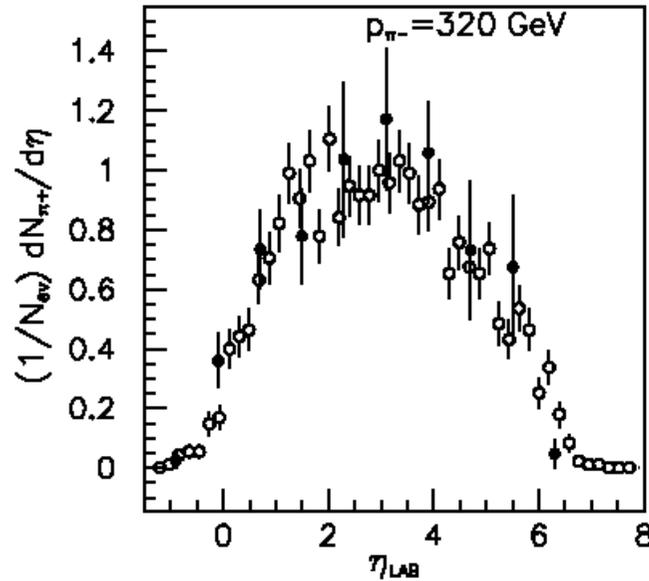
Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2010 (SNA + MC2010)
 Hitotsubashi Memorial Hall, Tokyo, Japan, October 17-21, 2010

Validation of GEANT4 Hadronic Generators versus Thin Target Data

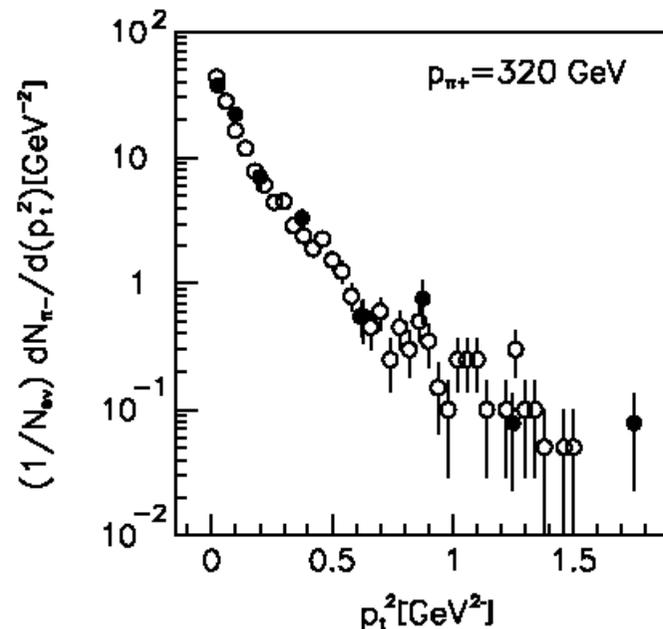
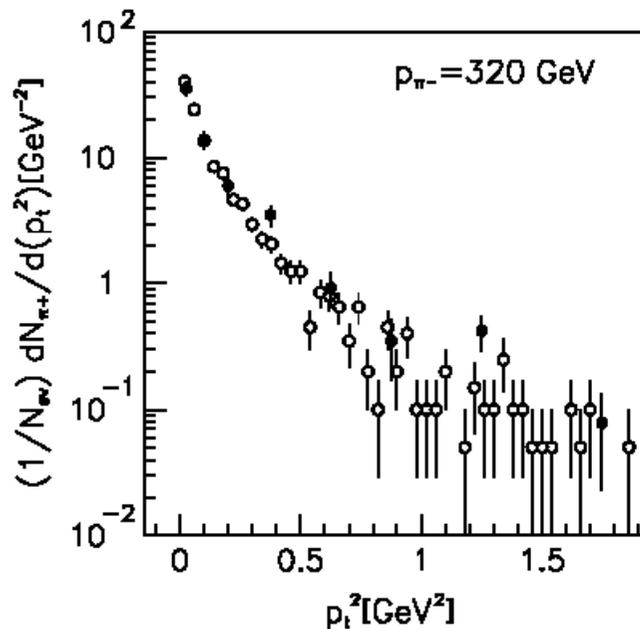
Banerjee¹, G. Folger², A. Ivanchenko^{2,3}, V. N. Ivanchenko^{2,4,5}, M. Kossov², J. M. Quesada⁶, A. Schalelicke⁷, V. Uzhinsky², H. Wenzel¹, D. H. Wright⁸ and J. Yarba¹

