

Geant4 Physics Validation

Refresher Course

Maria Grazia Pia
INFN Genova, Italy

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This Refresher Course includes Geant4 validation results from several sources: thanks to all the authors!

Special thanks to Sunanda Banerjee for help with Geant4 hadronic physics results

Geant 4

S. Agostinelli et al.

Geant4: a simulation toolkit

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

4332 citations)

Most cited NIM paper

Most cited publication in

- Nuclear Science and Technology
- Instruments and Instrumentation
- **Particle and Fields Physics** (264578 papers)

Most cited CERN publication in WoS (614810 papers)

J. Allison et al.

Geant4 Developments and Applications

IEEE Trans. Nucl. Sci., vol. 53, no. 1, pp. 270-278, 2006

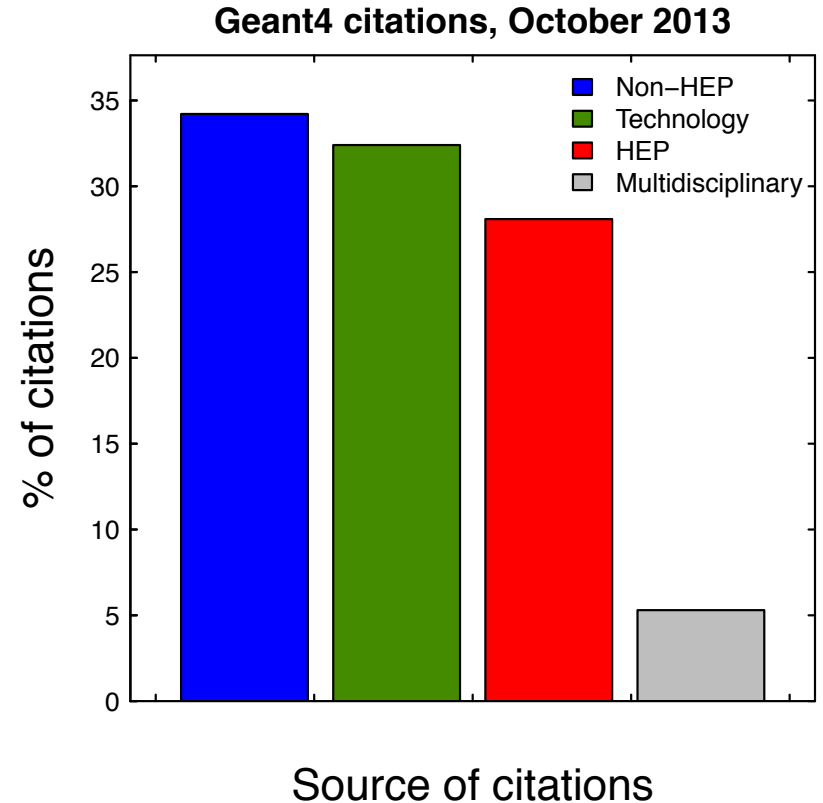
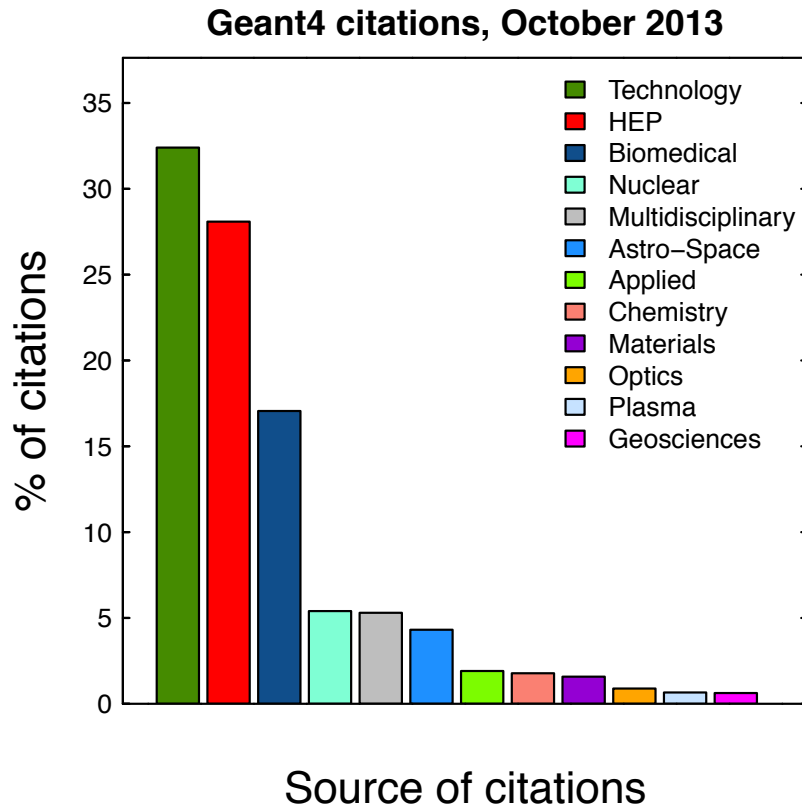
978 citations

Most cited TNS paper

*Many papers cite the NIM paper, but they omit citing the TNS one,
even though both are indicated in <http://cern.ch/geant4>*

Many papers that use Geant4 do not cite either reference

Who uses Geant4?



Based on Thomson-Reuters' Web of Science data

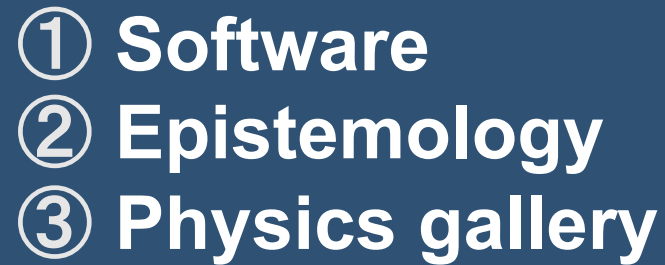
Foreword

- Geant4 is a huge and complex simulation toolkit
- It is used by a wide experimental community
- Practically impossible to cover all its physics validation in approximately one hour

- Emphasis on
 - **Concepts**
 - **Methods**

that let you

- appraise Geant4 physics validity
- select proper physics options for experimental applications

- 
- ① **Software**
 - ② **Epistemology**
 - ③ **Physics gallery**

Focus on Geant4 physics models



- Hardly any systematic, comprehensive, quantitative validation of the “**ingredients**” of Monte Carlo simulation codes is documented in the literature

This lecture: **focus on validation of Geant4 ingredients**

- Highlight quantitative Geant4 validation
 - Where it exists
- Identify differences and similarities of Geant4 models on the basis of quantitatively assessed validity



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 scattering
- γ conversion
- e^+e^- pair production
- Synchrotron radiation
- Transition radiation
- Cherenkov
- Refraction
- Reflection
- Absorption
- Scintillation
- Fluorescence
- Auger emission

Hadronic physics

● Ample variety of models

- Alternative/complementary
- It is possible to mix-and-match, with fine granularity
- **Data-driven, parameterised** and **theory-driven** models

● Sound framework design

- transparent (in the original design)
- clear separation between data and their use in algorithms

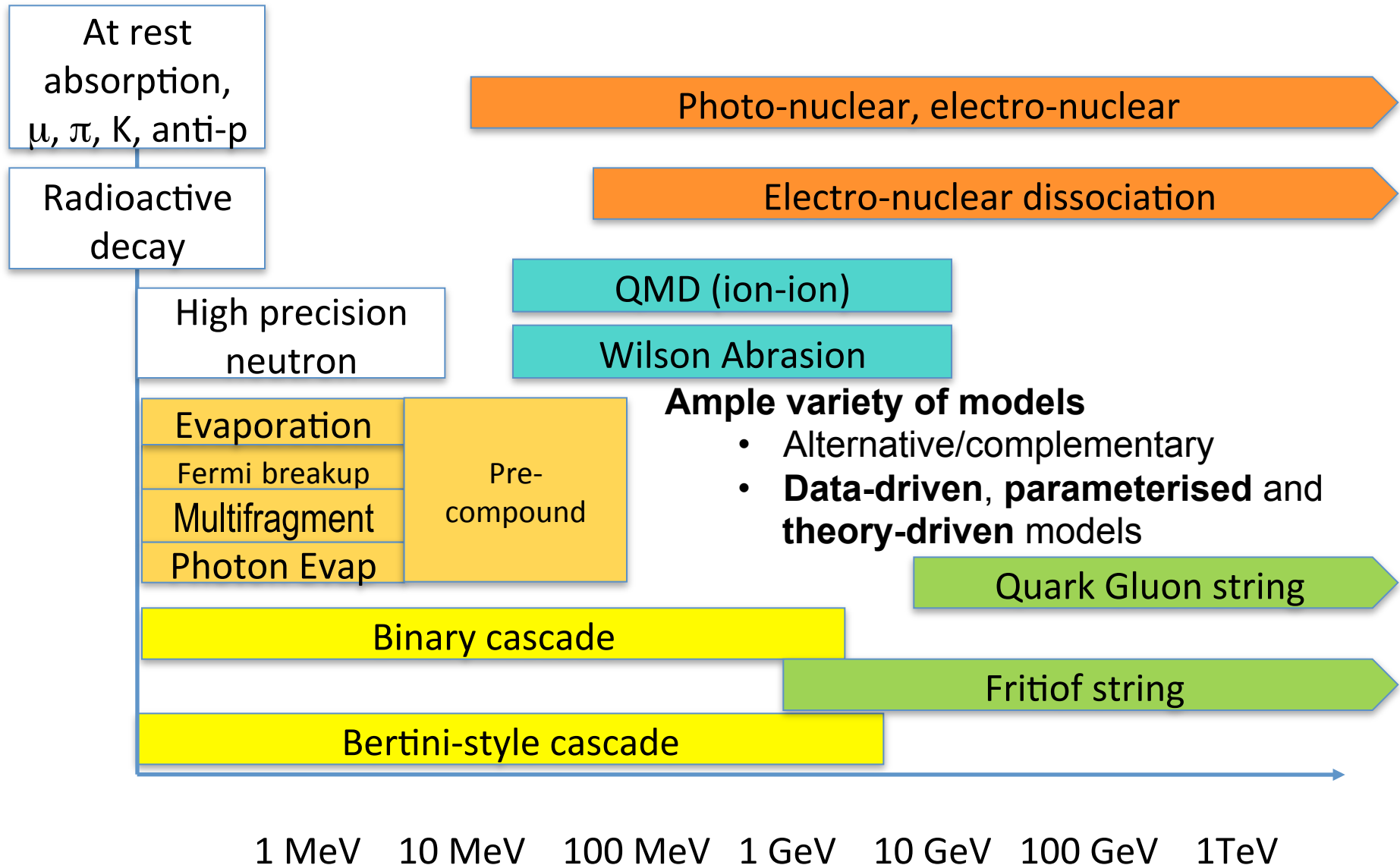
● Cross section data sets

- Transparent and interchangeable

● Final state calculation

- Models by particle, energy, material

Partial Hadronic Model Inventory



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**

G4VUserPhysicsList

- 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 wants to transport particles
 - the **thresholds** to produce secondary particles
- Pure virtual methods
 - ConstructParticles()
 - ConstructProcesses()
 - SetCuts()

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

The user is responsible for selecting the
physics processes and models
to be used in the simulation



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

What is what

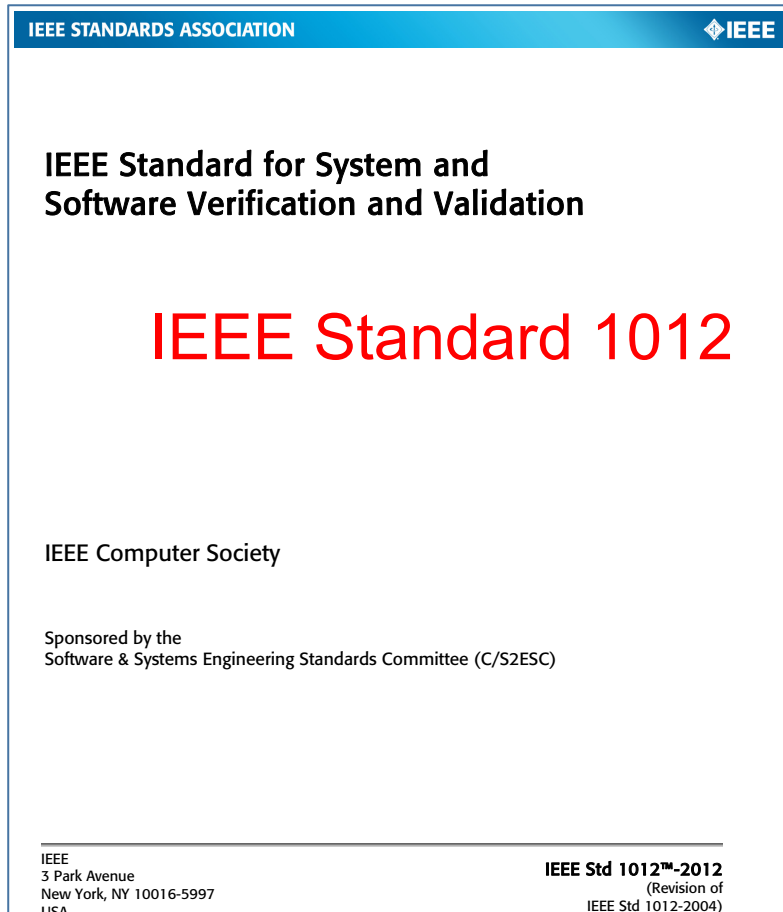
● **Verification**

● **Validation**

● **Calibration**

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

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

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

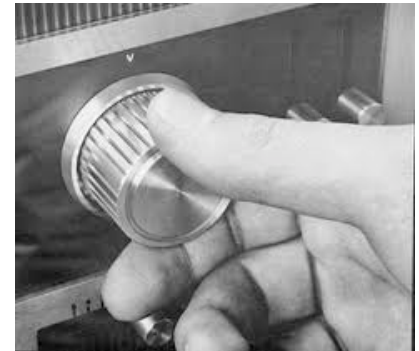
validation = consistency with experimental measurements

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

Calibration

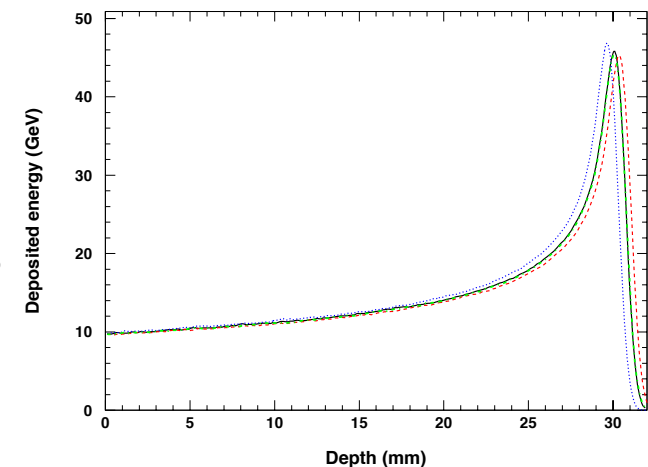
AKA “tuning”

- 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 using different Monte Carlo codes
 - Or comparison of different simulation models
- Comparison of simulation with theory
- Comparison of simulation 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!

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 published²⁶⁾ 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, Haifa Ben ABDELOUAHED⁵, Rachel BLACK⁶, Alexey BOGDANOV⁷, Helmut BURKHARD¹, Stéphane CHAUVIE⁸, Pablo CIRRONE⁹, Giacomo CUTTONE⁹, Gerardo DEPAOLA¹⁰, Francesco DI ROSA⁹, Sabine ELLES¹¹, Ziad FRANCIS¹², Vladimir GRICHINE¹, Peter GUMPLINGER¹³, Paul GUEYE⁸, Sébastien INCERTI¹⁴, Anton IVANCHENKO¹⁴, Jean JACQUEMIER¹⁵, Anton LECHNER^{1,15}, Francesco LONGO¹⁶, Omrane KADRI⁹, Nicolas KARAKATSANIS¹⁷, Mathieu KARAMITROS¹⁴, Rostislav KOKOULDN⁷, Hisaya KURASHIGE¹⁸, Michel MAIRE^{11,19}, Alfonso MANTERO²⁰, Barbara MASCIALINO²¹, Jakub MOSCICKI¹, Luciano PANDOLA²², Joseph PERL²³, Ivan PETROVIC⁹, Aleksandra RISTIC-FIRA⁹, Francesco ROMANO⁹, Giorgio RUSSO⁹, Giovanni SANTINI²⁴, Andreas SCHAELOCKE²⁵, Toshiyuki TOSHITO²⁶, Hoang TRAN¹⁴, Laszlo URBAN²⁷, Tomohiro YAMASHITA²⁷ and Christina ZACHARATOU²⁸

Comparisons of Monte Carlo codes

Phys. Med. Biol. **56** (2011) 811–827

[doi:10.1088/0031-9155/56/3/017](https://doi.org/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](https://doi.org/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](https://doi.org/10.1088/0031-9155/57/5/1231)

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

2012 IEEE Nuclear Science Symposium and Medical Imaging Conference Record (NSS/MIC)

N14-81

Comparison of GEANT4 and MCNPX-PoliMi Fission Models

SHOWER SIMULATIONS, COMPARISON OF FLUKA, GEANT4 AND EGS4
COMPARISON OF GEANT4 WITH EGSnrc FOR SIMULATION OF GAMMA-RADIATION DETECTORS BASED ON SEMI-INSULATING MATERIALS



Shower simulations, comparison of FLUKA, GEANT4 and EGS4



and



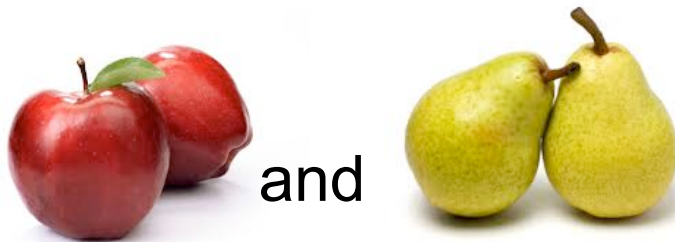
Comparison of GEANT4 very low energy cross section models with experimental data in water

4692 Med. Phys. 37 (9), September 2010

0094-2405/2010/37(9)/4692/17/\$30.00

© 2010 Am. Assoc. Phys. Med. 4692

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



and



Korean?

Validation is holistic

One has to validate the entire calculation system

Including:

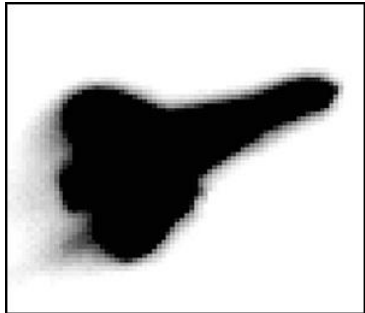
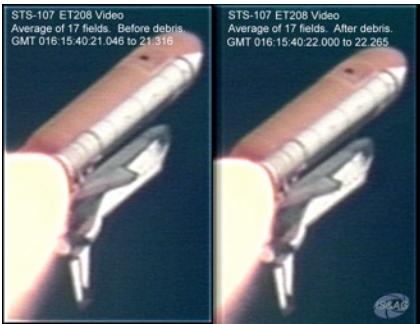


- User
- Computer system
- Problem setup
- Running
- Results analysis



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

Columbia Space Shuttle damage



Columbia breakup



Columbia re-entry

- 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
- Shortly after launch, Boeing did an analysis using the code CRATER to evaluate the likelihood that the wing was seriously damaged
- Problems with analysis:
 - The analysis was carried out by an inexperienced user
 - CRATER was designed to study the effects of micrometeorite impacts, and had been validated only for projectiles less than 1/400 the size and mass of the piece of foam that struck the wing
 - Didn't use a code like LS-DYNA that was the industry standard for assessing impact damage
- The prior CRATER validation results indicated that the code gave conservative predictions
- Analysis indicated that there might be some damage, but probably not at a level to warrant concern
- *(Maybe there was no way to fix the problem and avoid the accident)*

— NASA Columbia Shuttle Accident Report

Establishing validity



Agreement
Good agreement
Excellent agreement
Satisfactory agreement
...

Comparison of simulation results and experimental data in the literature mainly rests on

- qualitative visual appraisal of figures
- indicators (%) deprived of any statistical relevance

Statistics

- Mathematical foundation of Monte Carlo physics validation
- Rigorous statistical methods assess
 - Whether a **simulation model is consistent with nature**
 - ▷ well, whether a simulation model is not inconsistent with nature...
 - Whether different simulation models produce (or do not produce) equivalent results in terms of compatibility with experiment
- **Hypothesis testing**
 - Well established methods

Goodness-of-fit tests

- χ^2
- Kolmogorov-Smirnov
- Anderson-Darling
- Cramer-von Mises
- etc.

Categorical data analysis

- Fisher exact test
- Barnard test
- χ^2
- etc.

