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# Geant4 Low Energy Electromagnetic Physics

M.G. Pia

On behalf of the LowE EM Working Group

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

Geant4 Workshop

Lisbon, 9-14 October 2006

# Vision

## Technology

Advanced software technology at the service of physics

**User Requirements**  
+  
**Our own scientific background**

## Transparency

Within the Collaboration  
Towards the users

## Software process

Rigorous  
For quality  
For productivity  
For maintainability

## High scientific profile

Publications  
Physics Book

## People

Collaborative environment  
**No internal competition**  
Investment in the young  
Geant4 generation

## Analysis & Design

Transparency  
Openness  
Maintainability

## Physics Modeling

High precision  
Collaboration with theorists

**Synergy with  
Advanced Examples**

## Physics Validation

Rigorous, quantitative

Experimental investigation  
and feedback

# Photoelectric effect

- **New model for precise angular distribution**
  - Andreia, Pedro and Luis + MG integration
- **Difficulties encountered because of errors(?) in the theoretical reference paper**
  - Contacts with other theorists
- **Released June 2006 (K-L shells)**
  - Further improvements depending on clarification of the theoretical calculations

Barbara – MG – Sébastien – Ziad

- **Processes down to the eV scale**
  - At this scale physics interactions depend on the detailed structure of the medium
  - Processes specialised by material
  - 1<sup>st</sup> cycle: processes in water
- **Releases**
  - $\beta$ -version in Geant4 8.1 (June 2006)
  - Refined version in progress
  - Further extensions to follow
- **Processes for other materials to follow**
  - Interest for radiation effects on components
  - User requirements for gaseous materials

Particle	Processes
e	Elastic scattering Excitation Ionisation
p	Excitation Charge decrease Ionisation
H	Charge increase Ionisation
He <sup>++</sup>	Excitation Charge decrease Ionisation
He <sup>+</sup>	Excitation Charge decrease Charge increase Ionisation
He	Excitation Charge increase Ionisation

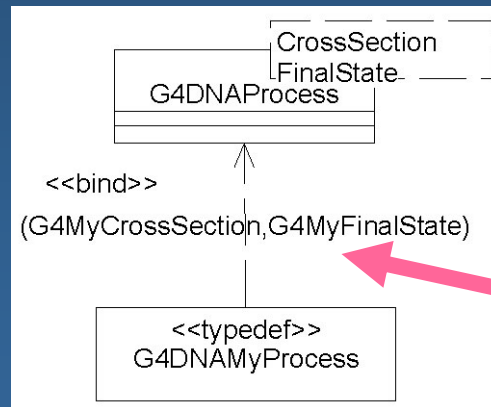
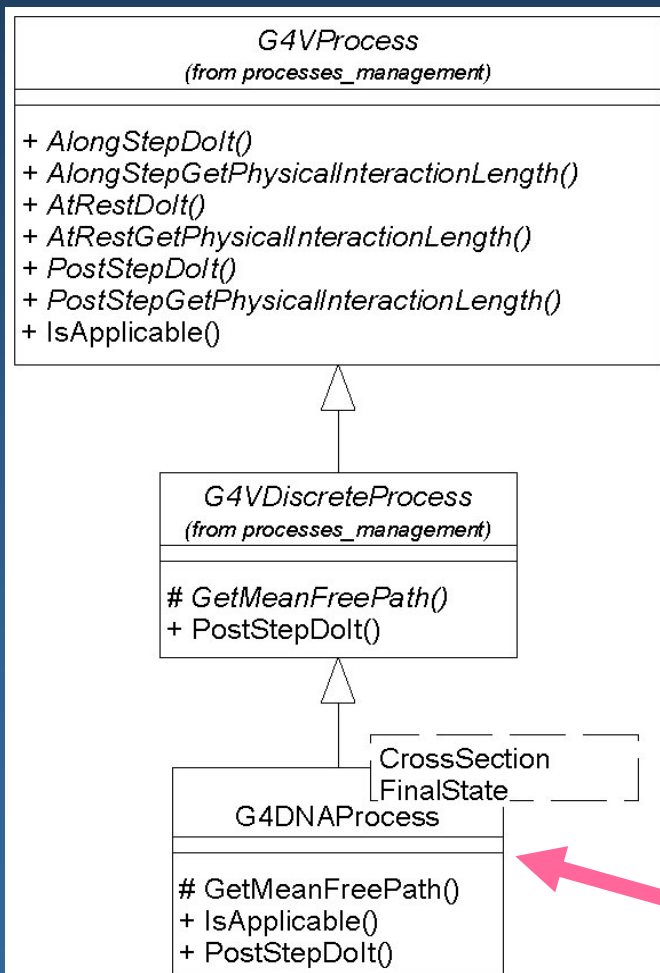
# Software design