Experimental comparisons: QGS

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

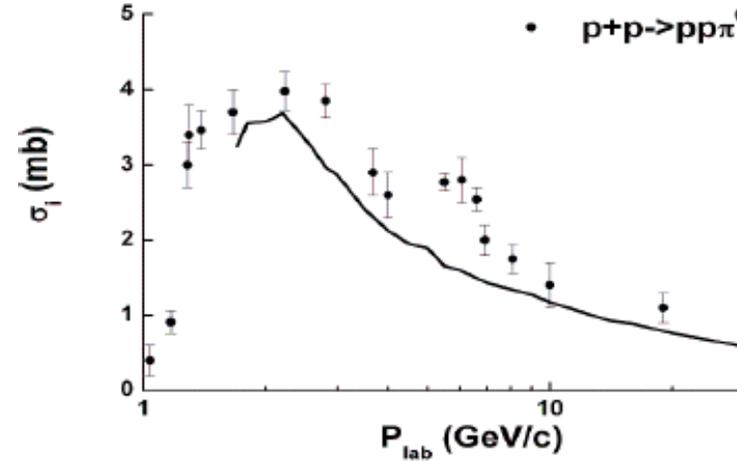
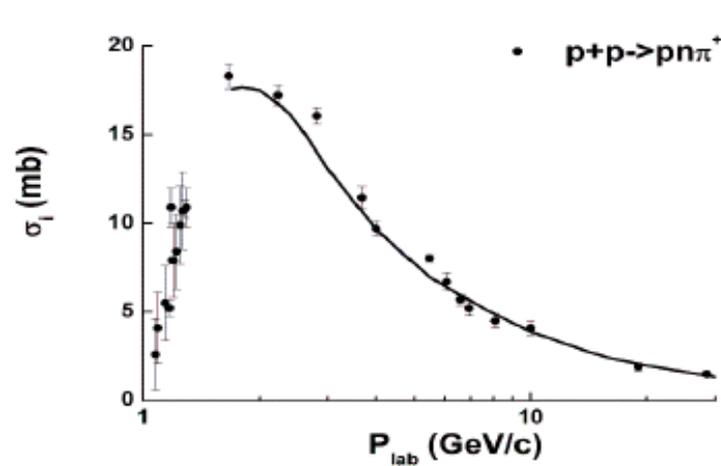


Comparison of differential pion yields for positive and negative pions in pion-Mg reactions at 320 GeV lab momentum



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

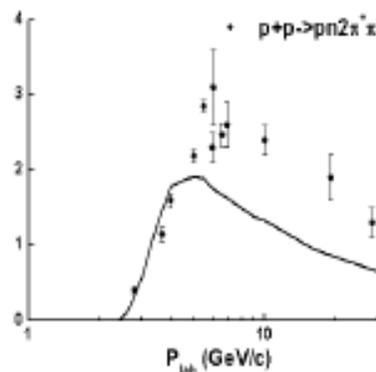
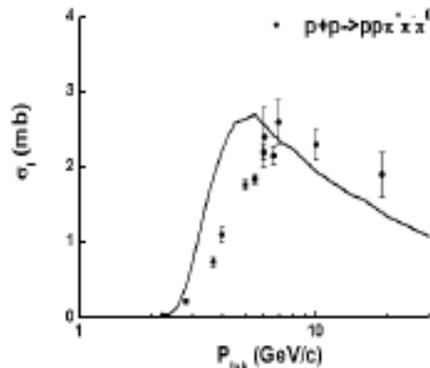
Experimental comparisons - FRITIOF