Mainly applied to contingency tables

What is validated

- Validation of the “**ingredients**” of Geant4
 - The foundation of Geant4 physics models
 - Cross sections
 - Differential cross sections (angular distributions, secondary particle energy spectra etc.)
 - Modeling assumptions
- Validation of **simulated observables** produced by Geant4 in **use cases**
 - Largely represented in the literature
 - Often qualitative only
 - Seldom related to “physics ingredients”

Data for software validation



Passive observations of physical events (*e.g. supernovae explosions or the weather*)

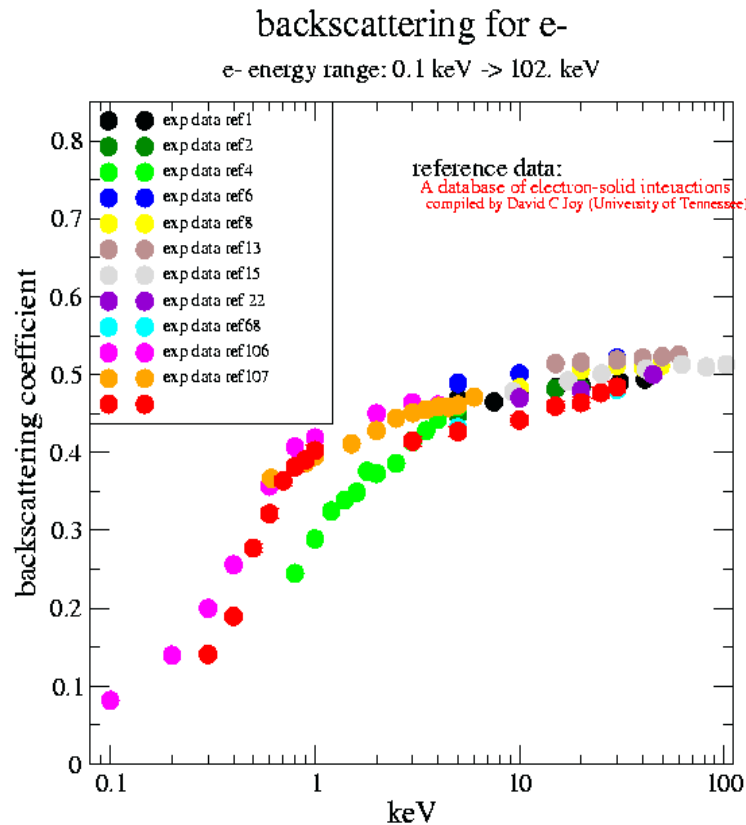
Experiments designed to elucidate a general physics principle or law
(*e.g. typical HEP experiments*)

Experiments designed to certify a detector
(*e.g. test beams*)

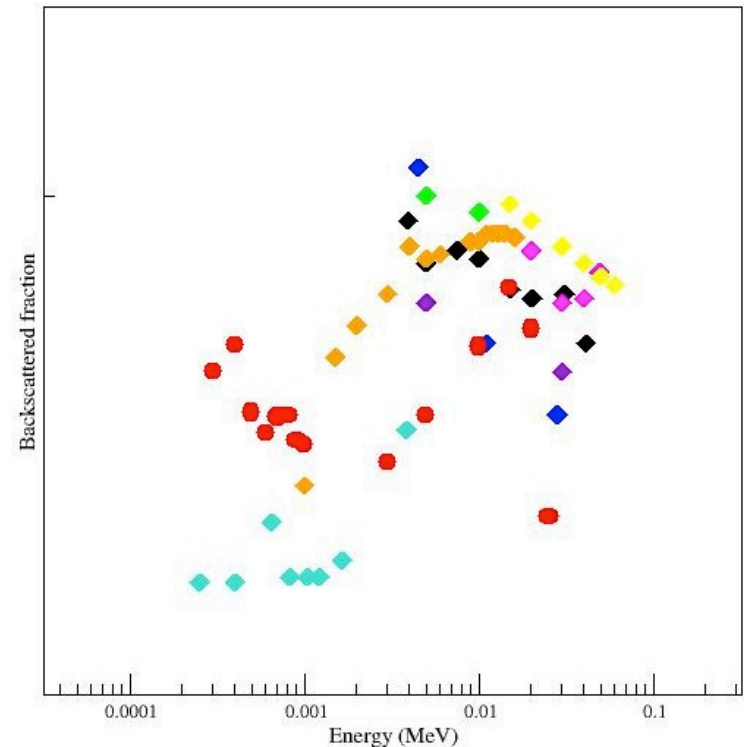


Experiments **specifically designed** to **validate a software** system/component

Validation: retrieving reliable data



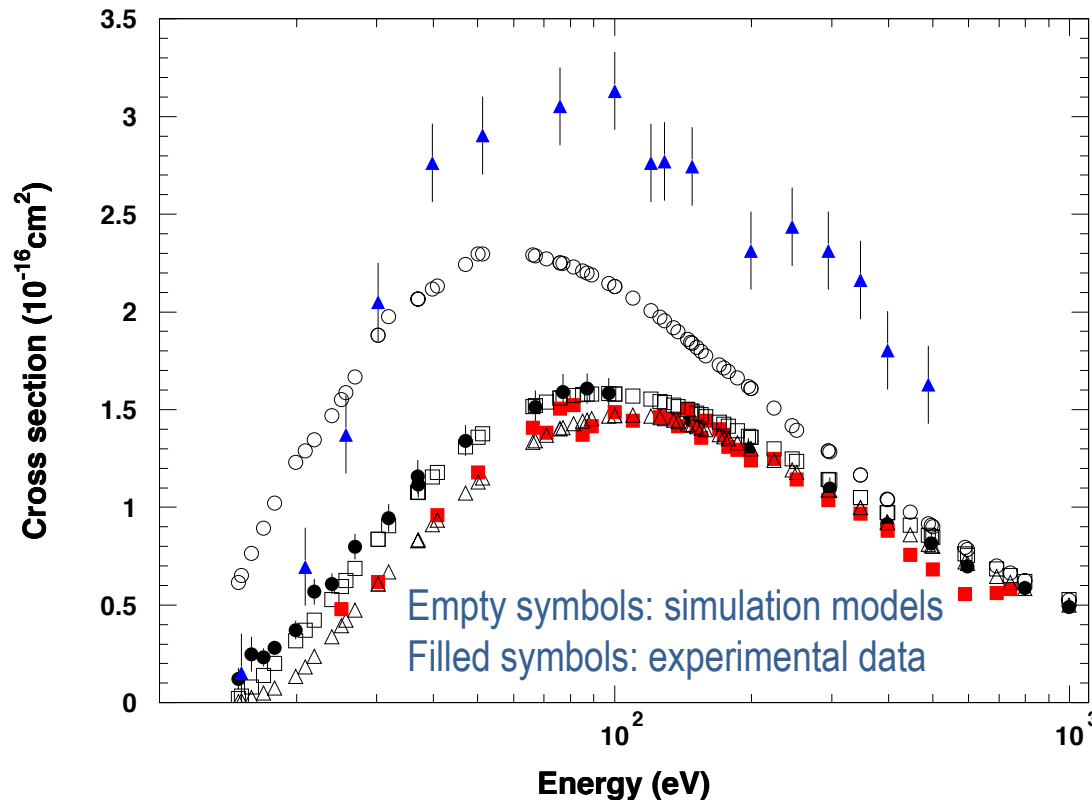
error bars?



experimental data often exhibit
large differences!

... or there are no data, or the details of the experimental setup are not documented, or the systematic is not analyzed, or experimenters are not keen to share their data, or...

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 with a given CL, rather than black & white*)

H. Seo, M. G. Pia, P. Saracco, C. H. Kim, **Ionization cross sections for low energy electron transport**, *IEEE Trans. Nucl. Sci.*, vol. 58, no. 6, pp. 3219-3245, 2011

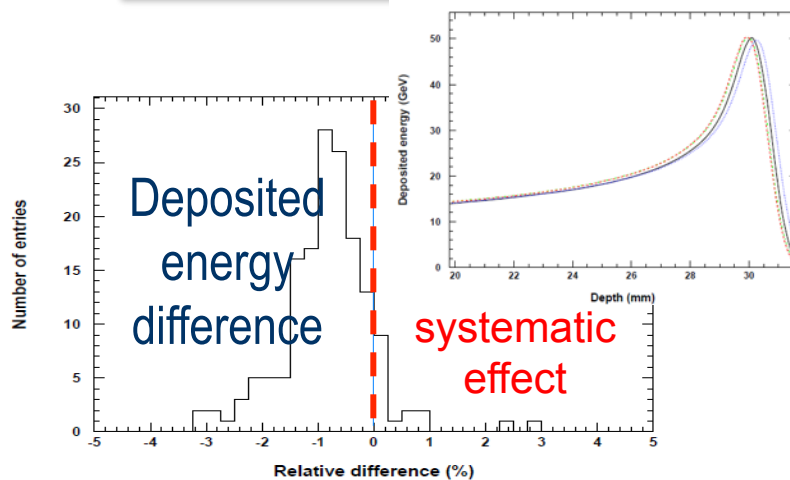
Can we quantify our ignorance?

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

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

What you validated yesterday, is still valid today?

2007 IEEE Nuclear Science Symposium Conference Record

N36-4

Best Student paper, IEEE NSS 2007

Validation of Geant4 low energy physics models against electron energy deposition and backscattering data

Anton Lechner, *Student Member, IEEE*, Maria Grazia Pia and Manju Sudhakar



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TNS, 2009

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

How does it look like a few years later?

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*

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 APOSTOLAKIS¹, Alexander BAGULYA⁴, Haifa Ben ABDELOUAHED⁵,
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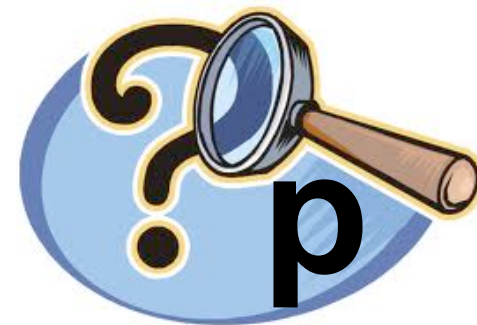
RADECS 2011 Proceedings - PA-19

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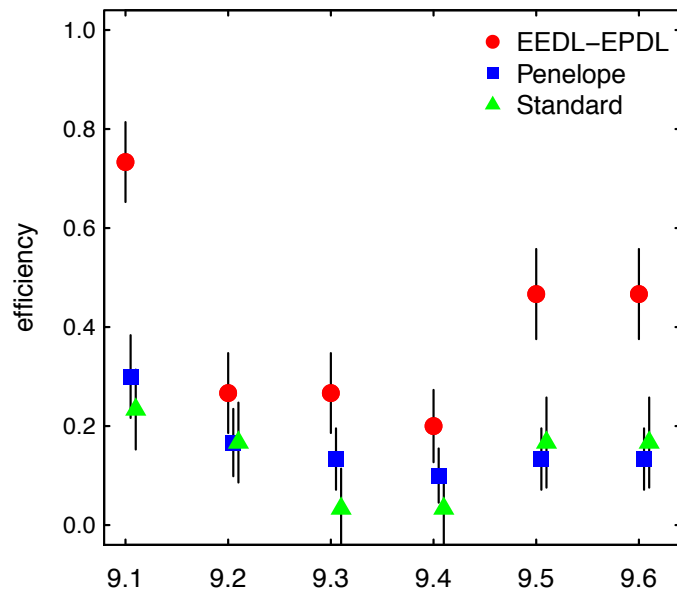
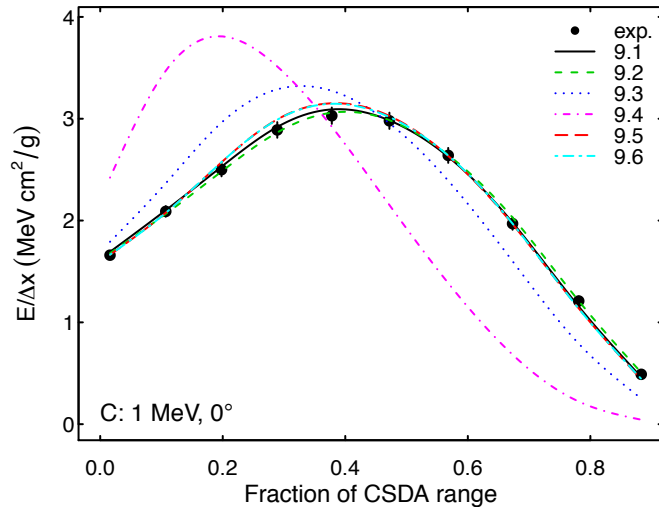
New Geant4 Model and Interface Developments for **Improved** Space Electron Transport Simulations: First results

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

Improvements



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
Be	4	58	0	0.071	0.014	0.124	0.311	0.149
Be	4	109	0	0.021	< 0.001	< 0.001	< 0.001	0.015
Be	4	314	0	0.015	0.764	< 0.001	< 0.001	0.013
Be	4	521	0	0.092	0.967	< 0.001	< 0.001	0.832
Be	4	1033	0	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
C	6	1000	0	0.917	0.994	< 0.001	< 0.001	0.290
Al	13	314	0	0.182	< 0.001	< 0.001	< 0.001	0.004
Al	13	521	0	0.574	< 0.001	< 0.001	< 0.001	0.091
Al	13	1033	0	0.484	0.123	< 0.001	< 0.001	< 0.001
Al	13	314	60	0.396	0.596	< 0.001	< 0.001	0.001
Al	13	521	60	0.137	0.011	0.001	< 0.001	0.056
Al	13	1033	60	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
Fe	26	300	0	0.832	< 0.001	0.351	0.741	0.787
Fe	26	500	0	0.055	< 0.001	0.314	0.003	0.814
Fe	26	1000	0	< 0.001	< 0.001	0.169	0.003	< 0.001
Cu	29	300	0	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
Cu	29	500	0	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
Mo	42	100	0	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
Mo	42	300	0	0.062	< 0.001	0.001	< 0.001	0.008
Mo	42	500	0	0.020	< 0.001	< 0.001	0.001	0.128
Mo	42	1000	0	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
Mo	42	300	60	0.023	0.002	0.049	0.043	0.029
Mo	42	500	60	0.022	< 0.001	0.011	0.006	0.003
Mo	42	1000	60	0.037	< 0.001	0.010	0.028	0.001
Ta	73	300	0	0.043	0.511	0.242	0.272	0.364
Ta	73	500	0	0.025	0.003	< 0.001	< 0.001	0.012
Ta	73	1000	0	0.030	< 0.001	< 0.001	< 0.001	0.002
Ta	73	500	60	0.011	0.003	0.040	0.042	0.010
Ta	73	1000	60	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
Ta	73	500	30	0.034	0.005	0.004	0.006	0.020

CMS simulation



Full Simulation Results for CMS Calorimeters

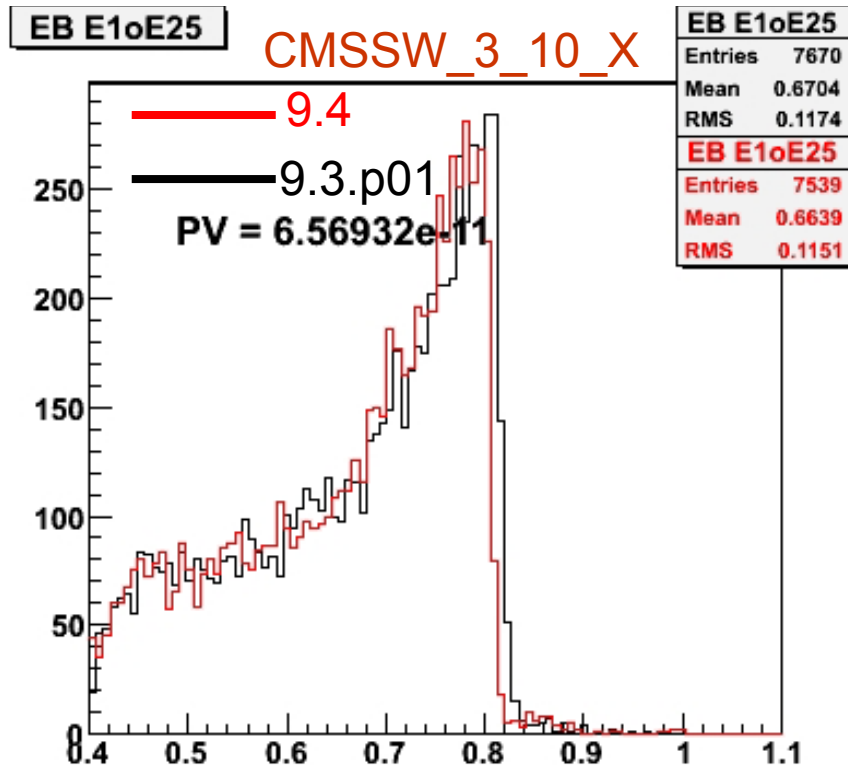


Outline

- 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

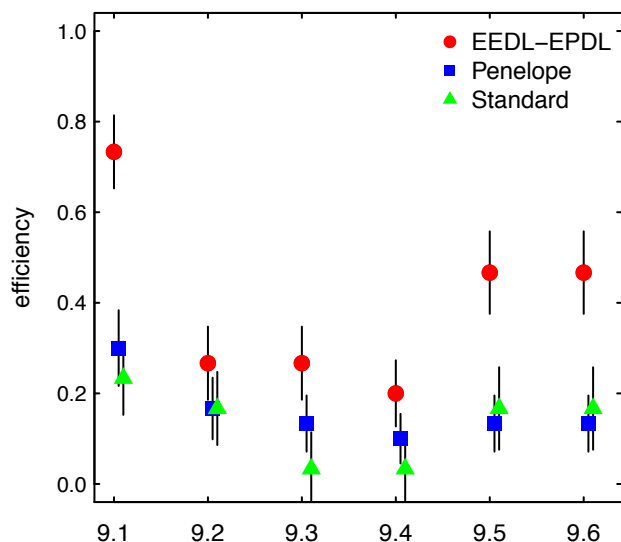
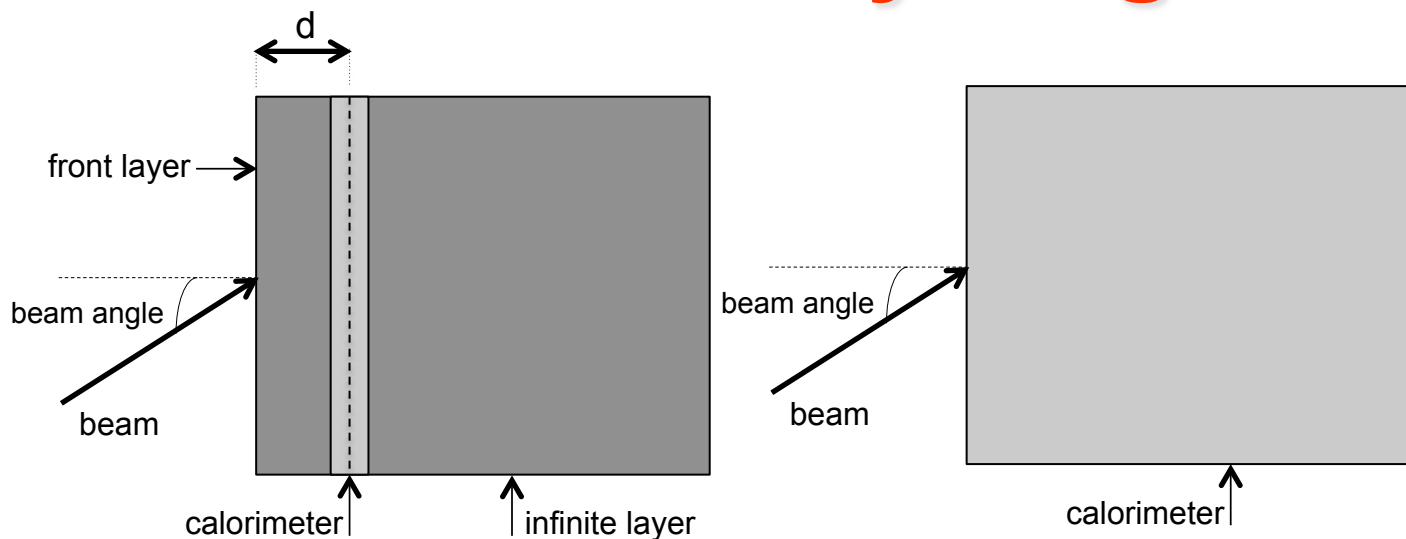
LHC Detector Simulations
October 6, 2011

Sunanda Banerjee
(On behalf of CMS collaboration)

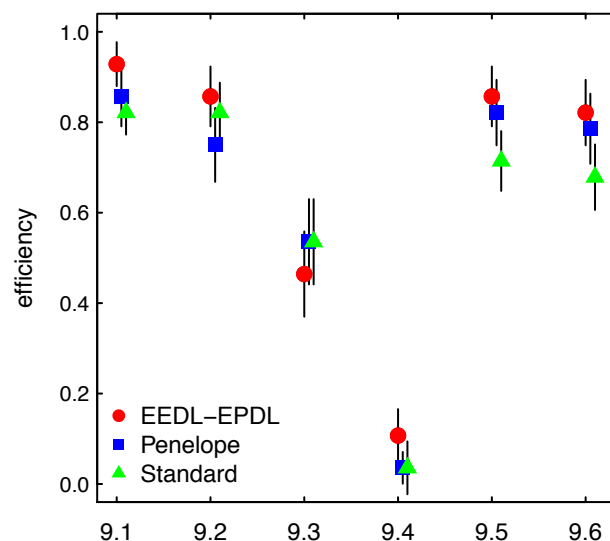


- The lateral shower profile for photons (and e^\pm) is changing with the Geant4 version from 9.3.p01 to 9.4 to 9.4.p02. This is not yet understood and we need some help to get some of the key distributions agreeing better with the data.

What is bad may be good



Geant4 version



Geant4 version

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.**

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.”*

Ongoing effort

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

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

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Validation of Geant4 Simulation of Electron Energy Deposition

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

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

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

2984

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

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 Zc

3269

Publications

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

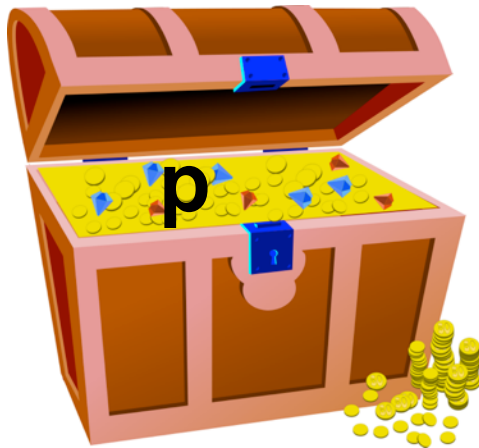
Validation of Proton Ionization Cross Section Generators for Monte Carlo Particle Transport

Maria Grazia Pia, and Paolo Saracco

...and more!

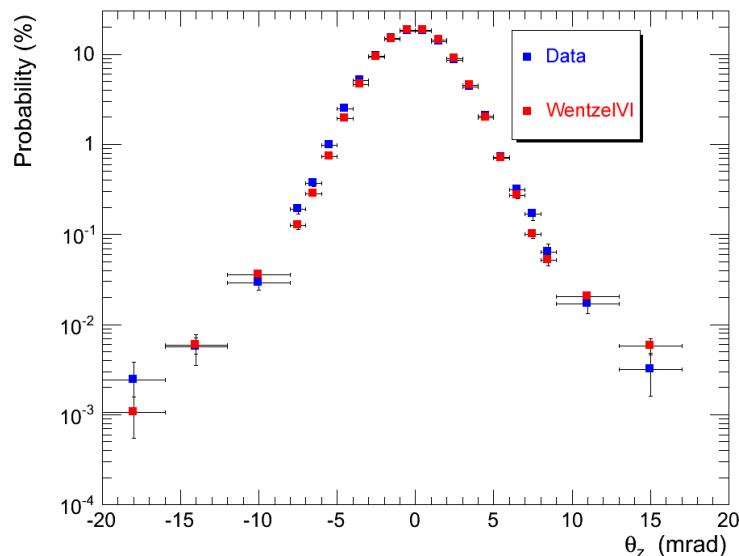


■ Geant4 collaboration ■ Our team



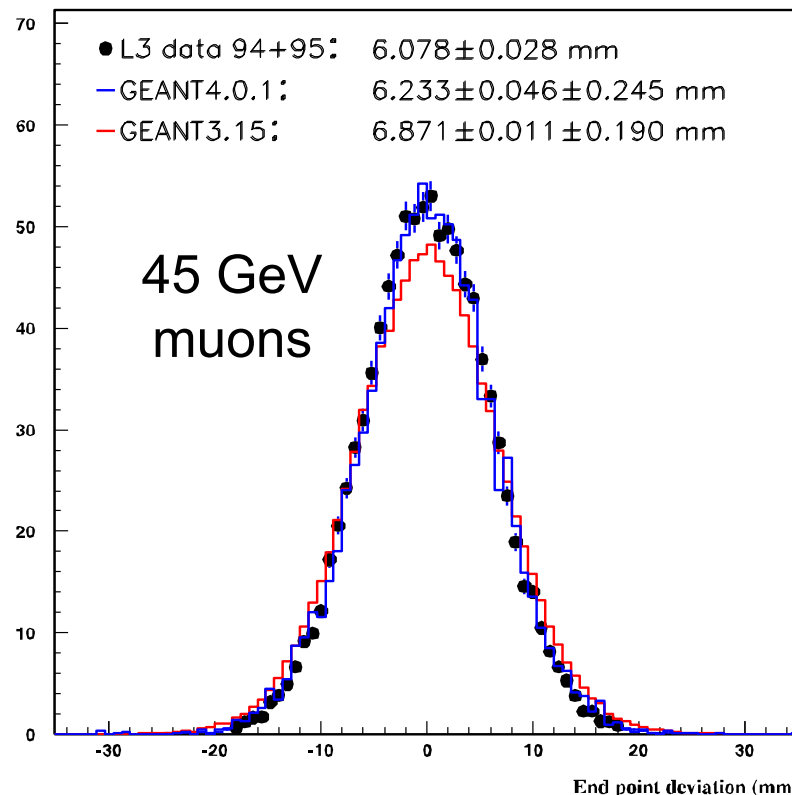
Muons

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



Muon scattering angular distribution for 7.3 GeV/c muon on a copper target (1 radiation length thick) Lassila-Perini and Urban1995 in comparison with the Wentzel-VI MSC model.