Innovative design introduced in Geant4: **policy-based class design**  
Flexibility of modeling + performance optimisation

Playground for further applications of this design technique in the LowE EM package

The process can be configured with a variety of physics models by template instantiation

Parameterised class



# Implementation

- First set of models implemented chosen among those available in literature
  - Direct contacts with theorists whenever possible
- Future extensions foreseen
  - Made easy by the design
  - Provide a wide choice among many alternative models
  - Different modeling approaches
  - Complementary models
- Unit test in parallel with implementation

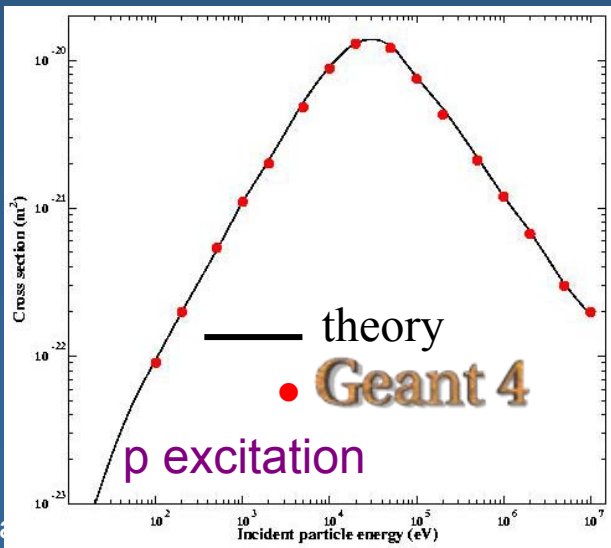
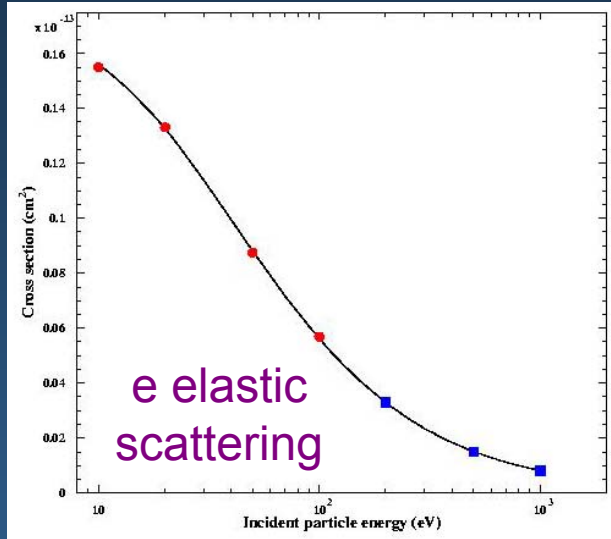
## References of models implemented