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

More in 

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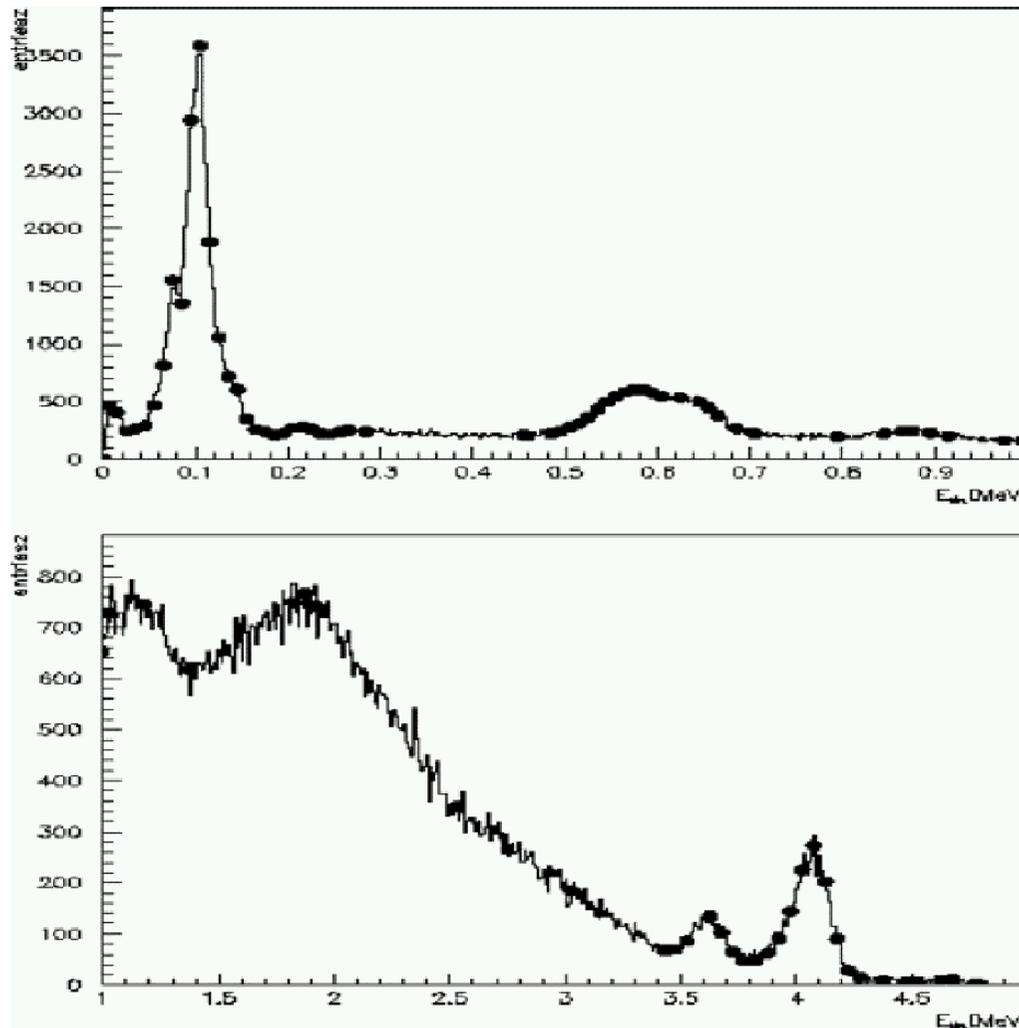
Development of the Fritiof Model in Geant4