Deviation of 45 GeV muons in L3



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.

Geant4 Simulation of Production and Interaction of Muons

Comparison with experimental data limited to stopping power in two materials

Multiple scattering

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

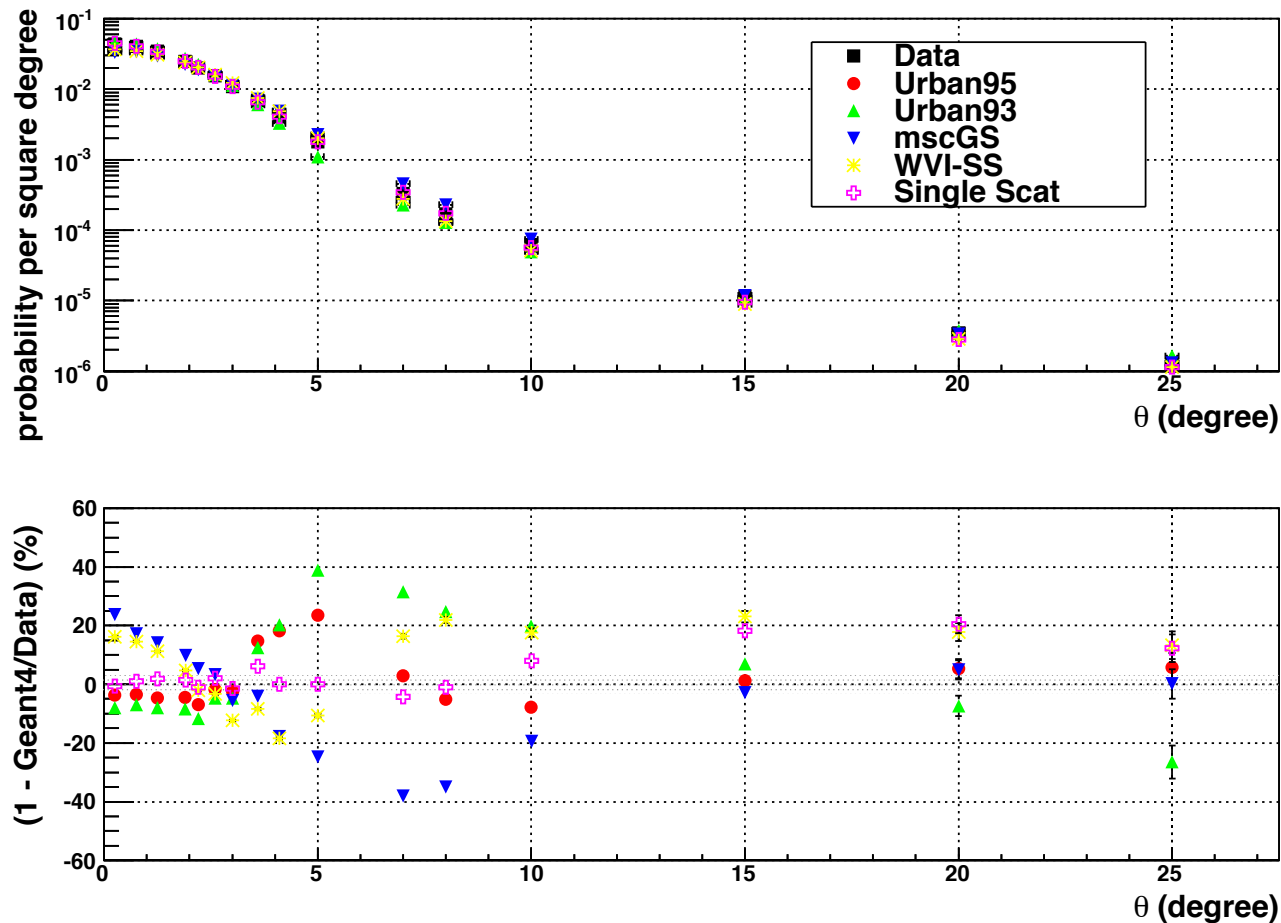


Figure 4. Comparison of different Geant4 MSC model predictions and experimental data [23] for 15.7 MeV electrons scattering off 9.68 μm Gold foil: angular distribution (top); Monte Carlo over data (bottom). Urban model 95 and the single scattering model provides overall better agreement with the data.

Electron energy loss

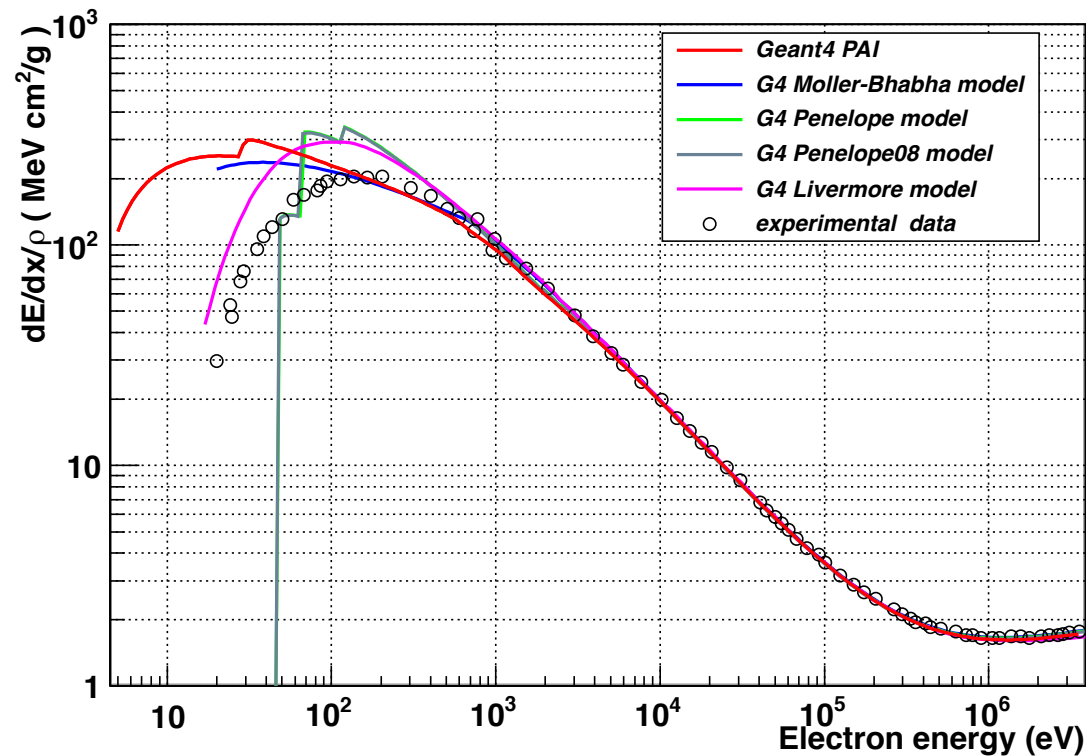
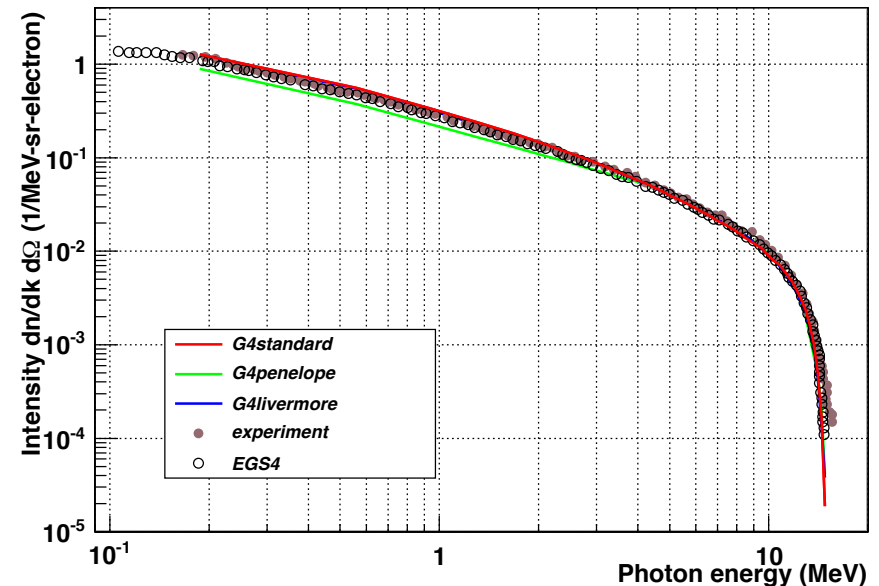


Figure 5. Electron mean energy loss in CO₂ vs. electron energy: points are data [30], solid lines - different Geant4 models. Moller-Bhabha and PAI model follow the data down to 100 eV. Below 200 eV Penelope and Livermore models show effects caused by the treatment of atomic shell effects.

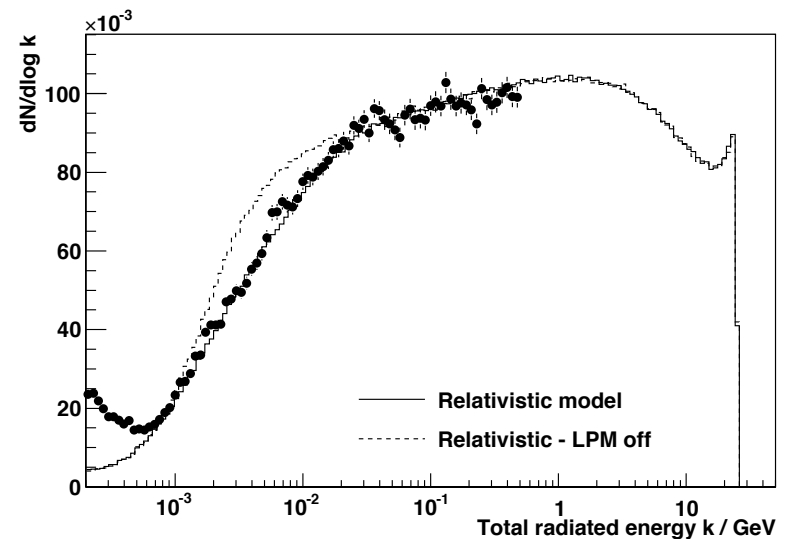
Bremsstrahlung

Bremsstrahlung intensity
spectrum for a 15 MeV electron
beam on Aluminum target
evaluated at the angle of 10° :
solid points – data [38], open
points – EGS4 published result,
histograms – Geant4 models



G4eBremsstrahlungRelModel
incorporates the
Landau-Pomeranchuk-Migdal effect

25 GeV electron beam on a thin
Aluminum foil, together with data
from the SLAC E-146 experiment



Electromagnetic physics revisited

- Wide scope project to assess **quantitatively** the **state-of-the-art** of electromagnetic physics modeling for Monte Carlo particle transport
 - Comparisons with large experimental data samples of various origin
 - Statistical data analysis for validation and for comparing the compatibility of different models with experiment

● Photons

- **Elastic scattering**: published
- **Compton scattering, photoionisation**: N29 session, talks 6-7
- **Pair production**: early stage, NP02-140

● Electrons

- **Ionisation** at low energies (challenge IPA and isolated atom assumption)

● Protons

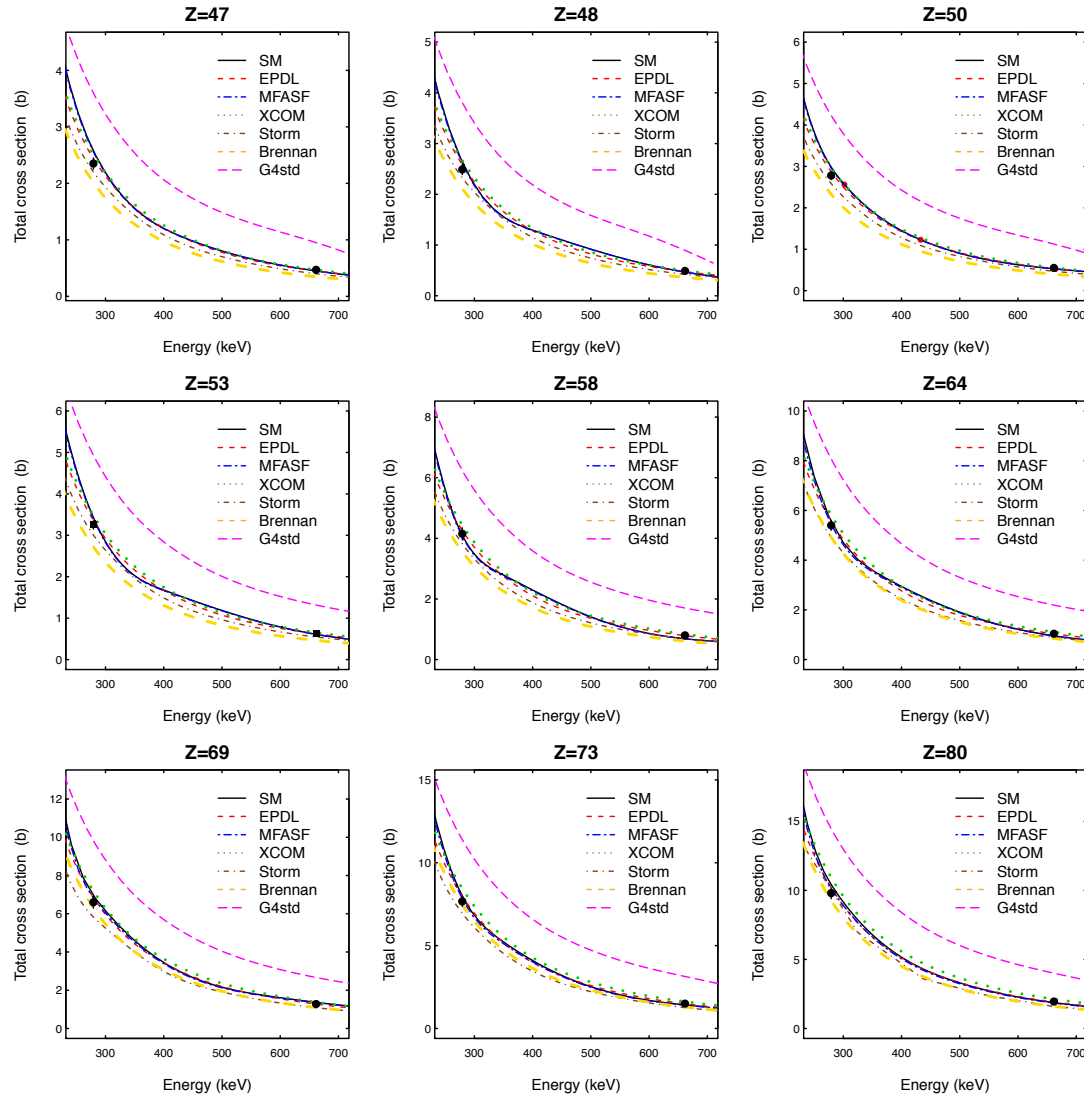
- **Ionisation** cross sections

Photon elastic scattering

- **Rayleigh scattering**
from the atomic electrons,
- **nuclear Thomson scattering**,
scattering from the nucleus
considered as a point charge,
- **Delbrück scattering**,
scattering from the field of the
nucleus,
- **nuclear resonance scattering**,
scattering from the internal
structure of the nucleus

Total cross section

Discriminant power despite the
very limited data sample



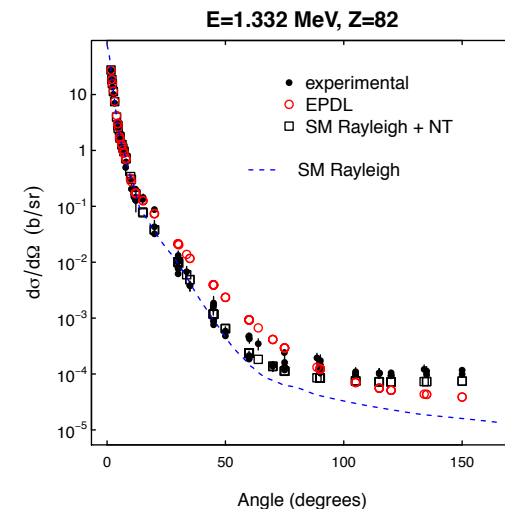
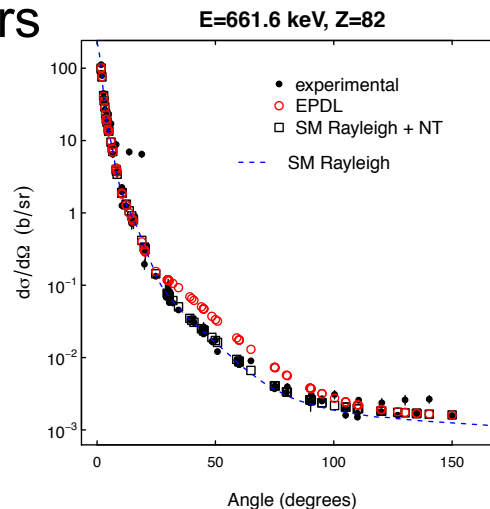
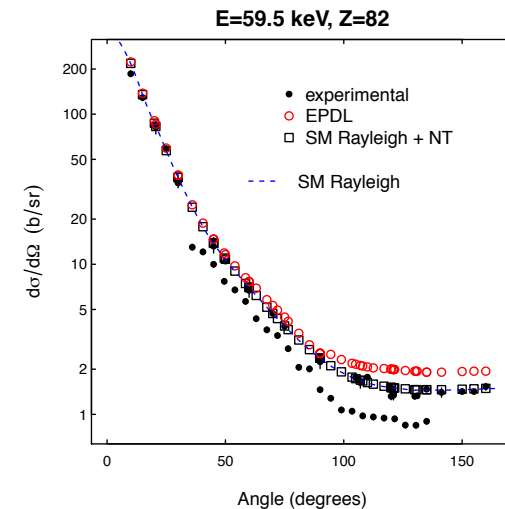
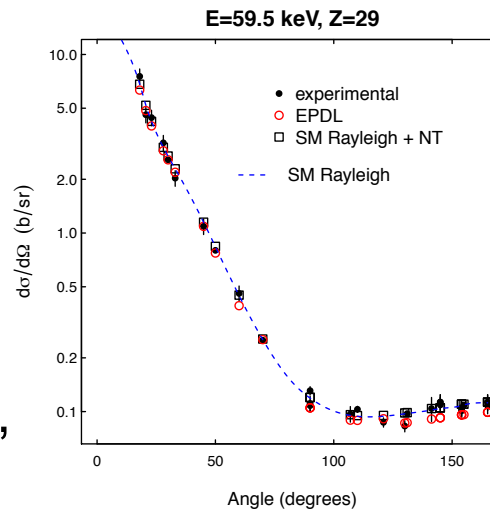
Photon elastic scattering models

Differential cross section

- numerical S-matrix calculations
- relativistic form factors (*EGS*)
- non-relativistic form factors
- modified relativistic form factors,
- modified relativistic form factors with anomalous scattering factors

Geant4

“Livermore” and à la Penelope
Non-relativistic form factors
by Hubbell et al.
(*EDPL*)



Quantitative

All angles		SM	EPDL
		Pass 55	27
		Fail 16	44
		p-value	
		Fisher test	< 0.001
		Pearson's χ^2	< 0.001
		Yates χ^2	< 0.001
		SM	MFASF
		Pass 55	37
		Fail 16	34
		p-value	
		Fisher test	0.003
		Pearson's χ^2	0.002
		Yates χ^2	0.002
$\theta \leq 90^\circ$		SM	EPDL
		Pass 55	27
		Fail 12	40
		p-value	
		Fisher test	< 0.001
		Pearson's χ^2	< 0.001
		Yates χ^2	< 0.001
		SM	MFASF
		Pass 55	36
		Fail 12	31
		p-value	
		Fisher test	< 0.001
		Pearson's χ^2	< 0.001
		Yates χ^2	< 0.001
		SM	EPDL
		Pass 10	1
		Fail 7	16
		p-value	
		Fisher test	0.002
		Yates χ^2	0.001
		SM	MFASF
		Pass 10	2
		Fail 7	15
		p-value	
		Fisher test	0.010
		Yates χ^2	0.012