1. D. Emfietzoglou, G. Papamichael, and M. Moscovitch, “An event-by-event computer simulation of interactions of energetic charged particles and all their secondary electrons in water”, *J. Phys. D: Appl. Phys.*, vol. 33, pp. 932-944, 2000.
2. D. J. Brenner, and M. Zaider, “A computationally convenient parameterization of experimental angular distributions of low energy electrons elastically scattered off water vapour”, *Phys. Med. Biol.*, vol. 29, no. 4, pp. 443-447, 1983.
3. B. Grosswendt and E. Waibel, “Transport of low energy electrons in nitrogen and air”, *Nucl. Instrum. Meth.*, vol. 155, pp. 145-156, 1978.
4. D. Emfietzoglou, K. Karava, G. Papamichael, and M. Moscovitch, “Monte Carlo simulation of the energy loss of low-energy electrons in liquid water”, *Phys. Med. Biol.*, vol. 48, pp. 2355-2371, 2003.
5. D. Emfietzoglou, and M. Moscovitch, “Inelastic collision characteristics of electrons in liquid water”, *Nucl. Instrum. Meth. B*, vol. 193, pp. 71-78, 2002.
6. D. Emfietzoglou, G. Papamichael, K. Kostarelos, and M. Moscovitch, “A Monte Carlo track structure code for electrons (~10 eV-10 keV) and protons (~0.3-10 MeV) in water: partitioning of energy and collision events”, *Phys. Med. Biol.*, vol. 45, pp. 3171-3194, 2000.
7. M. Dingfelder, M. Inokuti, and H. G. Paretzke, “Inelastic-collision cross sections of liquid water for interactions of energetic protons”, *Rad. Phys. Chem.*, vol. 59, pp. 255-275, 2000.
8. D. Emfietzoglou, K. Karava, G. Papamichael, M. Moscovitch, “Monte-Carlo calculations of radial dose and restricted-LET for protons in water”, *Radiat. Prot. Dosim.*, vol. 110, pp. 871-879, 2004.
9. J. H. Miller and A. E. S. Green, “Proton Energy Degradation in Water Vapor”, *Rad. Res.*, vol. 54, pp. 343-363, 1973.
10. M. Dingfelder, H. G. Paretzke, and L. H. Toburen, “An effective charge scaling model for ionization of partially dressed helium ions with liquid water”, in *Proc. of the Monte Carlo 2005*, Chattanooga, Tennessee, 2005.
11. B. G. Lindsay, D. R. Sieglaff, K. A. Smith, and R. F. Stebbings, “Charge transfer of 0.5-, 1.5-, and 5-keV protons with H<sub>2</sub>O: absolute differential and integral cross sections”, *Phys. Rev. A*, vol. 55, no. 5, pp. 3945-3946, 1997.
12. K. H. Berkner, R. V. Pyle, and J. W. Stearns, “Cross sections for electron capture by 0.3 to 70 keV deuterons in H<sub>2</sub>, H<sub>2</sub>O, CO, CH<sub>4</sub>, and C<sub>8</sub>F<sub>16</sub> gases”, *Nucl. Fus.*, vol. 10, pp. 145-149, 1970.
13. R. Dagnac, D. Blanc, and D. Molina, “A study on the collision of hydrogen ions H<sub>1</sub><sup>+</sup>, H<sub>2</sub><sup>+</sup> and H<sub>3</sub><sup>+</sup> with a water-vapour target”, *J. Phys. B: Atom. Molec. Phys.*, vol. 3, pp. 1239-1251, 1970.
14. L. H. Toburen, M. Y. Nakai, and R. A. Langley, “Measurement of high-energy charge transfer cross sections for incident protons and atomic hydrogen in various gases”, *Phys. Rev.*, vol. 171, no. 1, pp. 114-122, 1968.
15. P. G. Cable, Ph. D. thesis, University of Maryland, 1967.
16. M. E. Rudd, T. V. Goffe, R. D. DuBois, L. H. Toburen, “Cross sections for ionisation of water vapor by 7-4000 keV protons”, *Phys. Rev. A*, vol. 31, pp. 492-494, 1985.