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

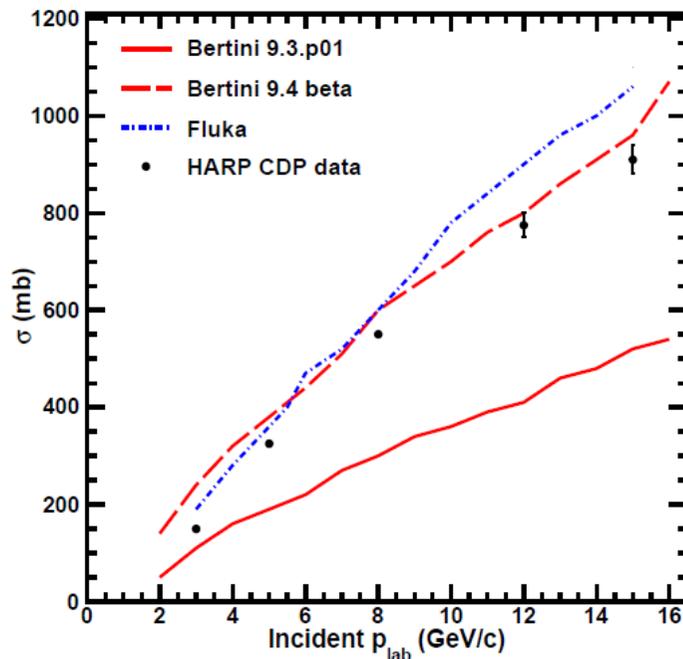
HP neutron models



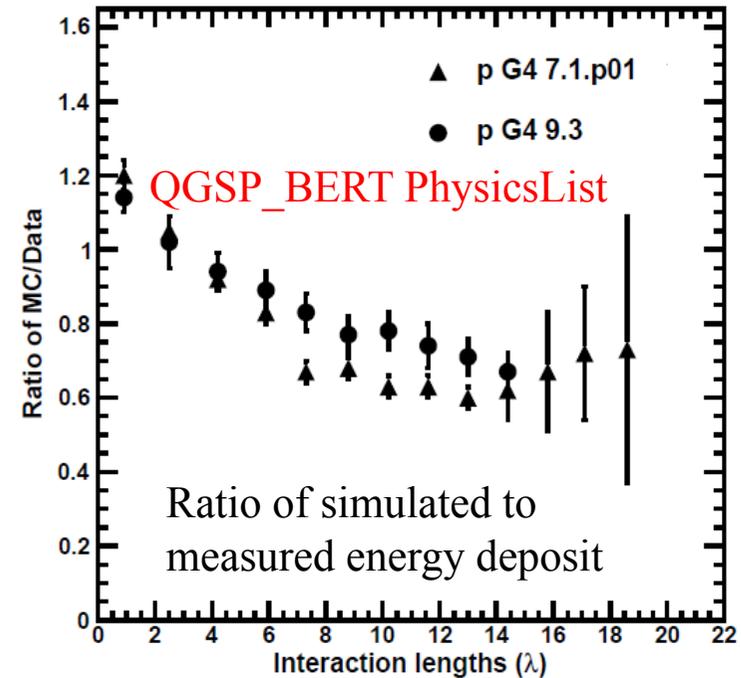
Geant4 simulation
of γ -rays from
14 MeV neutron
capture on uranium