E (keV)	Penelope 2001	Penelope 2008-2011	EPDL	EPDL ASF	SM	RF	NF	MF	MF ASF	RF ASF
5.45	0.998	0.996	0.992	0.297	1.000	0.952	0.996	0.999	1.000	1.000
5.93	0.706	0.745	0.741	0.049	0.999	0.432	0.732	0.775	1.000	1.000
6.4	0.860	0.830	0.863	0.148	1.000	0.728	0.829	0.923	1.000	1.000
6.93	0.913	0.877	0.876	0.008	1.000	0.722	0.883	0.944	1.000	1.000
7.47	0.695	0.626	0.614	0.041	1.000	0.386	0.637	0.749	1.000	1.000
8.04	0.053	0.001	0.001	< 0.001	0.696	< 0.001	0.001	< 0.001	0.736	0.727
8.63	0.144	0.249	0.241	< 0.001	0.759	0.020	0.199	0.232	0.820	0.812
9.23	0.023	0.033	0.030	< 0.001	0.652	0.002	0.024	0.029	0.719	0.708
13.95	< 0.001	< 0.001	< 0.001	0.002	0.154	< 0.001	< 0.001	< 0.001	0.046	0.064
14.93	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	0.001	< 0.001	< 0.001	< 0.001	< 0.001
16.58	0.956	0.908	0.901	0.587	0.218	1.000	0.947	0.947	0.305	0.281
17.44	< 0.001	< 0.001	< 0.001	< 0.001	0.102	< 0.001	< 0.001	< 0.001	0.013	0.025
17.75	< 0.001	< 0.001	< 0.001	< 0.001	0.105	< 0.001	< 0.001	< 0.001	0.009	0.025
21.12	0.008	0.001	0.001	0.017	0.099	< 0.001	0.001	0.001	0.124	0.118
22.1	< 0.001	< 0.001	< 0.001	< 0.001	0.014	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
23.1	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	0.002	< 0.001	< 0.001	< 0.001	< 0.001
24.14	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	0.002	< 0.001	< 0.001	< 0.001	< 0.001
25.2	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
26.27	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	0.001	< 0.001	< 0.001	0.001	< 0.001
26.36	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	0.772	0.758
30.85	< 0.001	0.280	0.322	< 0.001	0.011	0.955	0.399	0.507	0.028	0.015
30.97	0.001	0.011	0.020	0.004	0.377	0.001	0.006	0.002	0.667	0.509
32.06	0.003	0.078	0.100	0.197	0.602	0.030	0.066	0.036	0.885	0.749
33.3	0.004	0.077	0.082	0.048	0.306	0.154	0.104	0.072	0.589	0.422
34.6	< 0.001	< 0.001	< 0.001	0.005	0.033	0.006	0.001	0.001	0.071	0.046
35.86	0.001	0.001	0.001	0.008	0.148	0.195	0.002	0.002	0.314	0.179
39.9	< 0.001	< 0.001	< 0.001	< 0.001	0.061	0.043	0.004	0.003	0.083	0.072
42.75	< 0.001	0.001	0.001	0.002	0.183	0.001	0.003	0.002	0.082	0.089
47.24	< 0.001	0.011	0.021	0.003	0.019	0.005	0.002	0.065	0.022	0.044
59.54	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
81	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
84.3	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
88	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
122	0.196	0.500	0.541	< 0.001	0.107	< 0.001	0.478	0.287	0.033	0.182
136	0.534	0.837	0.790	< 0.001	0.913	0.047	0.893	0.836	0.669	0.891
145.4	< 0.001	< 0.001	< 0.001	< 0.001	0.037	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
244.7	< 0.001	0.025	0.032	0.006	0.038	< 0.001	0.027	0.024	0.037	0.036
279.2	< 0.001	< 0.001	< 0.001	< 0.001	0.201	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
317	< 0.001	< 0.001	< 0.001	0.019	< 0.001	0.200	< 0.001	< 0.001	< 0.001	< 0.001
320	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
334	0.031	0.873	0.801	< 0.001	0.118	< 0.001	0.617	0.757	< 0.001	0.022
344	< 0.001	0.047	0.033	< 0.001	0.080	< 0.001	0.040	0.140	< 0.001	< 0.001
411.8	< 0.001	< 0.001	< 0.001	< 0.001	0.136	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
443.96	< 0.001	< 0.001	< 0.001	< 0.001	0.053	< 0.001	< 0.001	0.111	0.012	< 0.001
465	0.758	0.542	0.518	0.488	0.285	0.120	0.535	0.302	0.287	0.290
468.1	< 0.001	< 0.001	< 0.001	< 0.001	0.053	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
511	0.754	0.752	0.756	0.756	0.730	0.746	0.753	0.727	0.731	0.731
661.6	< 0.001	< 0.001	< 0.001	< 0.001	0.044	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
723	< 0.001	< 0.001	< 0.001	< 0.001	0.096	< 0.001	< 0.001	0.114	0.009	< 0.001
779	< 0.001	< 0.001	< 0.001	< 0.001	0.683	< 0.001	< 0.001	0.333	< 0.001	< 0.001
811	4.561	6.060	6.245	6.295	5.822	8.857	6.174	5.828	5.881	5.784
847	< 0.001	< 0.001	< 0.001	< 0.001	0.598	< 0.001	< 0.001	0.870	0.278	< 0.001
868	0.005	0.162	0.141	0.043	0.919	< 0.001	0.142	0.925	0.854	< 0.001
878	0.026	0.140	0.119	0.115	0.164	0.001	0.123	0.153	0.140	0.156
889	< 0.001	< 0.001	< 0.001	< 0.001	0.323	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
952	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
964	< 0.001	< 0.001	< 0.001	< 0.001	0.152	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
1005	< 0.001	< 0.001	< 0.001	< 0.001	0.987	< 0.001	< 0.001	0.968	0.697	< 0.001
1019	0.280	0.053	0.045	0.045	0.075	< 0.001	0.049	0.073	0.066	0.095
1038	< 0.001	0.041	0.011	0.011	0.004	< 0.001	0.056	0.019	< 0.001	< 0.001
1086	< 0.001	< 0.001	< 0.001	< 0.001	0.125	< 0.001	< 0.001	0.011	< 0.001	< 0.001
1112	< 0.001	< 0.001	< 0.001	< 0.001	0.060	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
1120	< 0.001	< 0.001	< 0.001	< 0.001	0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
1173	< 0.001	< 0.001	< 0.001	< 0.001	0.029	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
1189	0.948	0.401	0.380	0.380	0.523	0.022	0.384	0.482	0.468	0.522
1238	< 0.001	< 0.001	< 0.001	< 0.001	0.011	< 0.001	< 0.001	0.008	< 0.001	< 0.001
1274	< 0.001	< 0.001	< 0.001	< 0.001	0.076	< 0.001	< 0.001	0.016	< 0.001	< 0.001
1302	0.054	0.039	0.031	0.031	0.050	< 0.001	0.032	0.048	0.044	0.057
1332	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
1359	< 0.001	< 0.001	< 0.001	< 0.001	0.382	< 0.001	< 0.001	0.325	0.133	< 0.001
1408	< 0.001	< 0.001	< 0.001	< 0.001	0.312	< 0.001	< 0.001	0.068	< 0.001	< 0.001
≥ 1600	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001

Photon elastic scattering

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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

State of the art

Form factor approximation:

non relativistic, relativistic, modified + anomalous scattering factors

2nd order S-matrix calculations

recent calculations, not yet used in Monte Carlo codes

Quantification

Statistical analysis, GoF + categorical

Differential cross sections

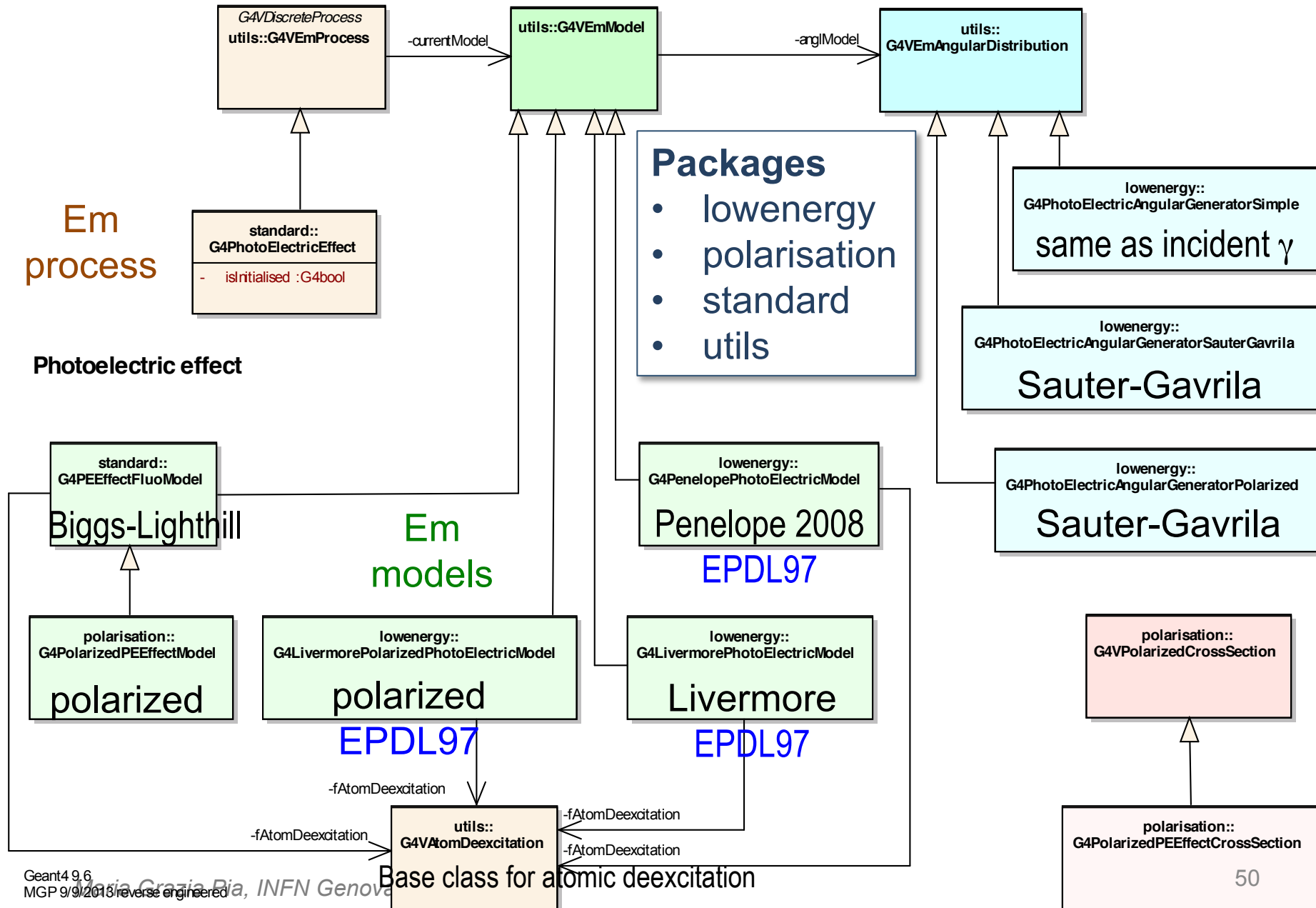
	Penelope 2001	Penelope 2008	EPDL	Relativ. FF	Non-Rel. FF	Modified FF	MFF ASF	RFF ASF	SM NT
ϵ	0.27	0.38	0.38	0.25	0.35	0.49	0.52	0.48	0.77
error	± 0.05	± 0.06	± 0.06	± 0.05	± 0.06	± 0.06	± 0.06	± 0.06	± 0.05

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

Photoionisation in Monte Carlo codes

	Cross sections	Angular distribution
EGS5	PHOTX	Sauter
EGSnrc	Storm-Israel Fit to XCOM EPDL97 (subshell)	Sauter
FLUKA	EPDL97	Sauter
Geant4	Revised Biggs-Lighthill (Henke) EPDL97	Sauter-Gavrila Same direction
ITS	Scofield 1973	Fischer+Sauter
MCNP(X)	EPDL89, EDPL97 ENDFB/IV+Storm-Israel	
Penelope	EPDL97	Sauter (K shell)

Photoelectric effect in Geant4 9.6



Validation environment

Streamlined software design consistent with Geant4 kernel

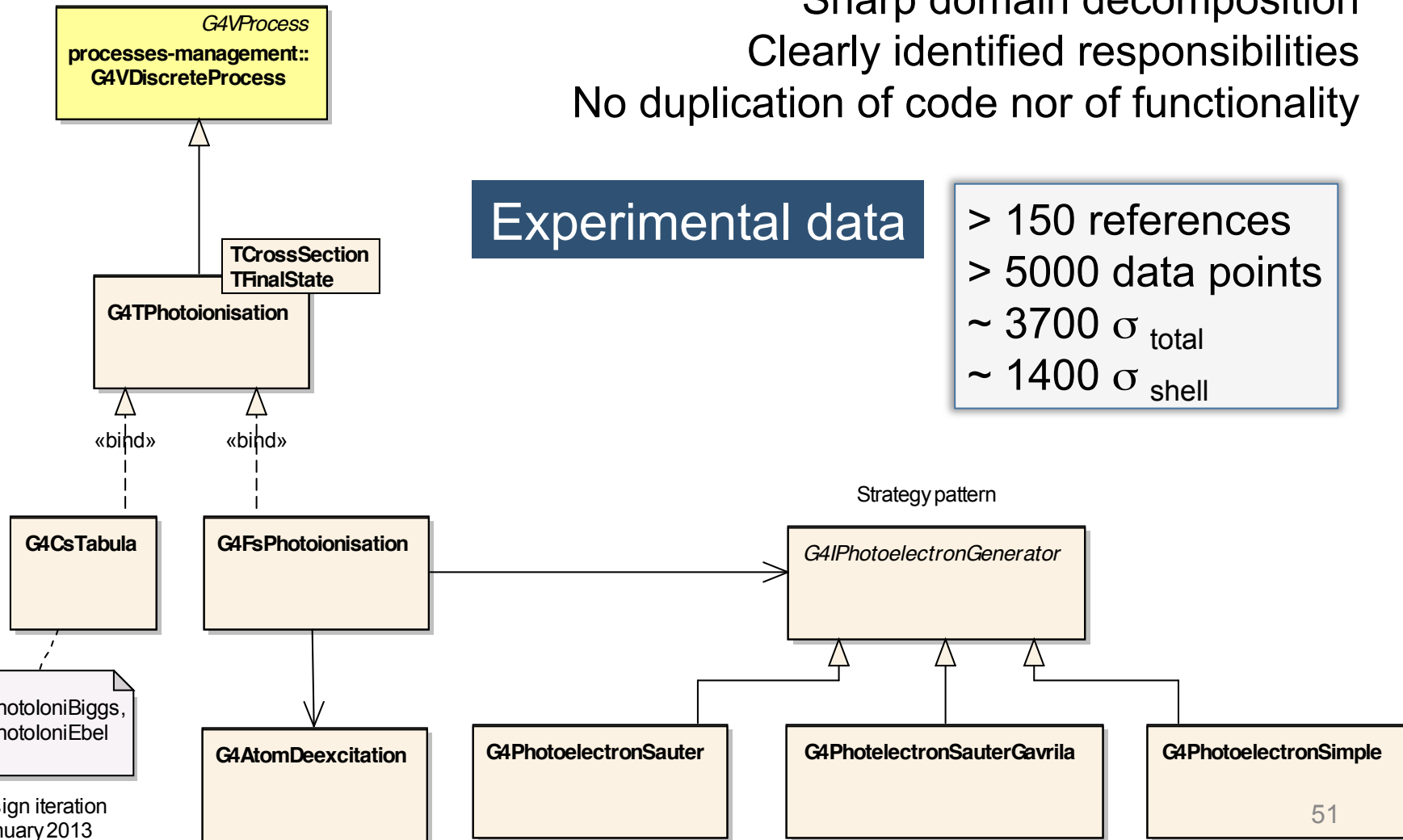
Sharp domain decomposition

Clearly identified responsibilities

No duplication of code nor of functionality

Experimental data

> 150 references
> 5000 data points
~ 3700 σ_{total}
~ 1400 σ_{shell}



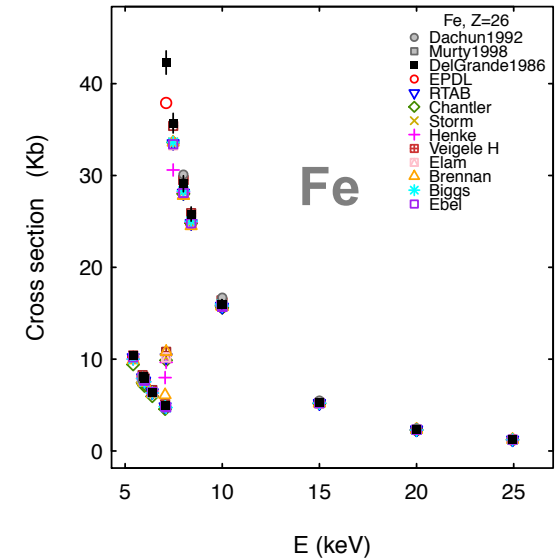
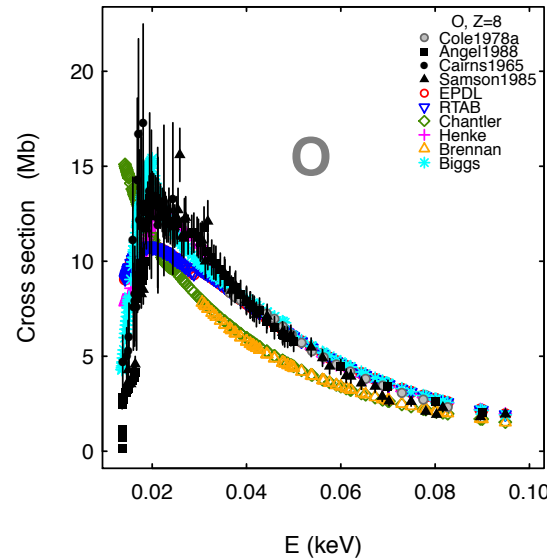
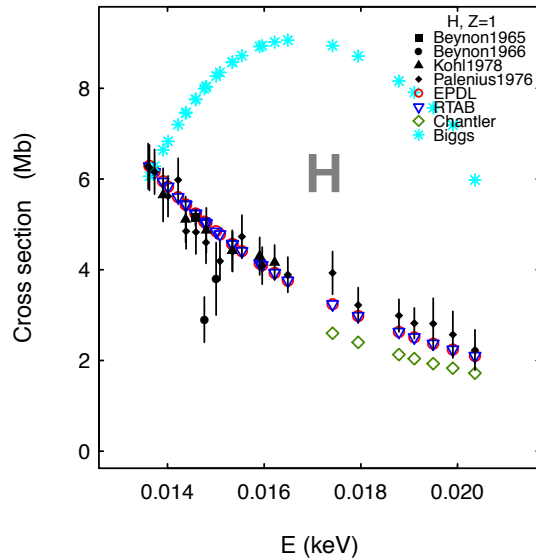
Photoionisation cross section sources

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 (<i>Scofield</i>)	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 (<i>Scofield</i>)	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 (<i>Scofield</i>)	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*

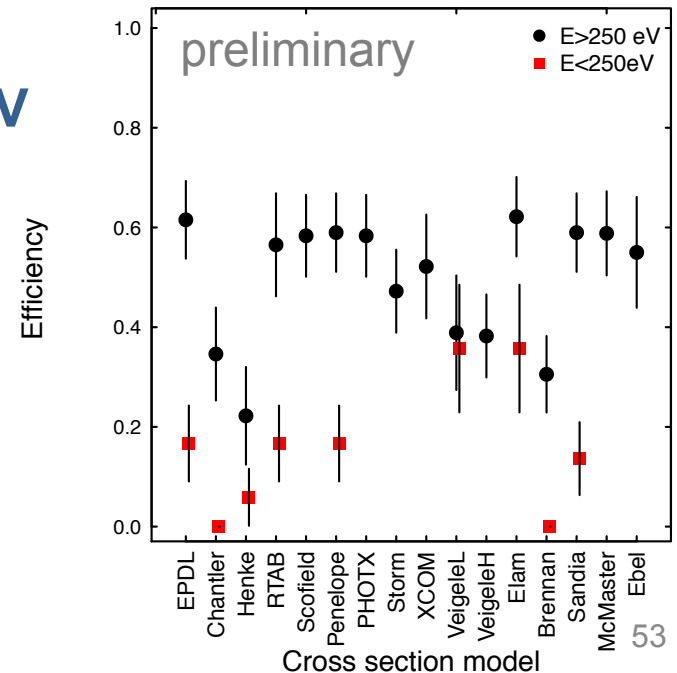
Total photoionisation cross sections



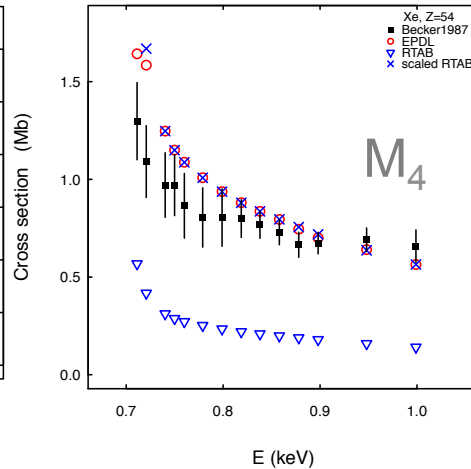
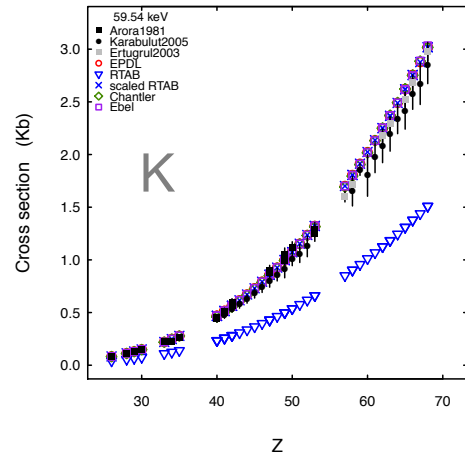
- Most calculation methods exhibit similar compatibility with experiment for **E > 250 eV**
 - Chantler, Brennan-Cowan look worse
- Degraded accuracy below 250 eV

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

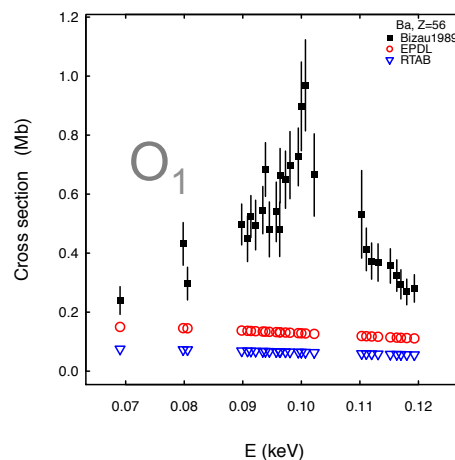
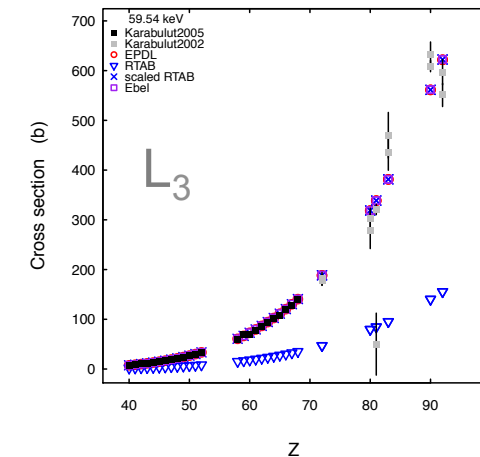