# Test

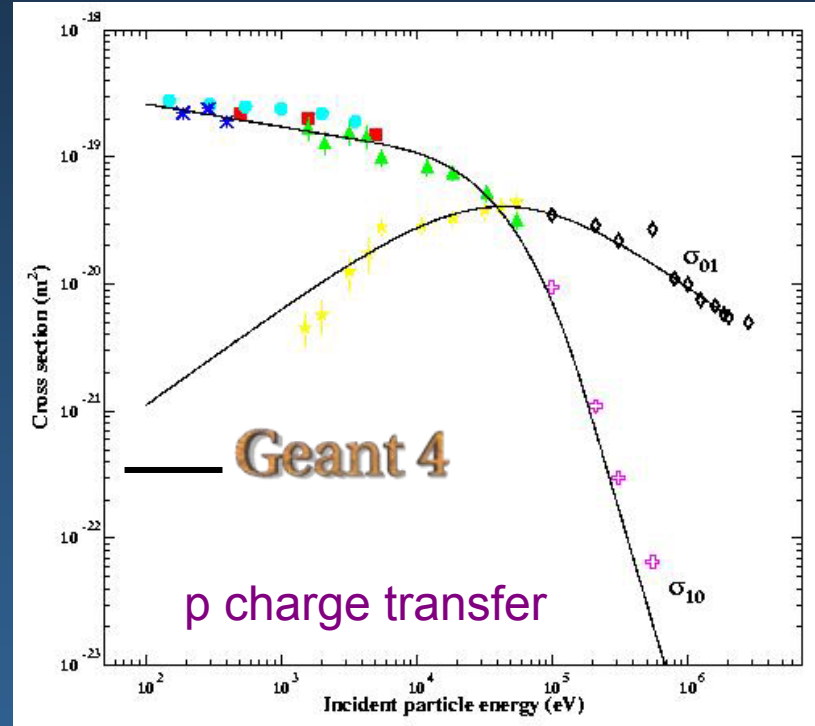
## Verification

against theoretical models



## Validation

against experimental data



Scarce experimental data

Large scale validation project planned



# Outlook

- IEEE NSS 2006
  - Talk
- Publication
  - 1<sup>st</sup> software development cycle
- Validation
  - Scarce experimental data
  - 2<sup>nd</sup> publication
- New models for water
  - Some already identified
- Models for other materials
  - Facilitated by the design

## Geant4 Models for Low Energy Particle Interactions with Water

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

**Abstract**— A set of processes specialized for the simulation of particle interactions with water has been developed in the Geant4 Low Energy Electromagnetic package. They address a physics domain relevant to the simulation of radiation effects in biological systems, where water represents an important component. The models cover the interactions of electrons, protons and light ions down to the electronVolt energy scale. The software design, the physics models implemented and a set of their tests are described.

### I. INTRODUCTION

THE simulation of radiation effects in biological systems is a critical concern in various domains, such as oncological radiotherapy and radiation protection. A common approach consists of describing the effects of the radiation of a biological system in terms of the dose released to it. Nevertheless the concern of dose fails when the biological effects of radiation on cellular structures and on the DNA (deoxyribonucleic acid) molecule are the object of study.

The Geant4-DNA project addresses the extension of the Geant4 [1]-[2] simulation toolkit to deal with radiation effects at the cellular and DNA scale. It exploits the Geant4 architectural design to equip an open source, general purpose Monte Carlo system for particle transport for the first time with functionality specific to radiobiology simulation. This novel approach provides the user the opportunity to combine specialized tools for the study of the biological effects of radiation with the rich simulation functionality of a full Monte

Carlo system for particle transport; nevertheless, thanks to the toolkit nature of Geant4, it does not carry any overhead for non essential functionality with respect to specialized Monte Carlo systems for radiobiology simulation: a user application only uses the toolkit components pertinent to it.

The Geant4-DNA software encompasses various domains: the extension of Geant4 physics processes down to the energy scale relevant to bio-molecular systems, the development of models to describe biological processes, and the description of biological entities, such as cells or the DNA molecule. The overall Geant4-DNA subsystem adopts a component-based architecture, where each domain is addressed by a software component.

This paper describes a new component of Geant4 physics developed in the context of the Geant4-DNA project: a set of specialized physics processes to model particle interactions in water, which is the main component of biological systems, down to the electronVolt energy scale. These new developments are identified in the following sections as the Geant4-DNA Physics Processes; they are part of the Geant4 Low Energy Electromagnetic Physics package [3]-[4].

The Geant4-DNA software is open-source; it is publicly released in the Geant4 Toolkit.