Recent improvements

Transition across models vs. energy



Shower shapes



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

More in 

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

An Overview of Geant4 Hadronic Physics Improvements

Validation

*Recognized as an
American National Standard (ANSI)*

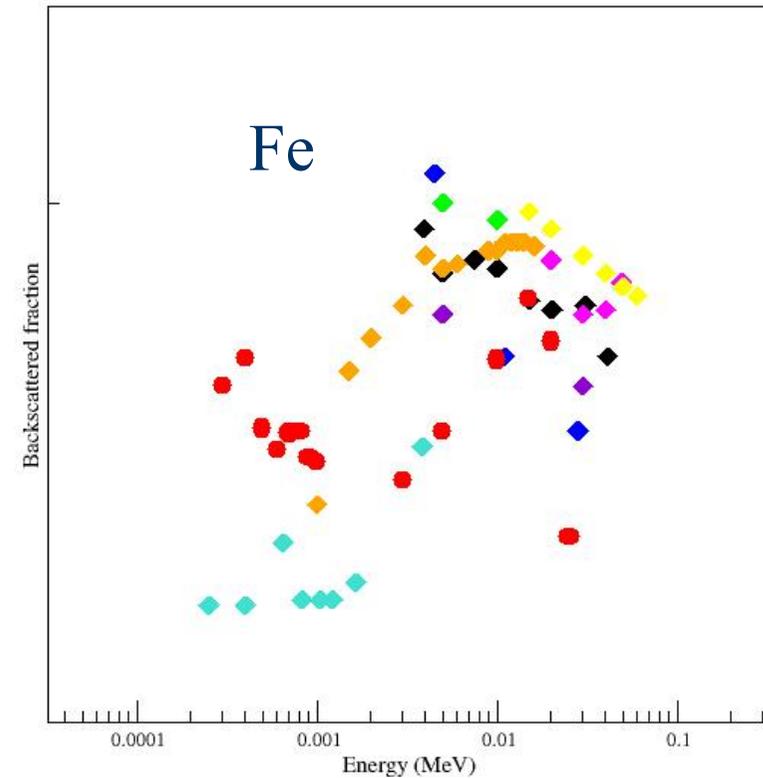
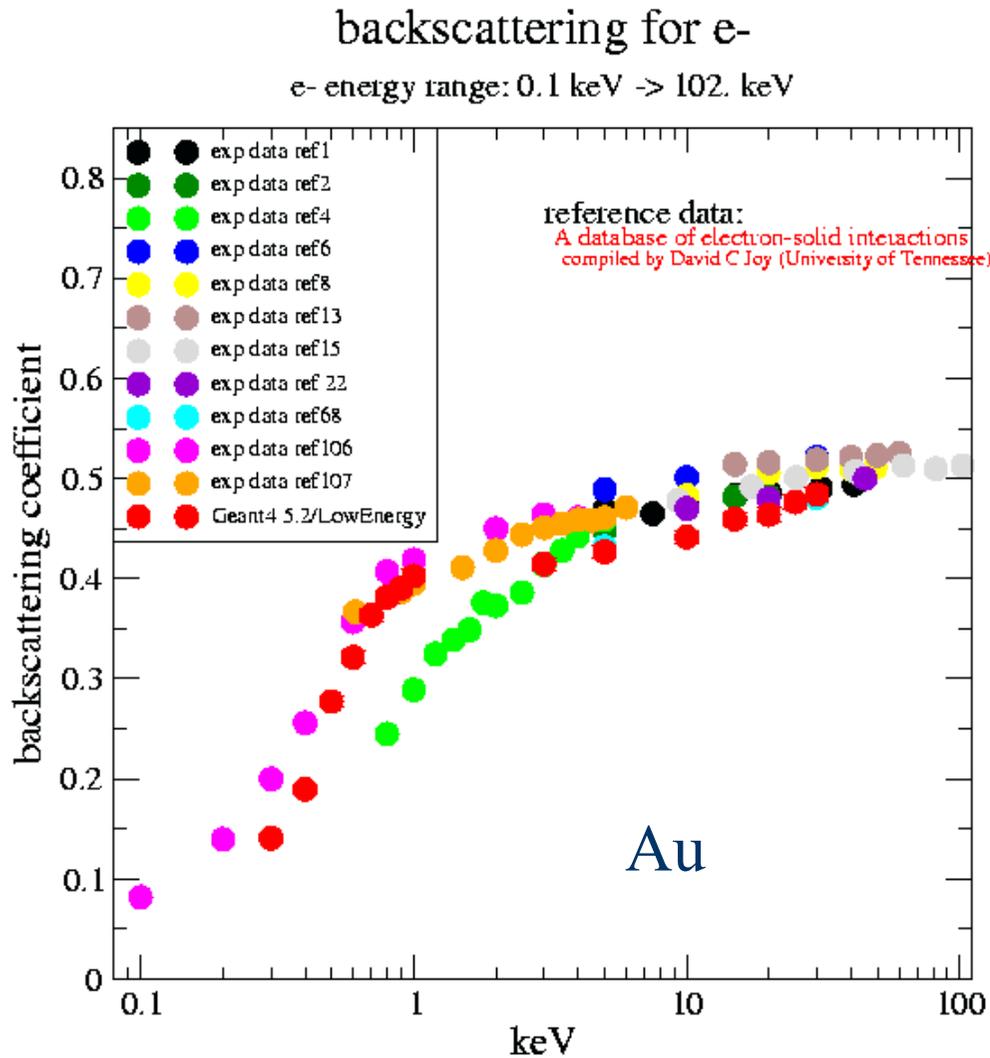
IEEE Std 1012™-2004
(Revision of
IEEE Std 1012-1998)