Shell cross sections



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

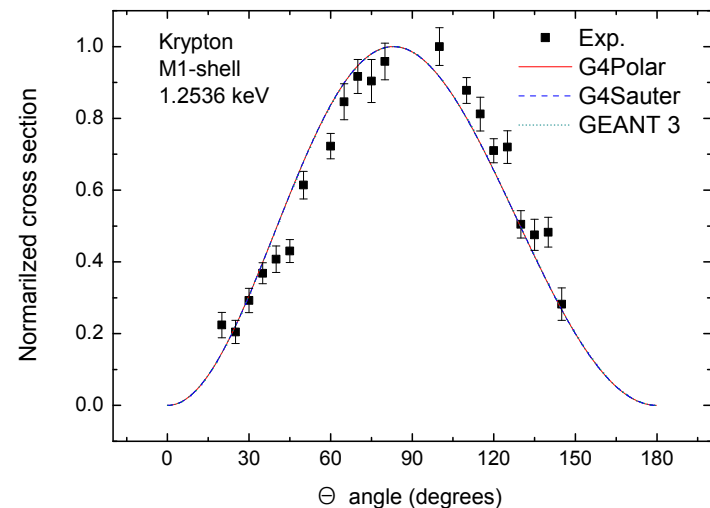
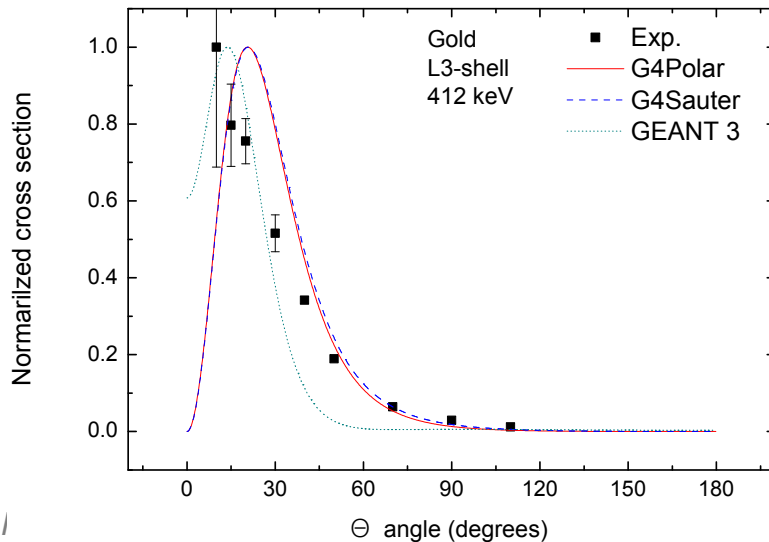
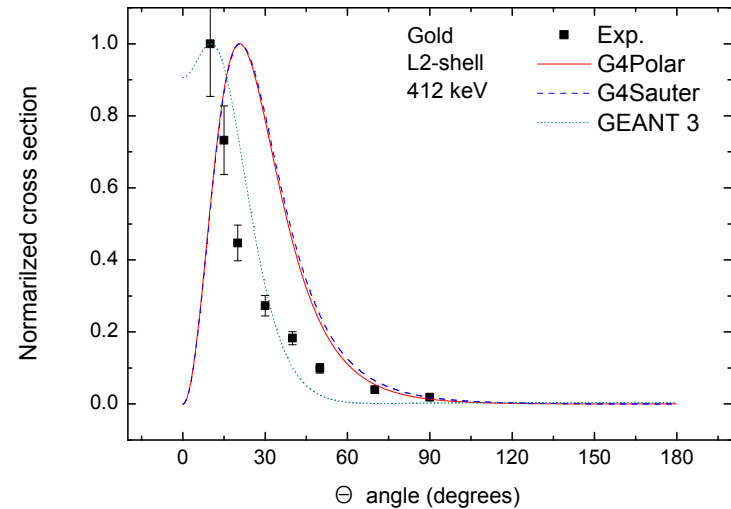
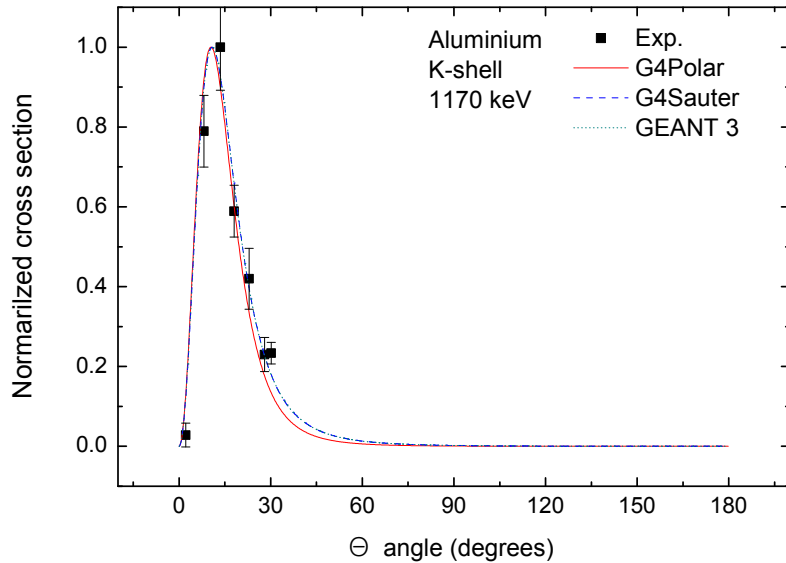
Systematic effect observed with RTAB shell cross sections
(presumably a missing factor in the calculation)

Maria Grazia Pia, INFN Genova

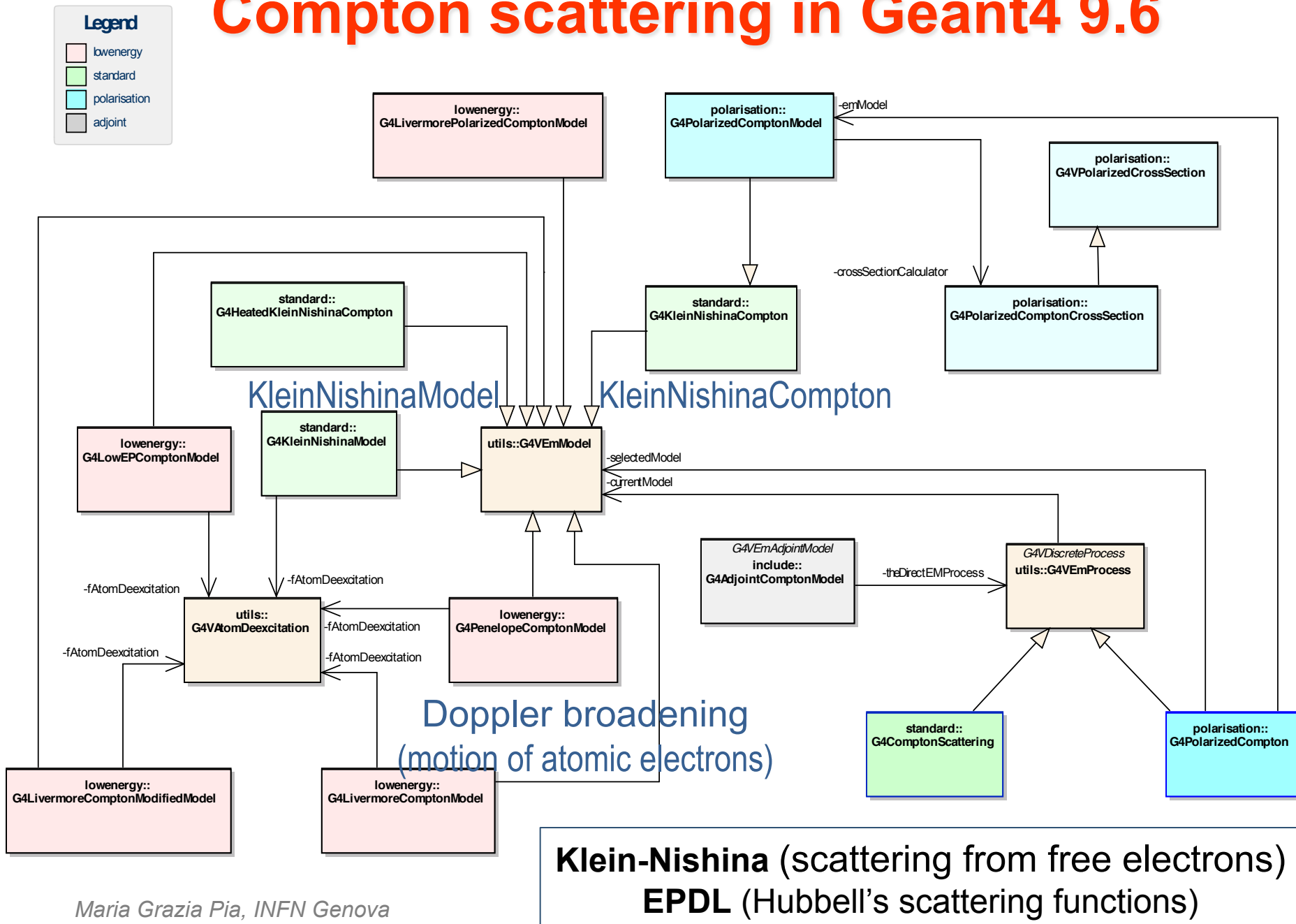
Angular distribution

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

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



Compton scattering in Geant4 9.6



Compton scattering: total cross section

- Small experimental data sample
- Most reported “measurements” of total Compton scattering cross section are measurements of total attenuation coefficients, from which theoretical Rayleigh scattering and photoelectric contributions are subtracted
 - Not appropriate for validation of simulation models
- Results of statistical analysis: **EPDL**, **Penelope-like** (integrated from differential cross section) and Geant4 **standard** electromagnetic (analytical paramerisation) total cross sections are statistically **equivalent** in comparison to experimental data

Differential Compton scattering cross section

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

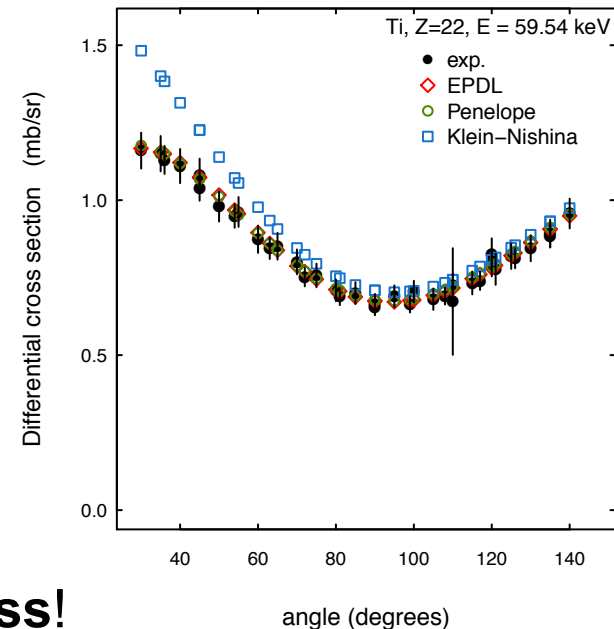
Various scattering functions are evaluated w.r.t. experimental data

model	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
<i>Hubbell</i>	<i>0.82</i>	<i>0.02</i>

>2300 experimental data

← Geant4 lowenergy

← Geant4 standard



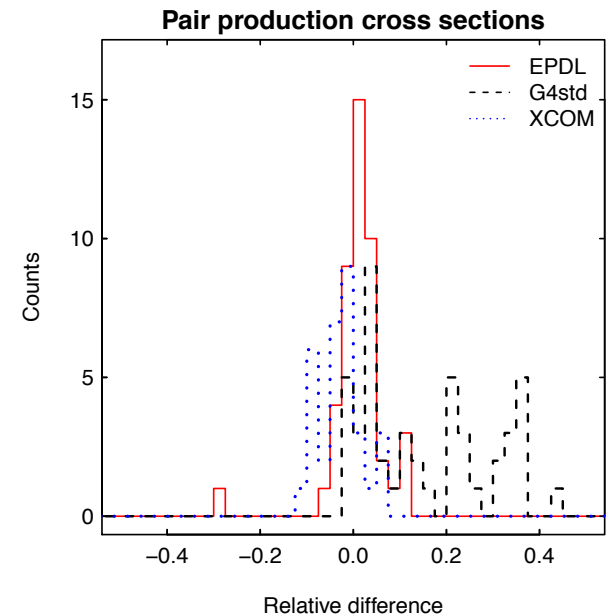
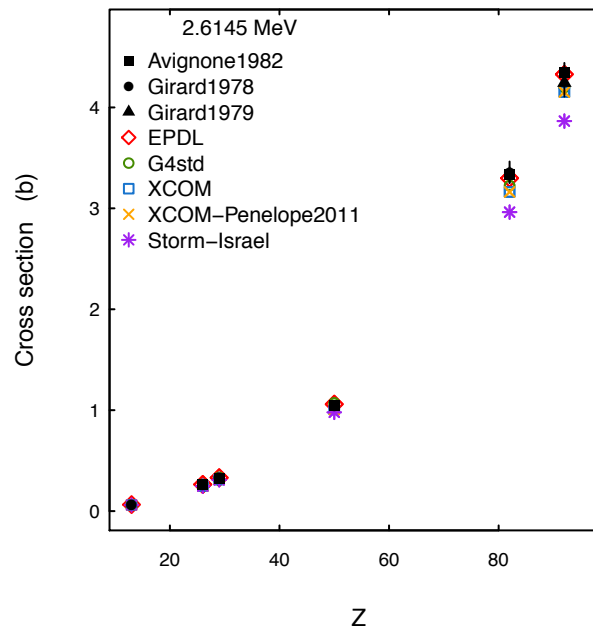
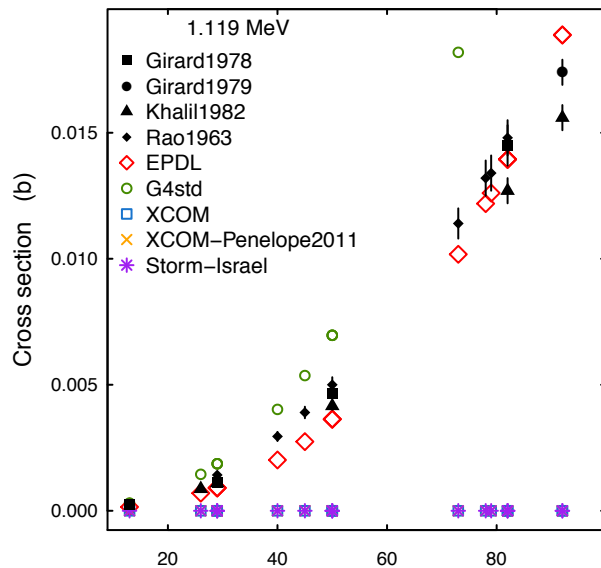
e^+e^- pair production

Validation at high energy in progress

- Total cross section: Bethe-Heitler with corrections (Hubbell, Gimm, Overbo)
- Near threshold

$E > 1.119 \text{ MeV}$

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



Further details

Simulation: N29, ASEM 203, 16.30

N29-5

N29-6

NP2-140

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

Publications on validation and improvements of Geant4 photoelectric effect, Compton scattering and pair production in preparation

Same format as previous paper on photon elastic scattering

- Evaluation of several models (in Geant4, in other MC codes, new)
- Ample set of experimental data
- Quantitative: rigorous statistical methods
- Computational performance
- Identify state-of-the-art

Electron impact ionisation

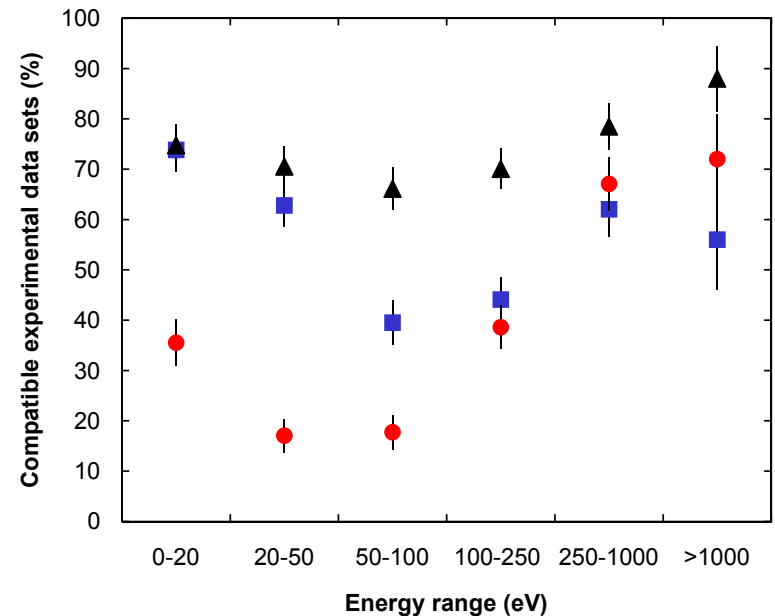
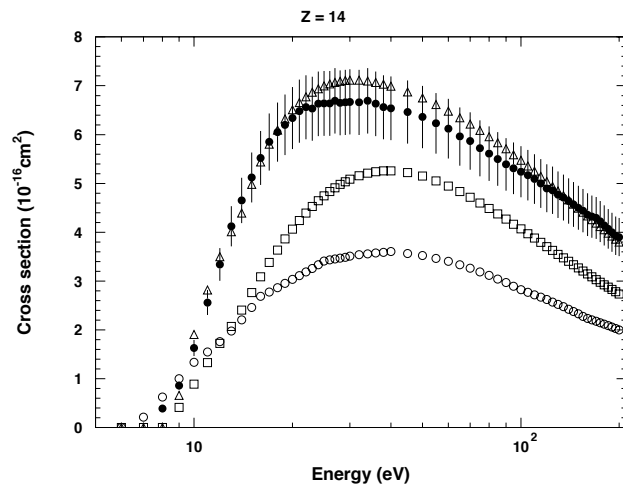
IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 58, NO. 6, DECEMBER 2011

3219

Ionization Cross Sections for Low Energy Electron Transport

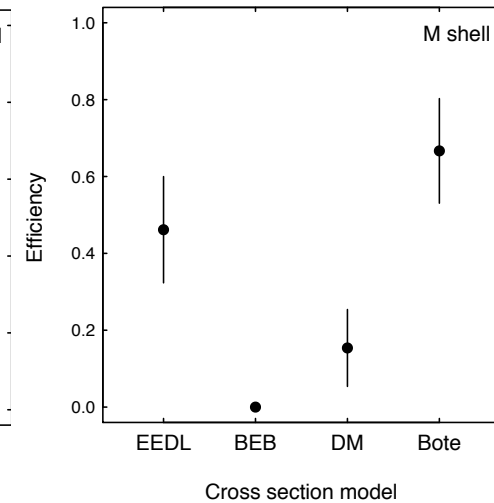
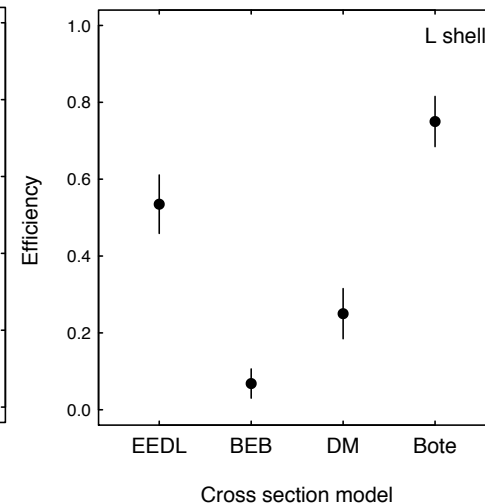
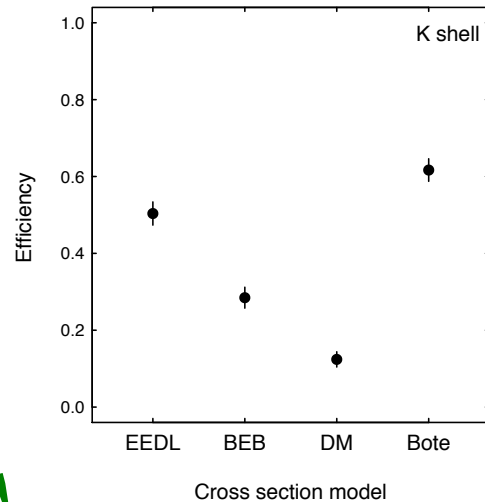
Hee Seo, Maria Grazia Pia, Paolo Saracco, and Chan Hyeong Kim

- 1) EEDL
 - 2) Binary-Encounter-Bethe (BEB)
 - 3) Deutsch-Märk
- (“Livermore” in Geant4)
- } new models



Electron impact ionisation: shells

- EEDL
- BEB
- DM
- Bote et al.



Preliminary!