### II. SOFTWARE PROCESS

The Geant4-DNA project addresses a very active scientific domain: the continuous progresses in biological research, as well as the availability of new accelerator facilities for cellular irradiation, contribute to a rapid evolution of the body of knowledge in fields pertinent to the project. The development of the Geant4-DNA software follows an iterative and incremental process. Such a process model is particularly suitable to address the complex, fast evolving research domain of radiation effects on biological systems: it allows building and refining the software taking into account the theoretical and experimental progresses in the field, at the same time producing concrete deliverables at each development cycle.

The software process of Geant4-DNA is based on the Unified Software Development Process [5] and adopts the Rational Unified Process™ (RUP) [6] as a process framework, tailored to the specific characteristics of the project and its scientific environment [7]. The rigorous software process,

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# Biological models

Barbara – MG – Stéphane – Susanna

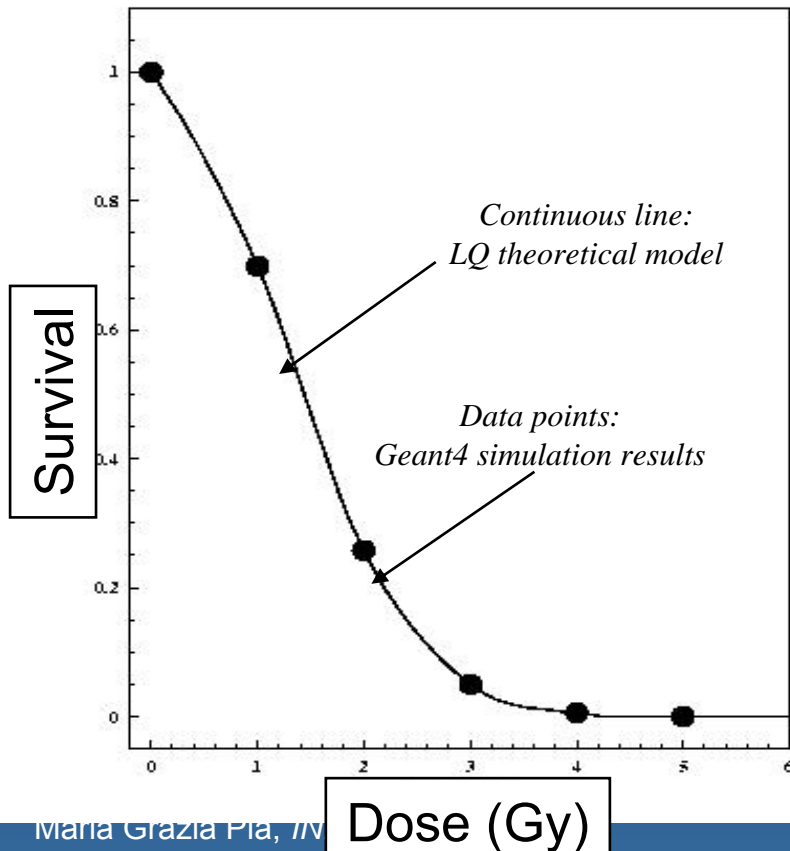
*In progress*

TARGET THEORY	Single-hit	$S = e^{-D / D_0}$	
TARGET THEORY	Multi-target Single-hit	$S = 1 - (1 - e^{-qD})^n$	<i>Revised model</i> $S = e^{-q_1 D} [1 - (1 - e^{-q_n D})^n]$
MOLECULAR THEORY	Radiation Action	$S = e^{-p(\alpha D + \beta D^2)}$	
MOLECULAR THEORY	Dual Radiation Action	$S = S_0 e^{-k(\xi D + D)^2}$	
MOLECULAR THEORY	Repair-misrepair Lin Rep / Quadmis	$S = e^{-\alpha D} [1 + (\alpha D T / \epsilon)]^\epsilon$	
MOLECULAR THEORY	Repair-misrepair Lin Rep / Mis	$S = e^{-\alpha D} [1 + (\alpha D / \epsilon)]^{\epsilon \Phi}$	
MOLECULAR THEORY	Lethal-Potentially Lethal	$S = \exp\left[-N_{TOT} \left[1 + \frac{N_{PL}}{\epsilon(1 - e^{-\epsilon B A_{tr}})}\right]^\epsilon\right]$	
MOLECULAR THEORY	Lethal-Potentially Lethal – Low Dose	$S = e^{-\eta_{AC} D}$	
MOLECULAR THEORY	Lethal-Potentially Lethal – High Dose	$-\ln[S(t)] = (\eta_{AC} + \eta_{AB}) D - \epsilon \ln[1 + (\eta_{AB} D / \epsilon)(1 - e^{-\epsilon B A_{tr}})]$	
MOLECULAR THEORY	Lethal-Potentially Lethal – LQ Approx	$-\ln[S(t)] = (\eta_{AC} + \eta_{AB} e^{-\epsilon B A_{tr}}) D + (\eta_{AB}^2 / 2\epsilon)(1 - e^{-\epsilon B A_{tr}})^2 D^2$	