IEEE Standard for Software Verification and Validation

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

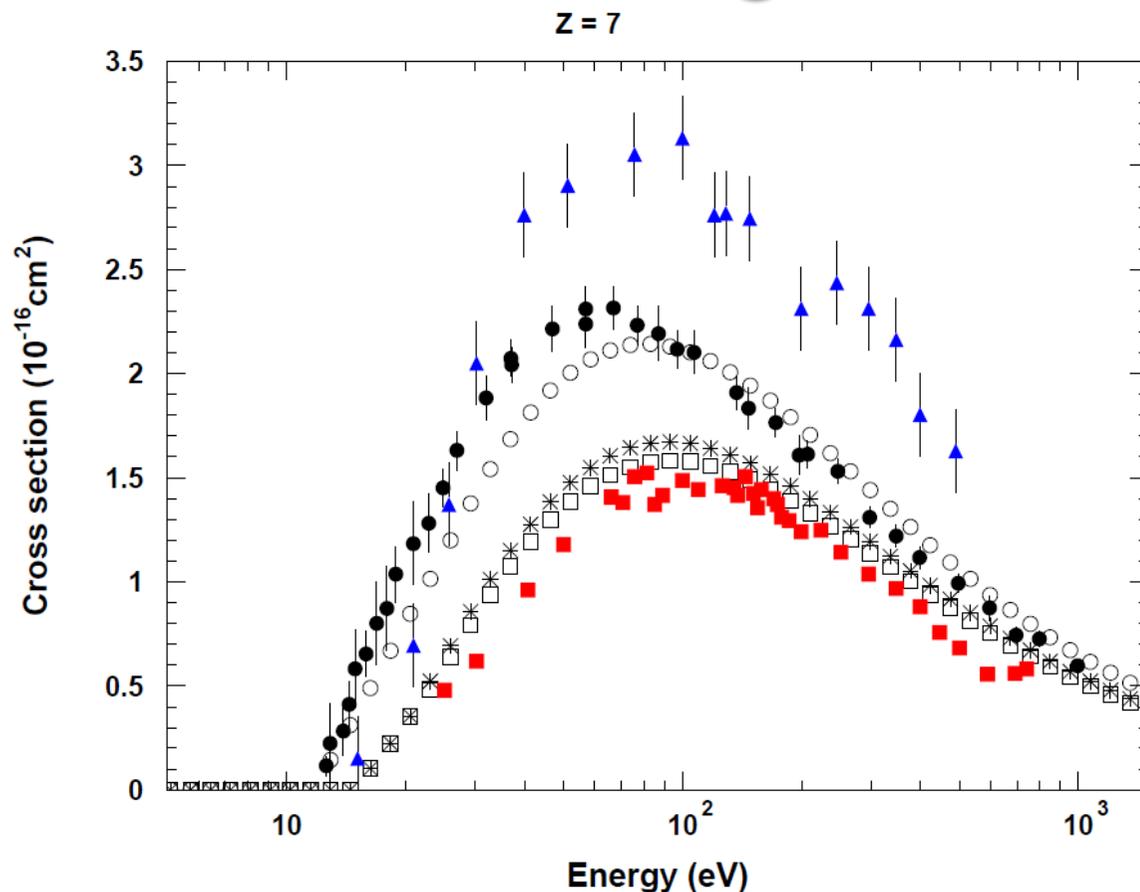
- 1) **Satisfy system requirements** allocated to software at the end of each life cycle activity
- 2) **Solve the right problem** (e.g., correctly model physical laws, implement business rules, use the proper system assumptions)
- 3) **Satisfy intended use and user needs**

The main problem of validation: experimental data!



Experimental data often
exhibit large differences!

Which one is right?