K shell

Pass

Fail

EEDL	Bote
138	169
136	105

L shell

EEDL	Bote
23	33
20	11

M shell

EEDL	Bote
6	8
7	4

Test

Fisher

Pearson χ^2

Barnard

Fisher

Pearson χ^2

Barnard

Fisher

Barnard

p-value

0.0098

0.0076

0.0079

0.0453

0.0362

0.0383

0.4283

0.3519

0.01

significance

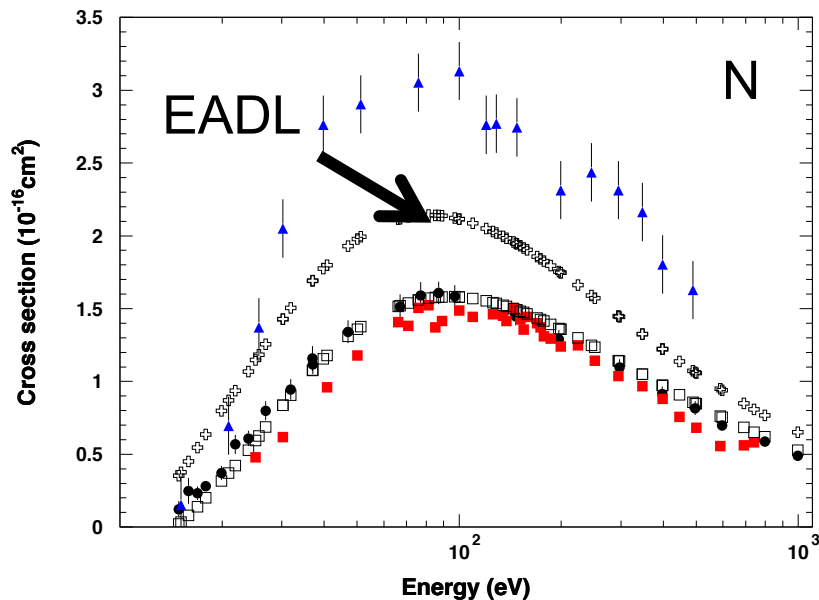
0.05

significance

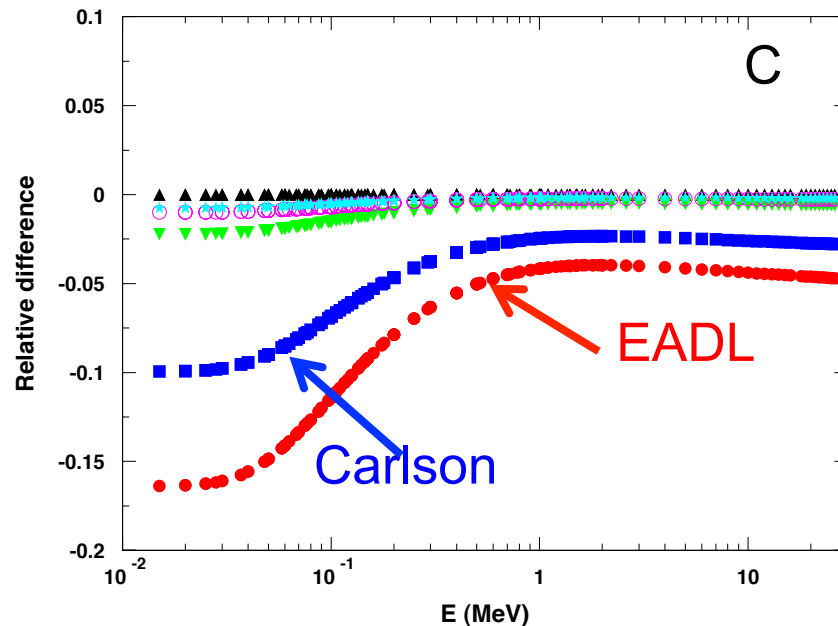
Small data
sample

Atomic parameters: binding energies

electron impact ionisation



proton impact ionisation

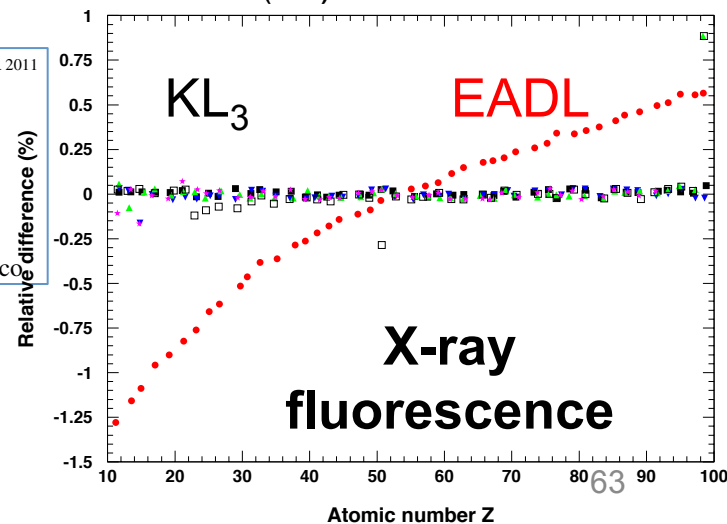


3246

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



Proton impact ionisation

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

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

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

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

	ISICS 2011					ERCS08	KIO
	ECPSSR	ECPSSR-HS	ECPSSR-UA	ECPSSR-HE	ECPSSR-HS-UA	Default	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

Theoretical and empirical models for proton ionisation cross sections
PWBA, ECPSSR (in various flavours), Paul-Sacher, Kahoul, Miyagawa, Orlic, Sow

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/](https://geant4.web.cern.ch/geant4/electromagnetic/pii/)

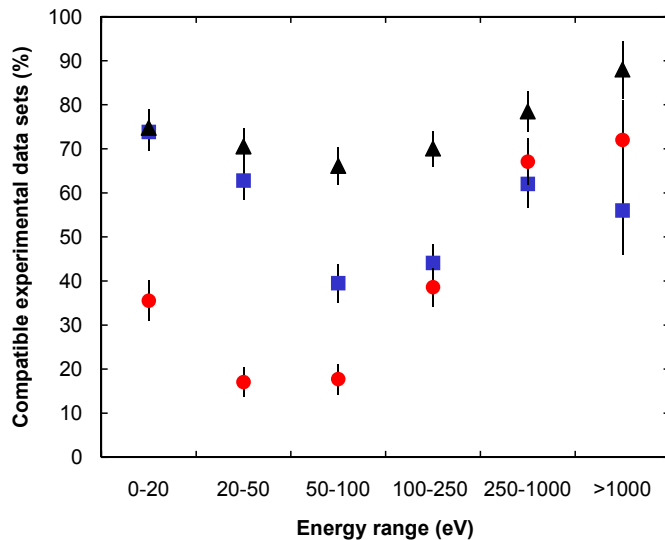
IPA and IA assumption

Micro/nano-dosimetry
Radiation effects

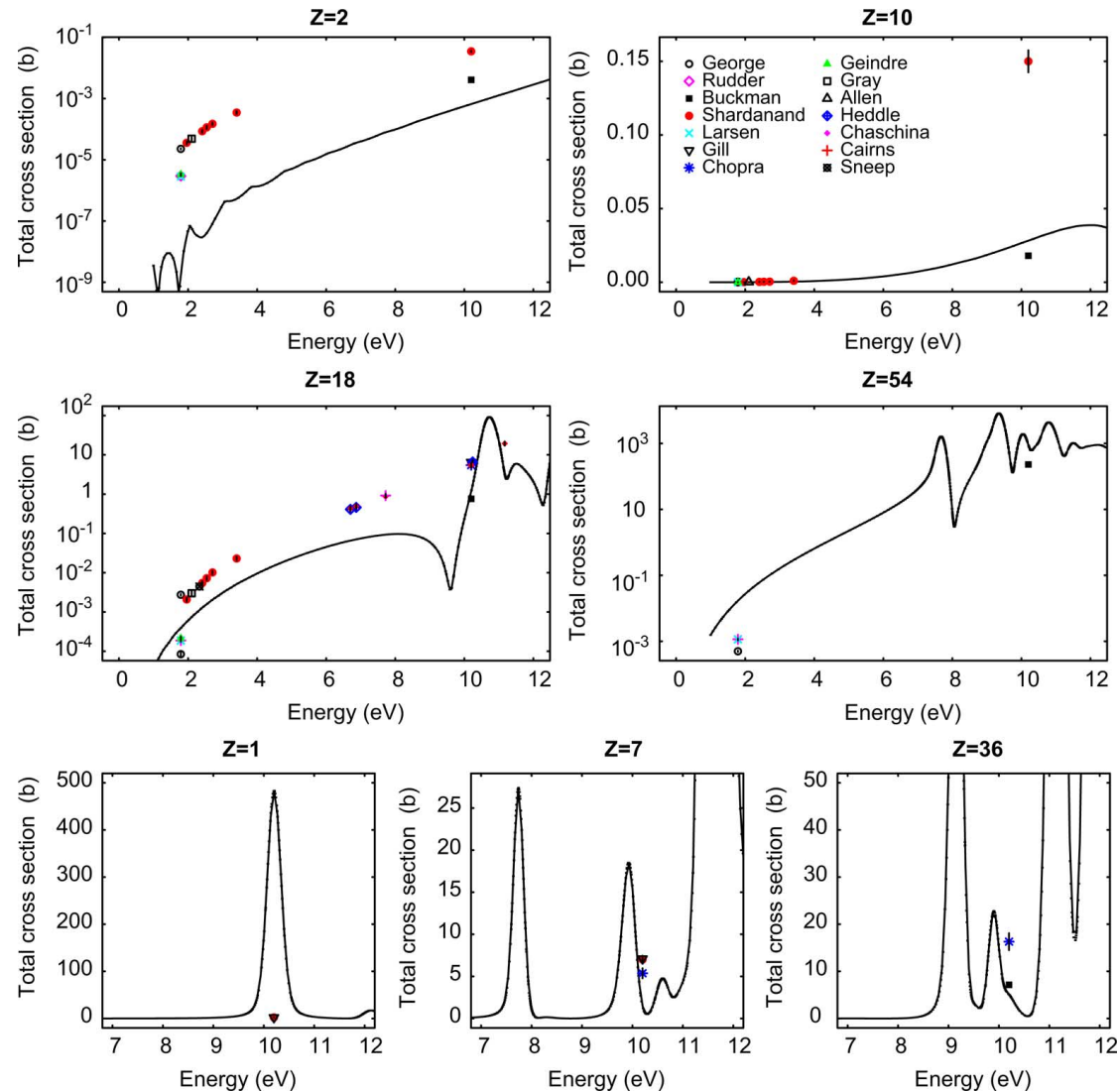
Photon elastic scattering

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

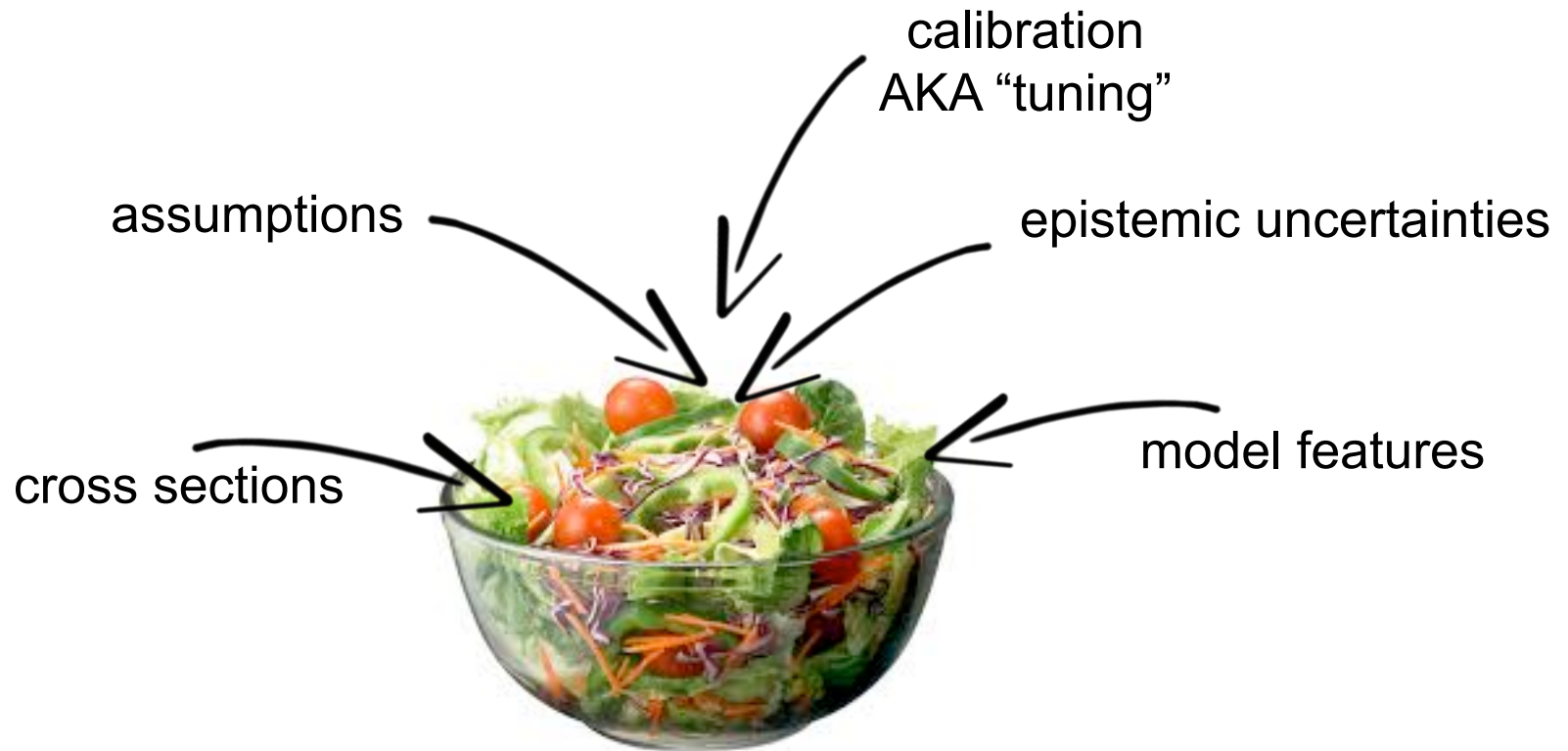
Electron impact ionisation



Maria Grazia Pia, INFN Genova



Hadronic transport models



What is (can be) validated?

Use cases (maybe)

Physics Validation Project

[Login](#) $H, A \rightarrow \tau \tau \rightarrow \text{two } \tau \text{ jets} + X, 60 \text{ fb}^{-1}$ [Info](#) ▾ [News](#) ▾ [Documents](#) ▾ [Results](#) ▾ [Contact](#)[CERN](#) ▸ [PH](#) ▸ [SFT](#) ▸ [SIMU](#) ▸ [VALI](#)

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News and announcements

2011-12-15

Status and perspectives of Geant4 physics

2011-12-15

Report on project

2011-09-22

LPCC Detector Simulation Workshop at CERN (6-7 October 2011)

2011-05-16

New report available: Geant4 simulation of target-diffraction process

2011-05-04

First plots added

FLUKA

Geant4

Geant3

ALICE

ATLAS

Our goal is to provide up-to-date comparison between LHC data and detector simulation toolkits. The detailed study of simulation results will allow for an in-depth improvement of the simulation code used by LHC experiments.

LCG Physics Validation Meeting

We regularly meet few times per year to discuss the status of simulation for experiments and any other subject.

Presentation from experiments, developers and experts are shown at the **LCG Physics Validation for LHC Simulations** meetings.

[Read more](#)

General Information

This website contains useful links and information on the activities of the physics validation project. As an activity of the [simulation project](#) area we deal with the simulation of the LHC experiments.

[Read more](#)

Report on project

[Report](#) on project status given at the LPCC Detector Simulation Workshop.

LPCC Detector Simulation Workshop at CERN (6-7 October 2011)

[LPCC \(LHC Physics Center at CERN\)](#) is organizing a 2 days workshop on the Simulation of LHC detectors.

HEP experiments

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High Energy Physics Experiments

Comparisons of the Geant4 predictions with experimental data obtained with High Energy Physics prototype detectors in the test beam runs.

- ATLAS (Simulation of Barrel, EndCal and Forward Hcal test beam results, etc.)
 - [Test Beam Runs 2000-2001, 2002, 2004](#)
- CMS (Calorimeter prototype beam test results, validation of various physics lists, etc.)
 - [Test Beam 2004](#)
 - [Test Beam 2006 and tuning of physics list towards LHC startup](#)

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Last updated: 6 Jan 2011

Medium energy

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Medium Energy Verifications

These tests compare Geant4 predictions with experimental data from about 100 MeV up to 20 GeV.

- [113-800 MeV protons \(various targets\)](#)
- [123, 151 MeV gammas](#)
- [380 MeV protons \(isotope production\)](#)
- [400 MeV heavy ions](#)
- [730 MeV protons](#)
- [1.5 GeV protons on Pb](#)
- [3.0 GeV protons on Pb](#)
- [1.4-9.0GeV proton and 1.4-5.0GeV pion on Be, C, Cu, Pb, and U](#)
- [14.6GeV/c proton on Be, Al, Cu, and Au](#)

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Last updated: 10/12/2013

Maria Grazia Pia, INFN Genova

Validation database at FNAL

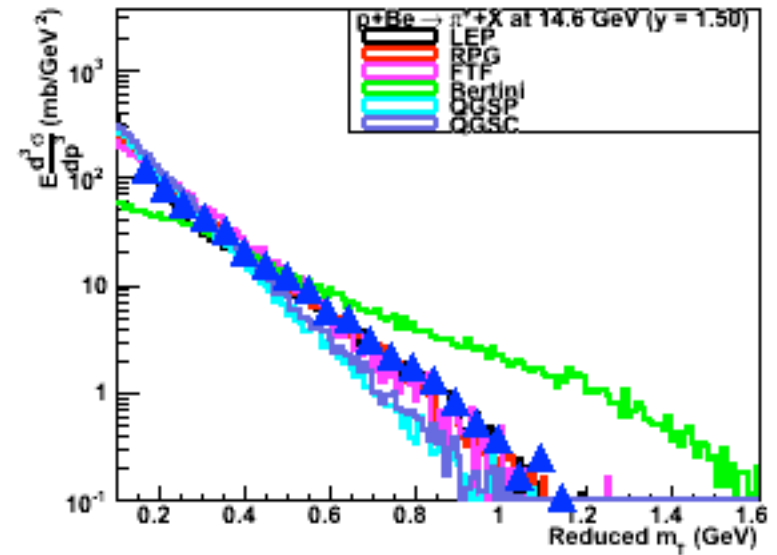
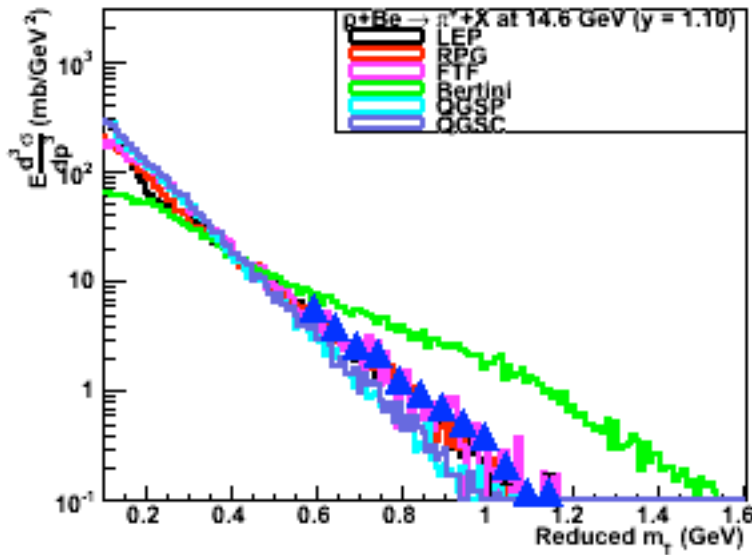
<http://g4validation.fnal.gov:8080/G4ValidationWebApp/index.jsp>

List of Tests

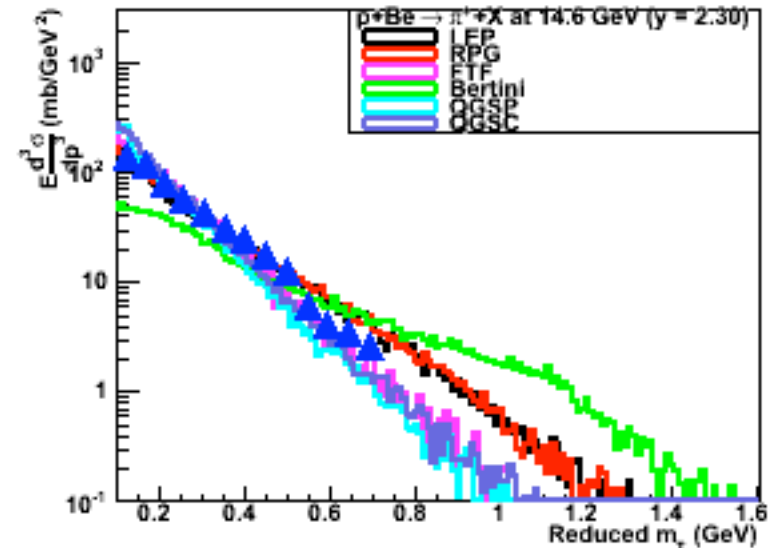
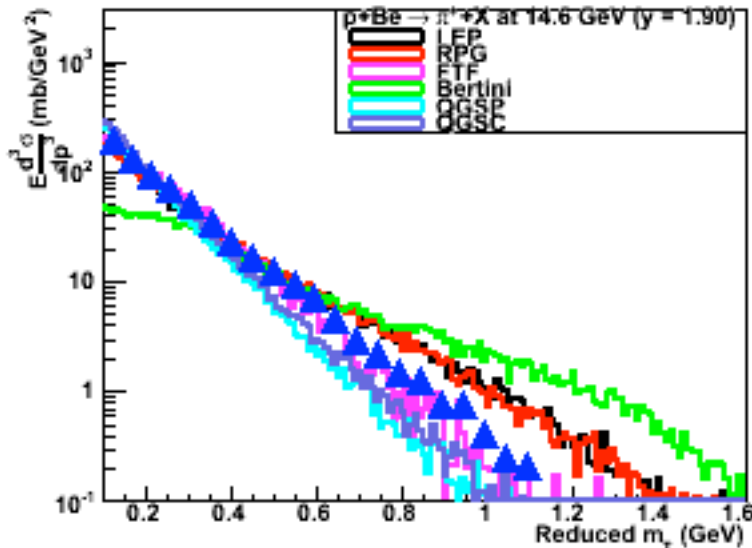
Name	Description	Working Group
ATLAS	shower characteristics of ATLAS Calorimeters	LHC-feedback
CMS	shower characteristics of CMS Calorimeters	LHC-feedback
HadrIon	Test of Physics Lists (thick targets, ion beams)	hadronic
HadrXS	Test of Physics Lists (cross sections)	hadronic
Hadrcap	is an analogous to 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 ATLAS 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 π^+ production in 14.6 GeV/c p-Be interactions



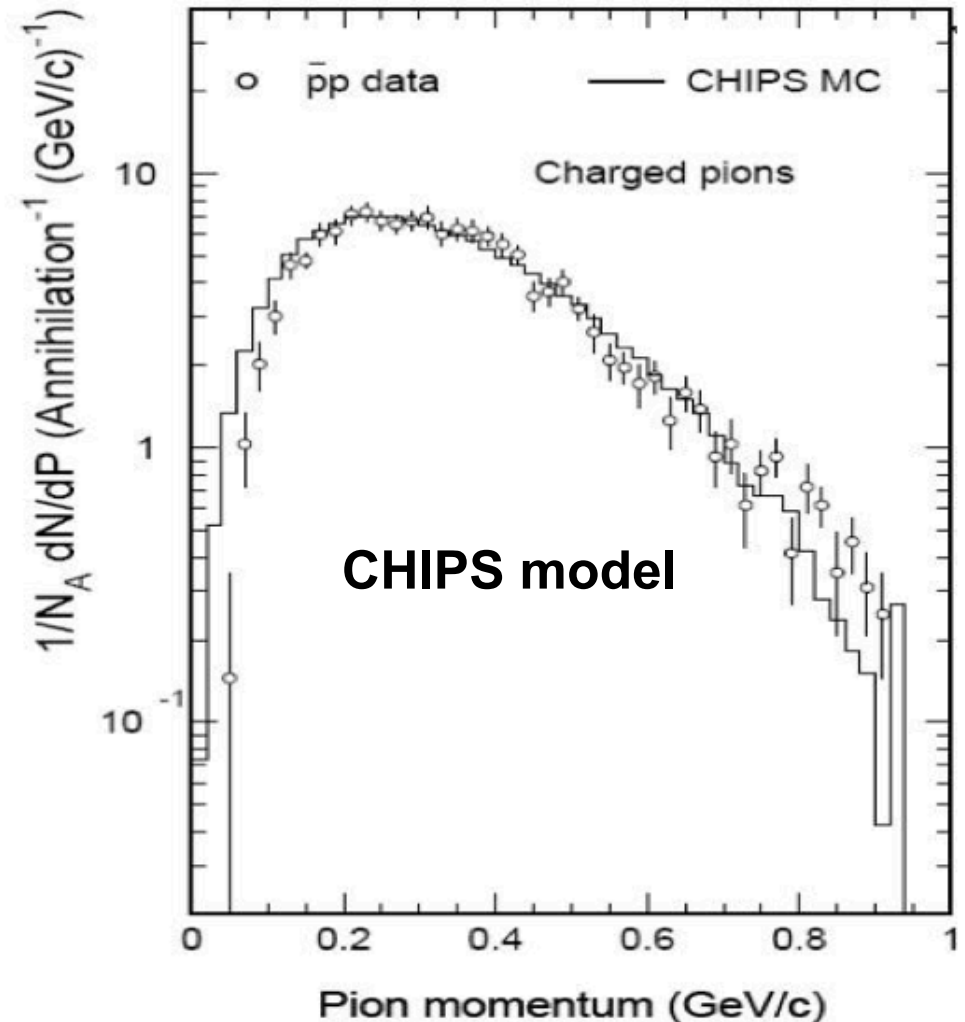
http://geant4.cern.ch/results/validation_plots/thin_target/hadronic/medium_energy/test_bnl_802/bnl_data.shtml