# Prototype development

Design, implementation and usage of  
one cell survival model in Geant4

## Verification



Monolayer

V79-379A cells

Proton beam  
E = 3.66 MeV

Linear-Quadratic  
model

$$S = e^{-\alpha D - \beta D^2}$$

$$\alpha = 0.32$$

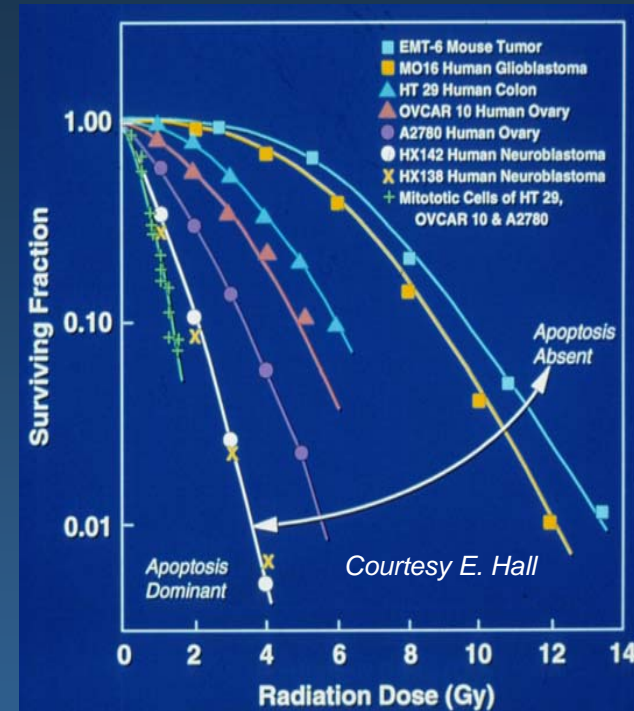
$$\beta = -0.039$$

Folkard et al., Int. J. Rad. Biol., 1996

# Outlook

- IEEE NSS 2006
  - Talk
- Publication
  - 1<sup>st</sup> software development cycle
- Analysis and design
  - Models
  - Mixed fields
- Physical design
  - New Geant4 domain
  - Consultation desirable
- Models
  - Other cell survival models
  - Models for other cellular processes

Human cell lines irradiated with X-rays



- Validation
  - Literature survey
  - Ad hoc data?

# Validation

- Atomic relaxation
- Bremsstrahlung
- + other validation activities in Advanced Examples
  
- Statistical Toolkit
  
- Common features of the validation activities
  - Collaborative, open, transparent work environment
  - Rigorous, quantitative analysis
  - Publication-quality methods and results

# Atomic relaxation

Alfonso – Barbara – MG – Susanna – Valentina

## ● Reference: NIST

- Fluorescence: R.D. Deslattes et al., X-ray transition energies: new approach to a comprehensive evaluation, Rev. Mod. Phys. 75 (2003), 35-99
- Auger: various sources