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

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



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 APOSTOLAKIS¹, Alexander BAGULYA⁴, Haifn Ben ABDELOUAHED⁵, Rachel BLACK⁶, Alexey BOGDANOV⁷, Helmut BURKHARD¹, Stéphane CHAUVIE⁸, Pablo CIRRONE⁹, Giacomo CUTTONE⁷, Gerardo DEPAOLA¹⁰, Francesco Di ROSA⁹, Sabine ELLES¹¹, Ziad FRANCIS¹², Vladimir GRICHINE¹, Peter GUMPLINGER¹³, Paul GUEYE⁸, Sébastien INCERTI¹⁴, Anton IVANCHENKO¹⁴, Jean JACQUEMIER¹¹, Anton LECHNER^{1,15}, Francesco LONGO¹⁶, Omrane KADRI⁹, Nicolas KARAKATSANIS¹⁷, Mathieu KARAMITROS¹⁴, Rostislav KOKOULIN⁷, Hisaya KURASHIGE¹⁸, Michel MAIRE^{11,19}, Alfonso MANTERO²⁰, Barbara MASCIALINO²¹, Jakub MOSCICKI¹, Luciano PANDOLA²², Joseph PERL²³, Ivan PETROVIC⁹, Aleksandra RISTIC-FIRA⁴, Francesco ROMANO⁹, Giorgio RUSSO⁹, Giovanni SANTIN²⁴, Andreas SCHAEELICKE²⁵, Toshiyuki TOSHITO²⁶, Hoang TRAN¹⁴, Laszlo URBAN¹⁹, Tomohiro YAMASHITA²⁷ and Christina ZACHARATOU²⁸

Validation or calibration?

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

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

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



Validation is holistic

One must validate the entire calculation system

Including:

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



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



The launch of STS-107 on January 16, 2003

Columbia Space Shuttle accident, 2003

Can we quantify our ignorance?

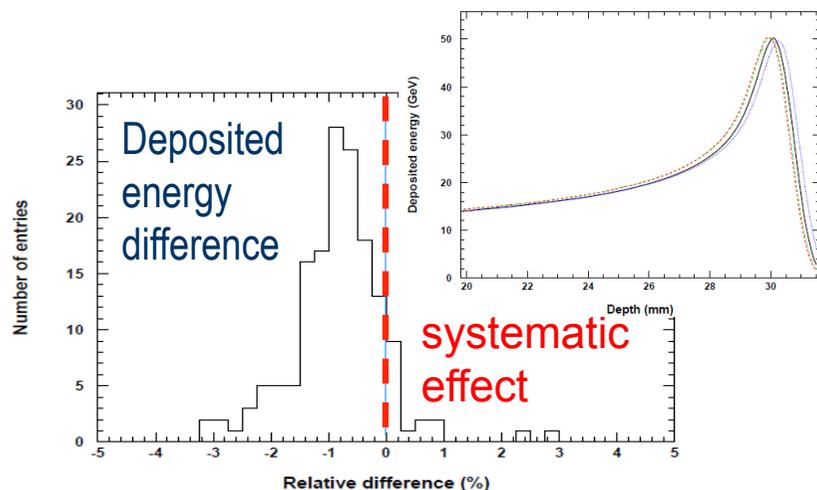
Simulation codes usually contain parameters or model assumptions, which are not validated (because of lack of experimental data, or conflicting data)

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

Or we may use a simulation model outside the range where it has been validated

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

Can we quantify them?



No generally accepted method of measuring epistemic uncertainties

Interval analysis

Dempster-Shafer theory of evidence

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

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

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

Dedicated INFN UQ project

Geant4 pre-assembled physics lists

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

Through the narrow gate

- **Think**

- **Learn**

- Master the technology
- Search the literature
- Read Geant4 documentation

- **Work**

- You do not run Geant4, you run your own application
- Understand what you are doing
- Understand what Geant4 does



Conclusion

- Geant4 is a rich and powerful tool for experimental research
- ...but it invests the user with responsibility of making **choices**
- **Validation** is ongoing
- Check what is documented in the literature, that may be relevant to your experimental problem
 - **Refereed journals** (conference papers)

Trust what you can document **quantitatively**
Document what you cannot trust *[yet]*

Slides available at

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

Collection of physics references

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

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

Acknowledgment: **Geant4 developers and users**