Stopped particles

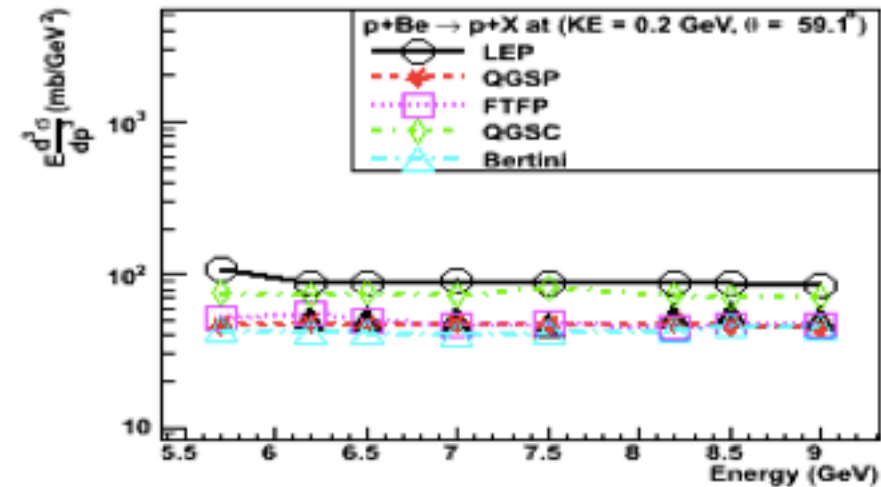
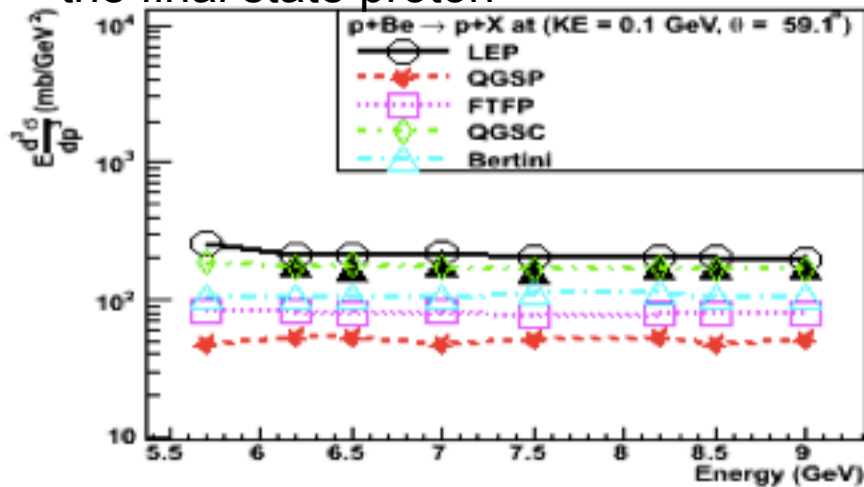
antiprotons
stopping in H:
**charged pion
production**

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

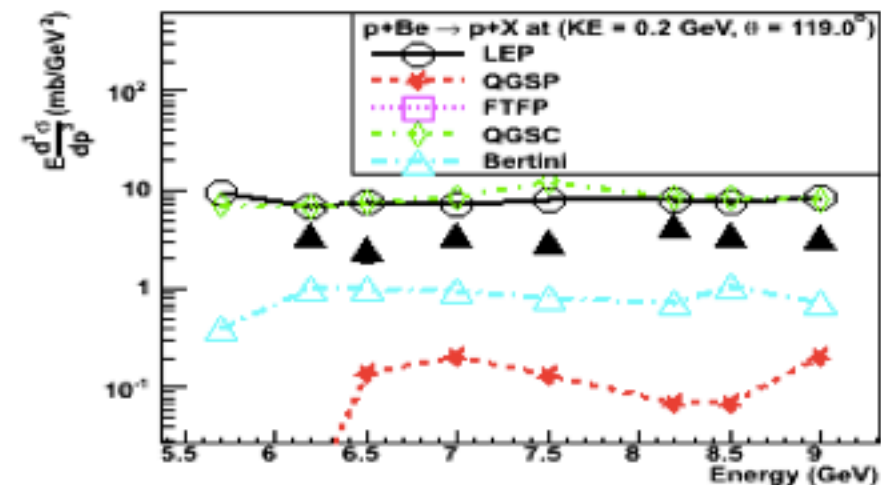
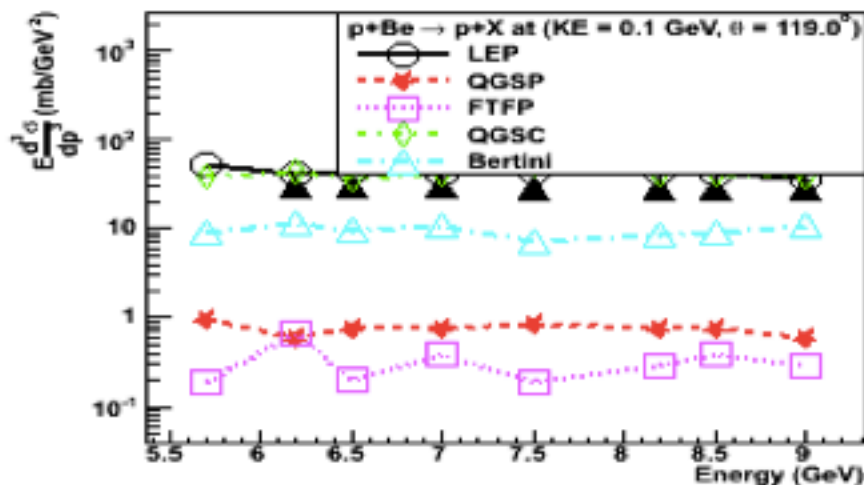


Inclusive proton production

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

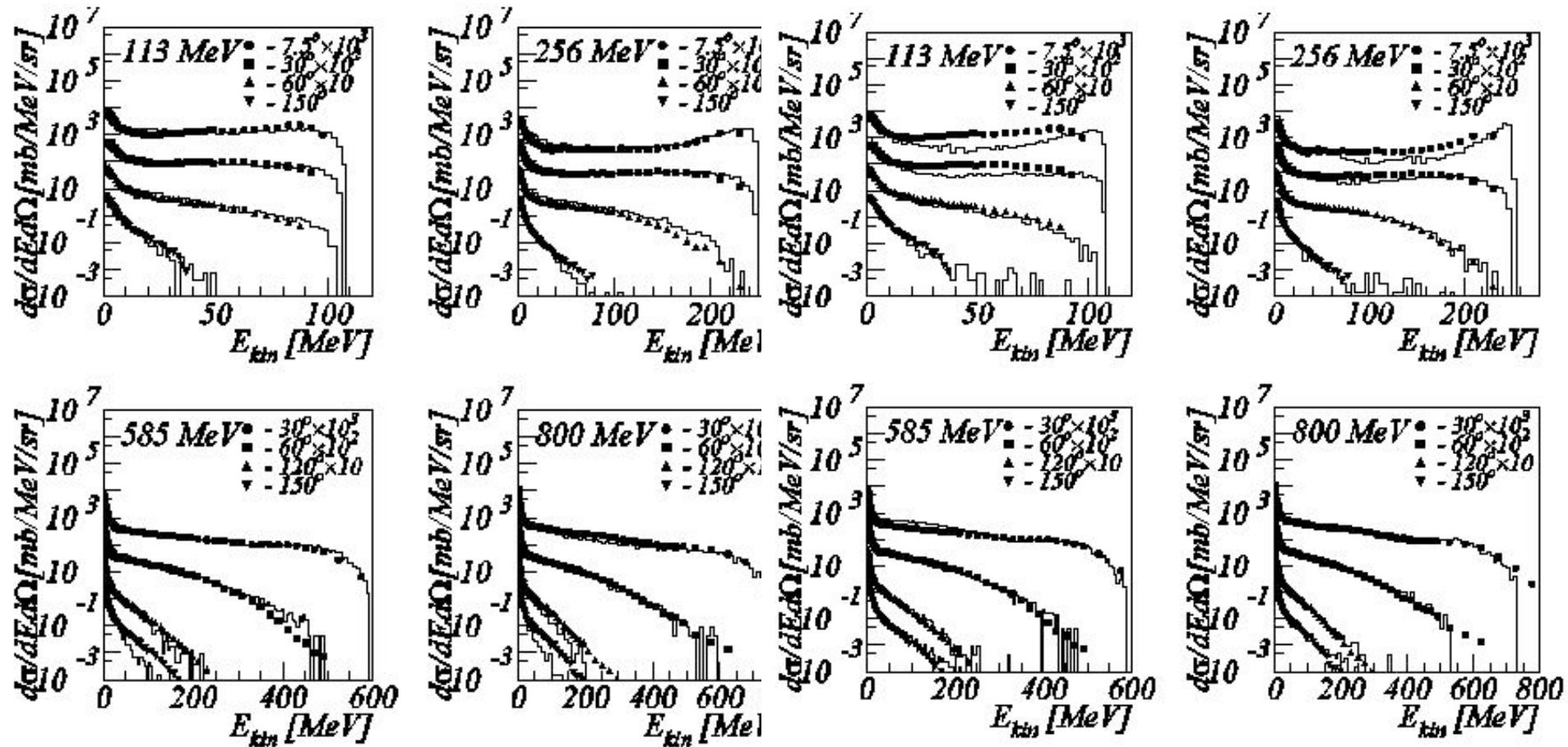


A sample of results

Impossible to show all!

Al(p,n) Binary cascade

Al(p,n) Bertini cascade



What does one evince from these plots?

Metaanalysis

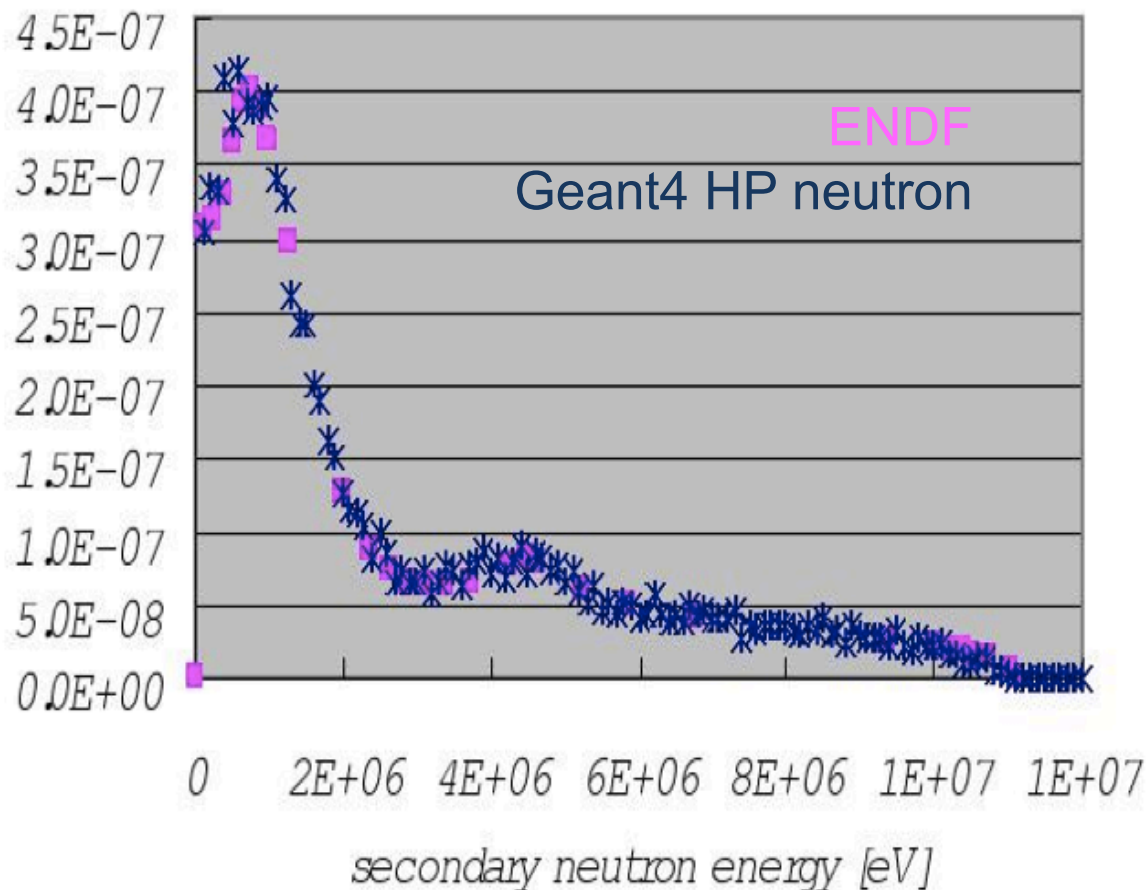
Needed!

Documentation of epistemic uncertainties
and their effects
Sensitivity analysis

HP neutrons

Reference: ENDF/B-VI
Release 8, Tape162

Geant4 version: 8.1



Data-driven model

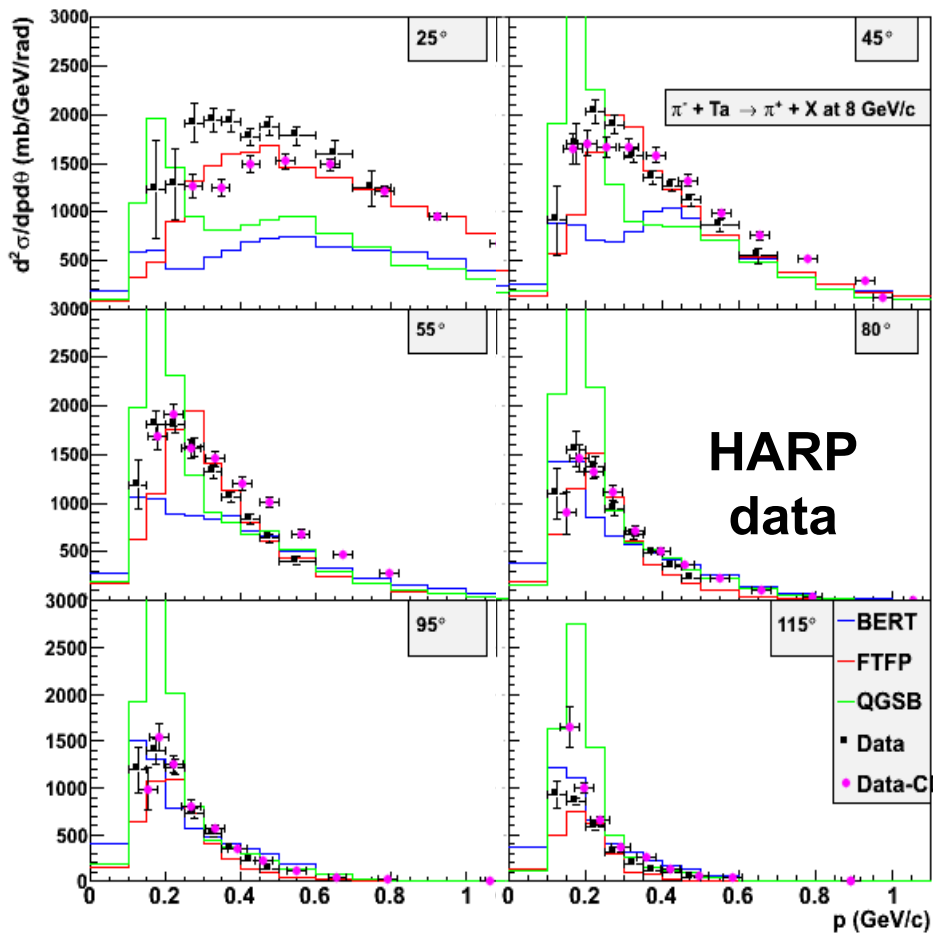
*The model is as
good as the data on
which it is based*

Systematics of
evaluated data
compilations

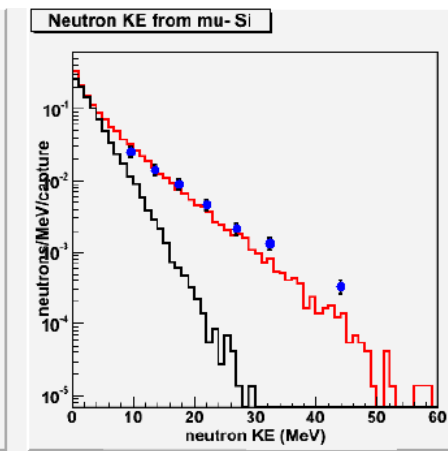
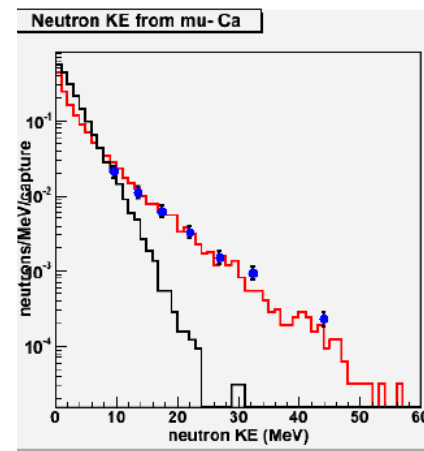
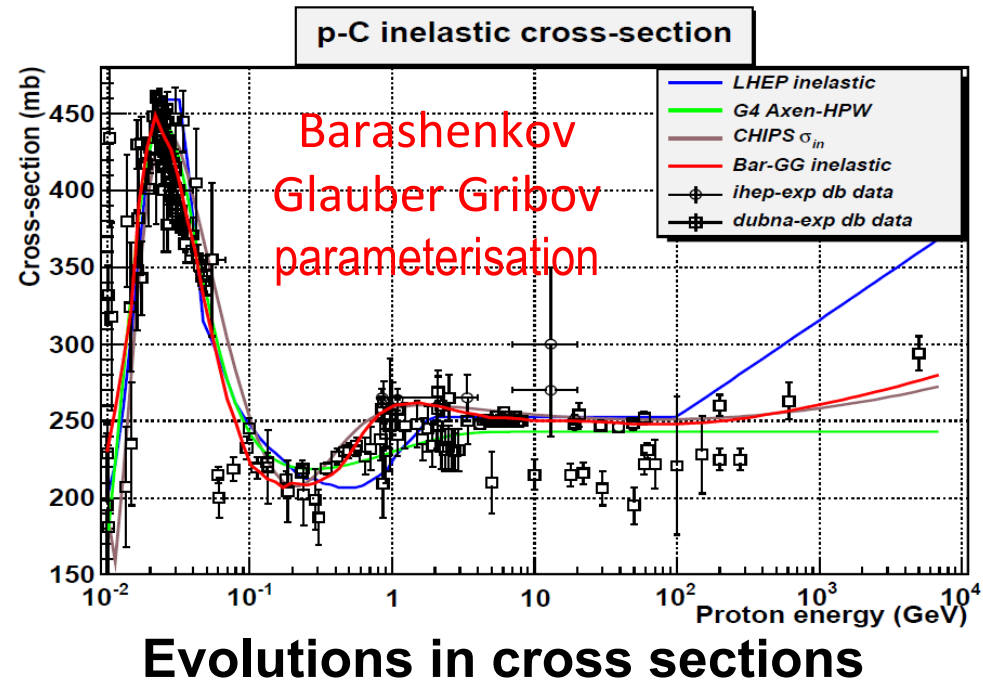
Recent developments

More in

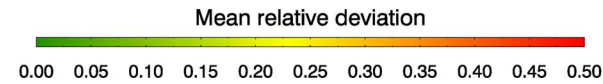
Simulation N29-3



Evolutions in Bertini cascade



Radioactive decay

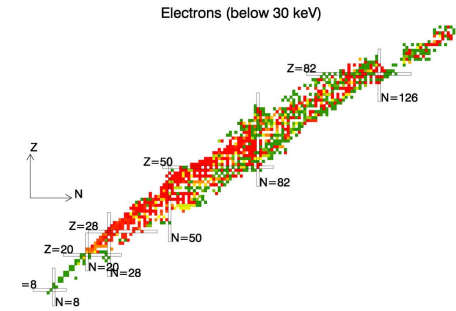


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IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 60, NO. 4, AUGUST 2013