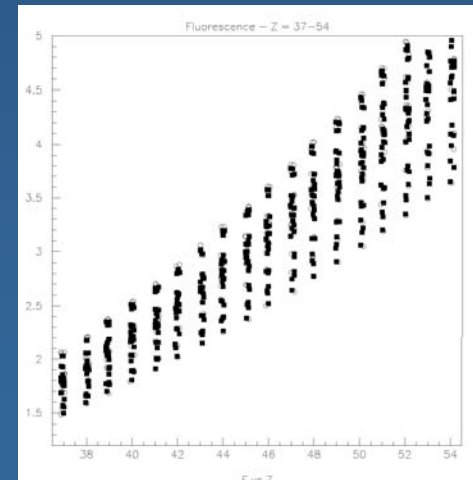
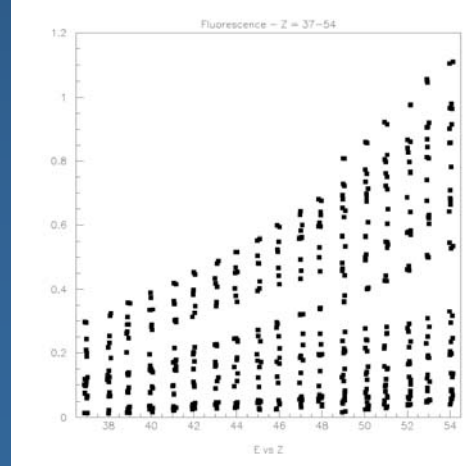
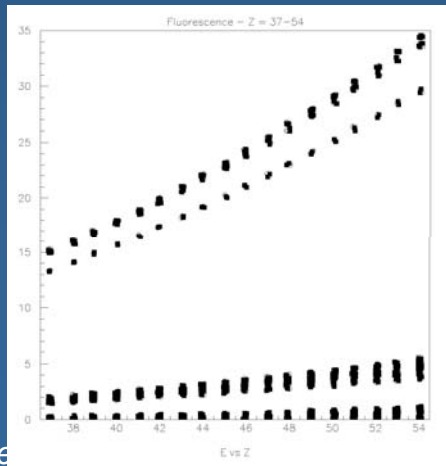
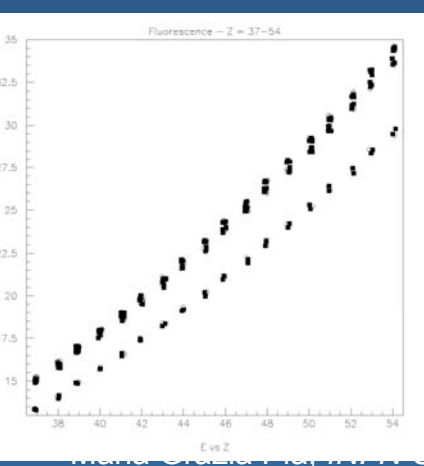
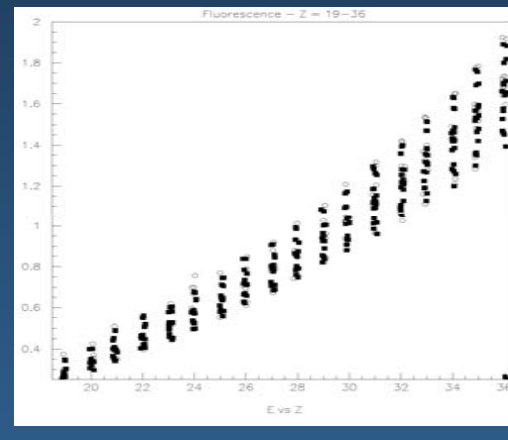
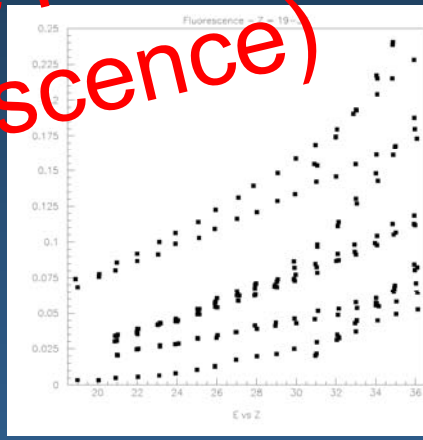
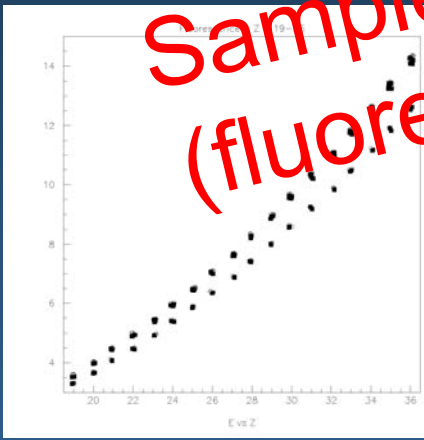