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

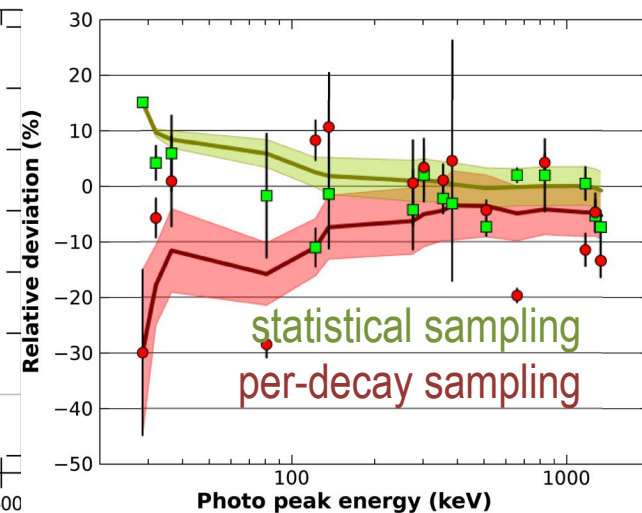
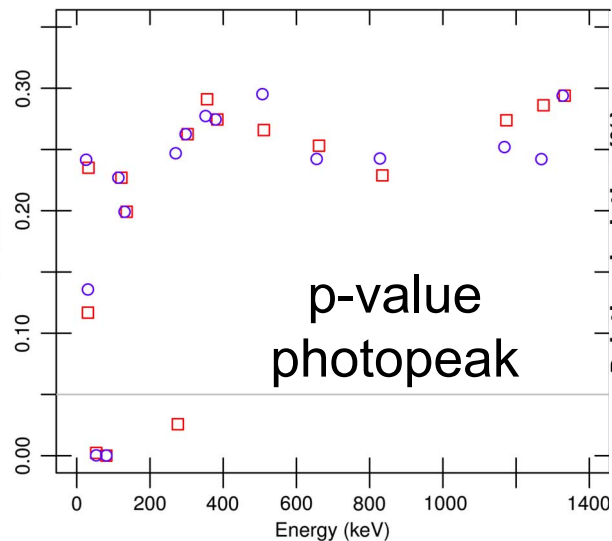
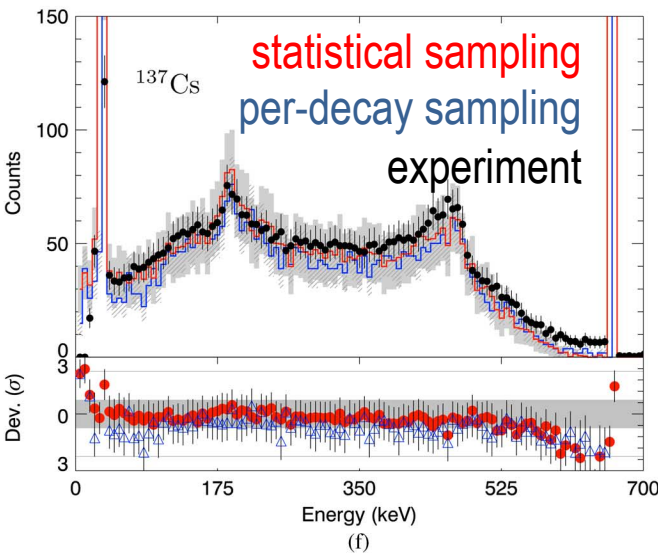
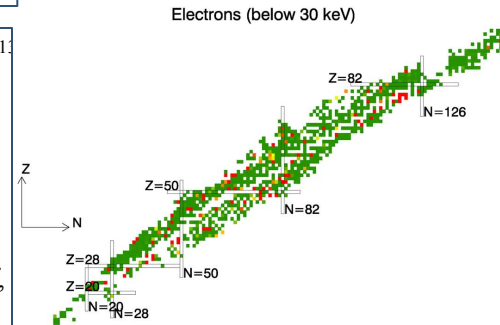


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IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 60, NO. 4, AUGUST 2013

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

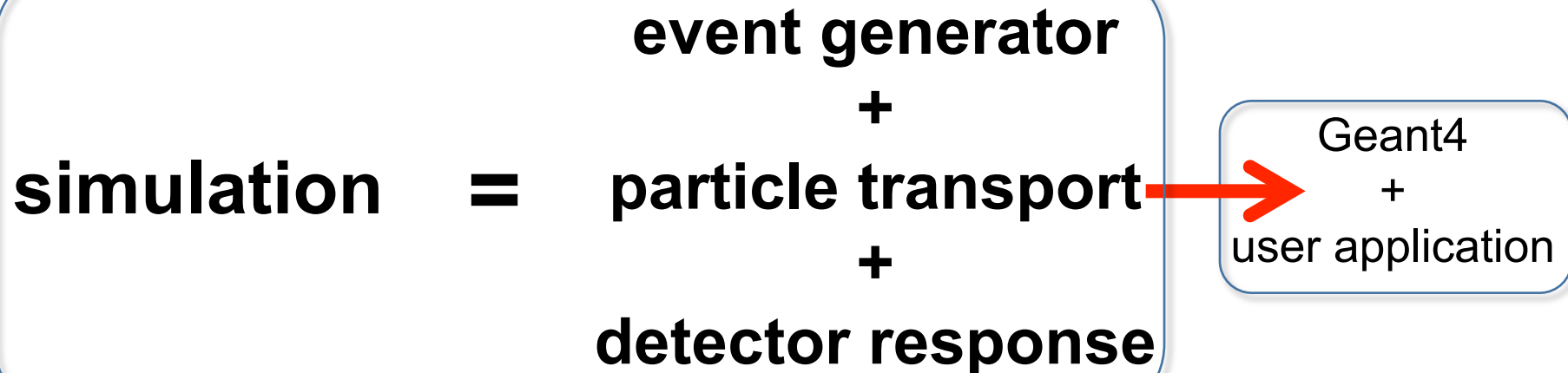


In LHC experiments

A lot of activity, by many people, for many years
Comparing Geant4-based simulations with test beam or full-scale data

No time to show the impressive wealth of results!

some highlights...



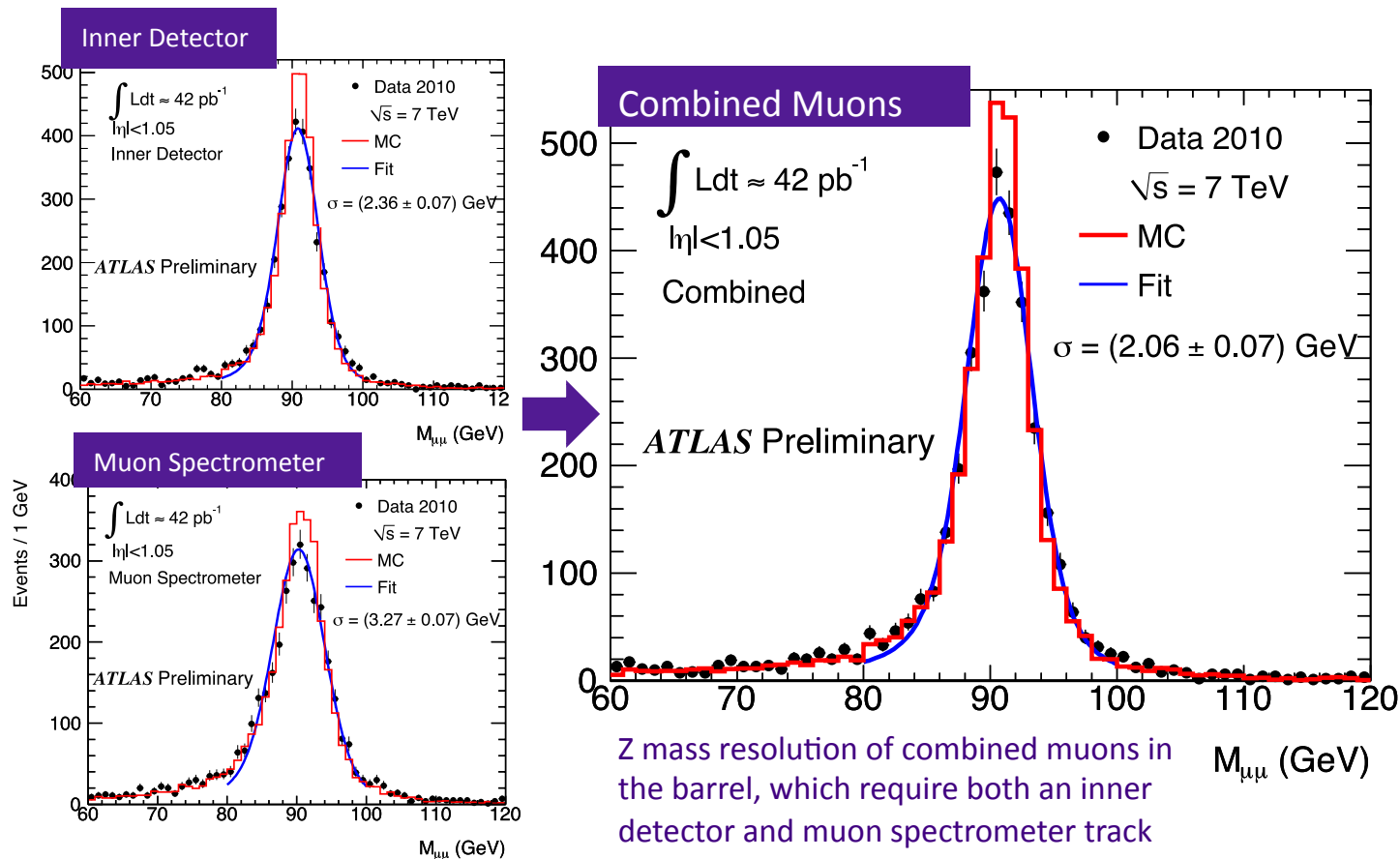
Muon simulation in ATLAS

ATLAS: Data and MC Comparisons for Muon Spectrometer, including Cavern Background

LPCC Simulation Workshop 6 October 2011

Laura Jeanty

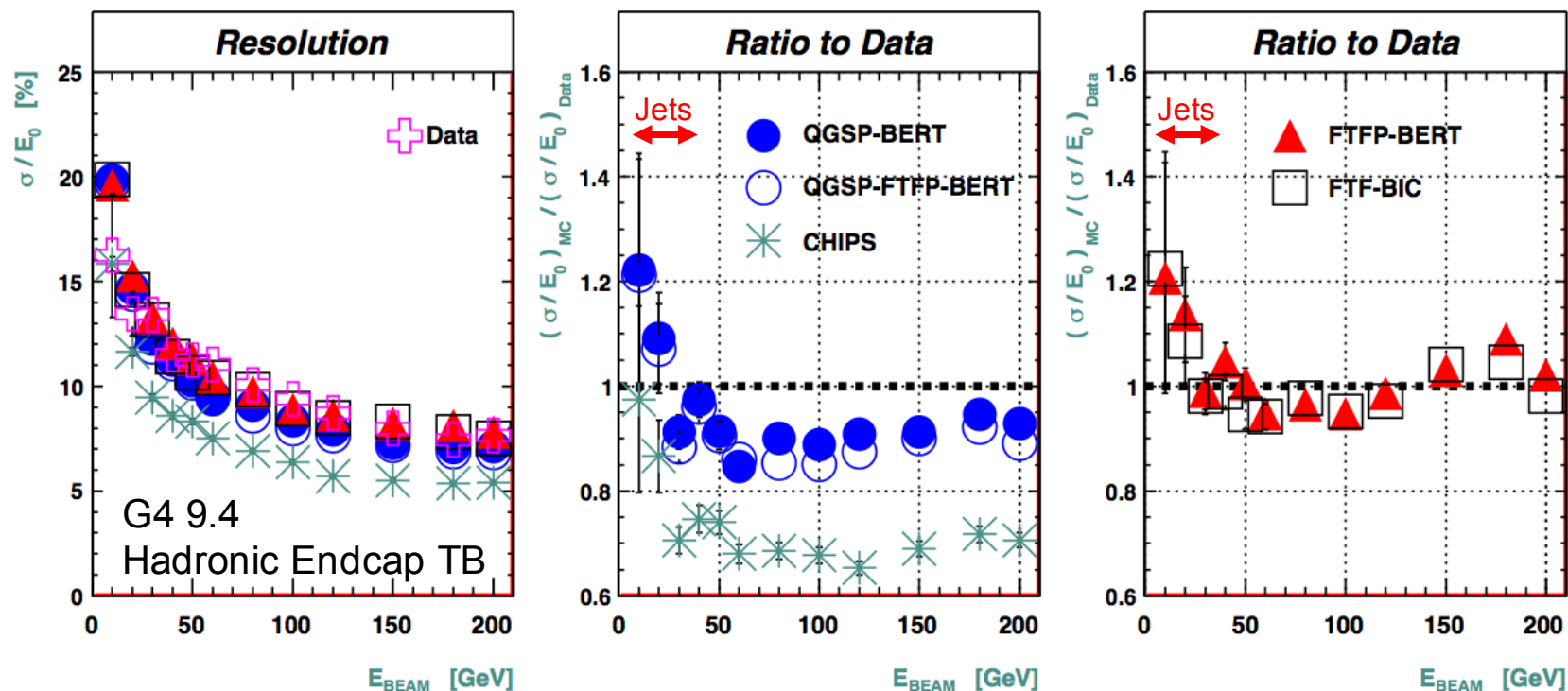
On behalf of the ATLAS Collaboration



Atlas Data/MC comparisons in hadronic physics

Resolution

- Considerably more variation in resolution
 - In situ, we have to also deal with background variations, which make resolution measurements very tricky - go to test beam!
 - Also varies against G4 release considerably more than response





CMS: Full Detector Simulation

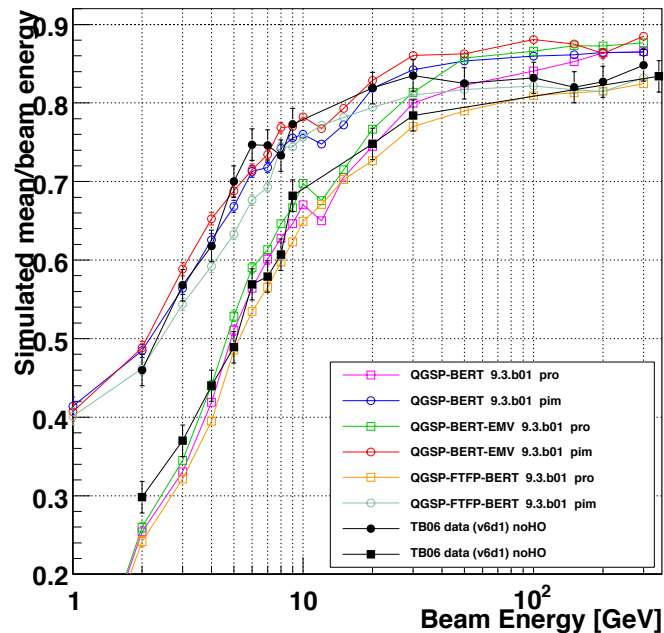
LHC Detector Simulations

October 6, 2011

Sunanda Banerjee

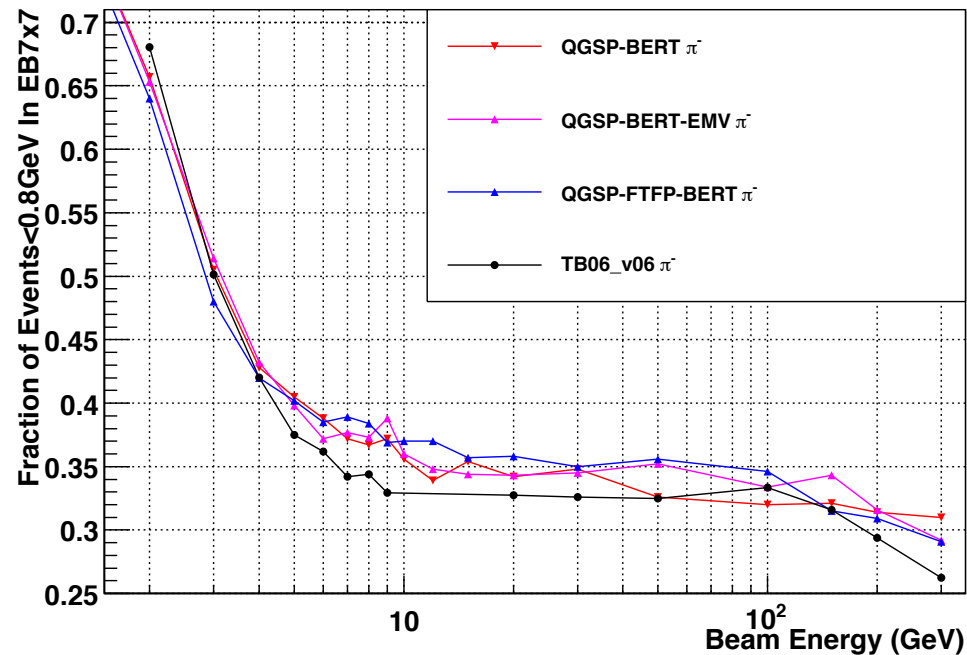
(On behalf of CMS collaboration)

Calo Response (MCidealMIP calib.: ele50)



October 6, 2011

MIP fraction G4.9.3.b01

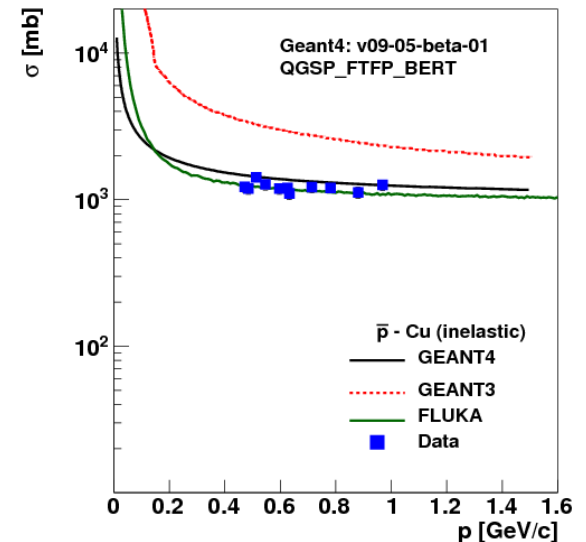
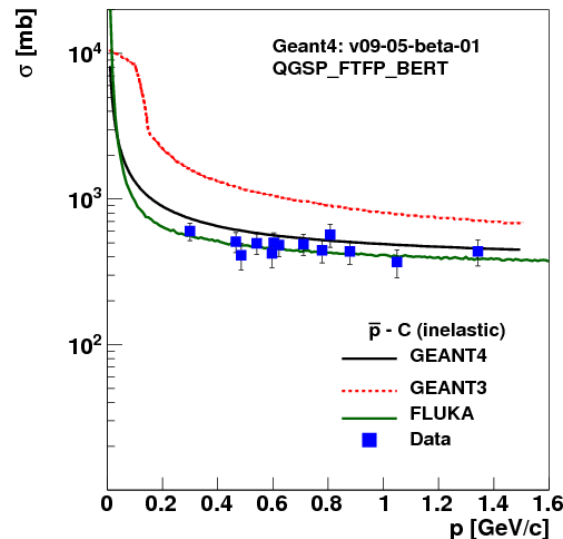
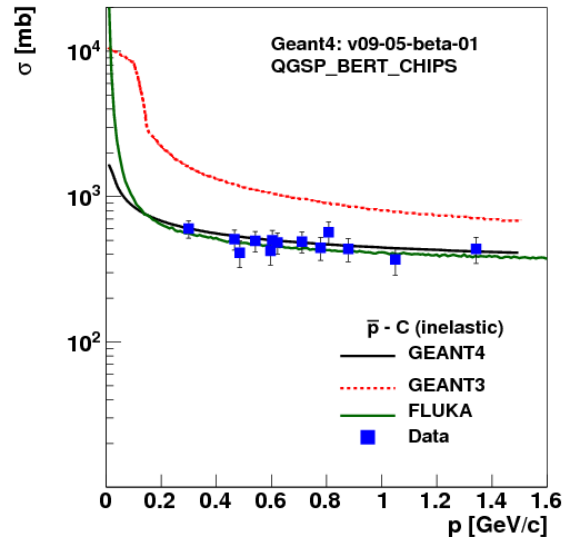


CI

(Low momentum) Hadron-Nucleus interactions in ALICE

Marco van Leeuwen, Utrecht University
For the ALICE collaboration

LHC Detector Simulation workshop
6-7 October 2011



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?*

LHC Detector Simulation Workshop

RICH Simulation in LHCb

S.Easo,
RAL,
6-10-2011

On behalf of LHCb–RICH group

Validation using Testbeams

(B)Performance of the LHCb RICH photo-detectors and readout in a system test using charged particles from a 25 ns- structured beam,

M.Adinolfi et.al. , NIM A 603 (2009) 287-293

Radiator	quantity	Data	MC
N ₂	resolution mrad	$0.296 \pm 0.003 \pm 0.006$	0.29 ± 0.003
C ₄ F ₁₀	resolution mrad	$0.166 \pm 0.002 \pm 0.002$	0.174 ± 0.005
N ₂	yield	$12.44 \pm 0.04^{+0.08}_{-0.09}$	12.15 ± 0.61
C ₄ F ₁₀	yield	8.9 ± 0.5	9.3 ± 0.5

Here, **resolution**: Single photon Cherenkov angle resolution

yield: Yield in a typical HPD. Similar yields in other HPDs

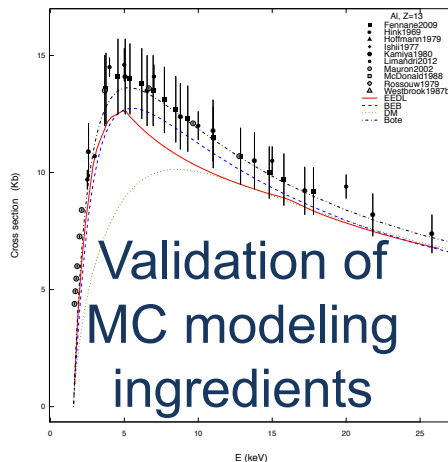
Using LHCb software framework and standard LHCb software chain

Uncertainty quantification

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

Input

Parameter uncertainties



Validation of
MC modeling
ingredients

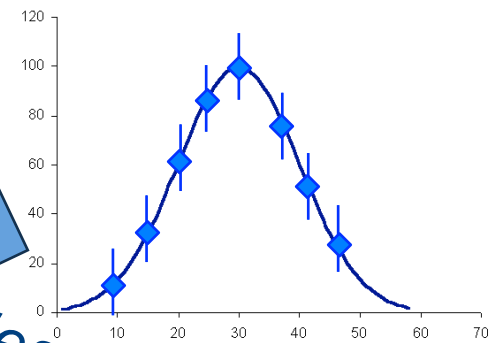
Beware: input uncertainties
can be hidden in the code
(in models and algorithms)



Monte Carlo method
Statistical uncertainty

Geant 4

observable
with uncertainties



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

N18-5

Progress with Uncertainty
Quantification in Generic
Monte Carlo Simulations

Uncertainty quantification is the ground for
predictive Monte Carlo simulation

No time for reviewing everything...

- Much more:
 - Geant4 electromagnetic and hadronic models
 - **Experimental use cases**
- Selection constrained by time, not by merit
- **Concepts** and **methods** to find your way across the wealth of information about Geant4 physics and its validation

Through the narrow gate

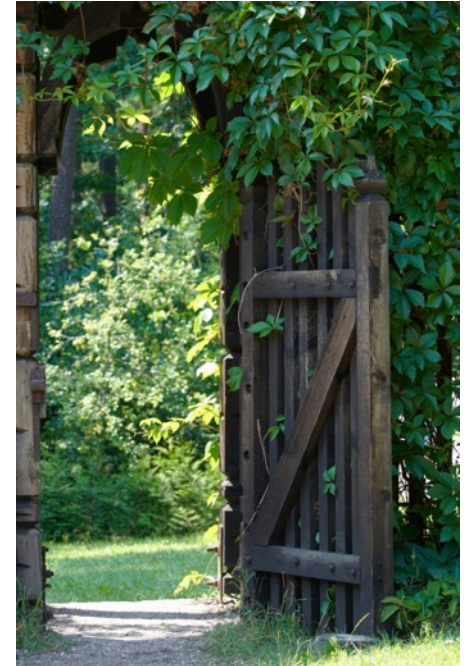
● Think

● Learn

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

● Work

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



We need a paradigm shift...

- Experimenters 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
 - NASA: experiments at accelerators
 - Military projects: e.g. weapon simulations
- What about particle/nuclear/astro/medical physics?

Conclusion

- Geant4 is a rich and powerful tool for experimental research
- It requires the user to be responsible for his/her **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**