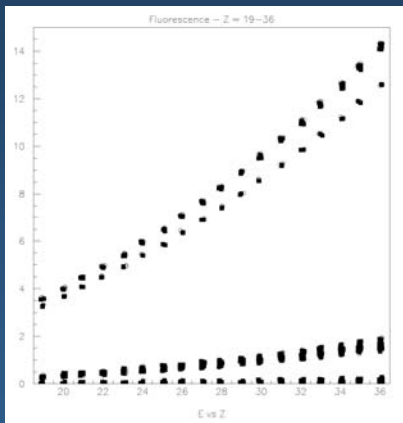
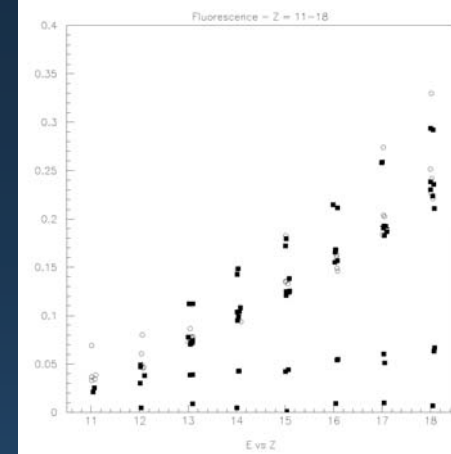
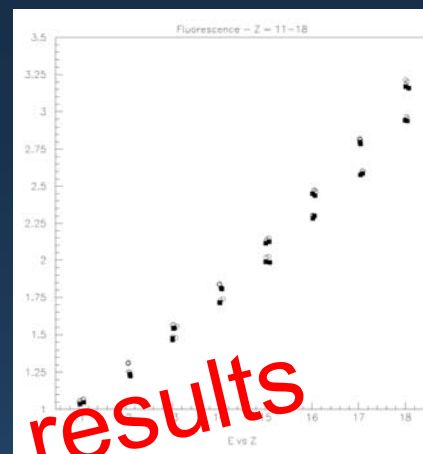
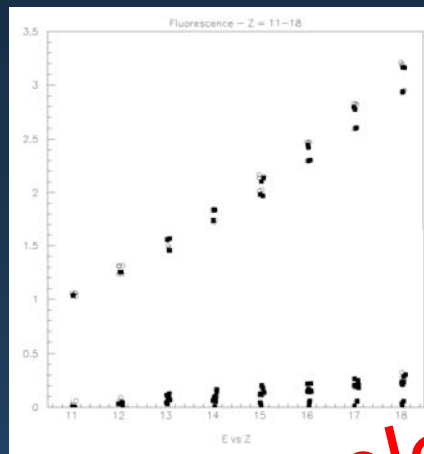
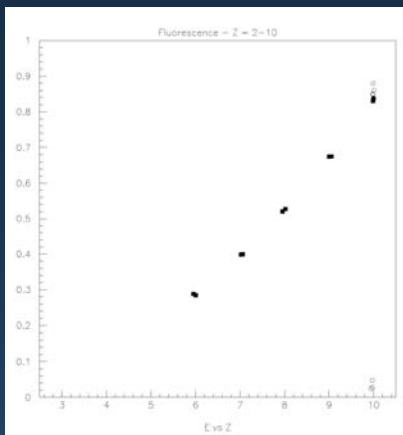
## ● Production completed, all Z (major effort!)

## ● Analysis in progress

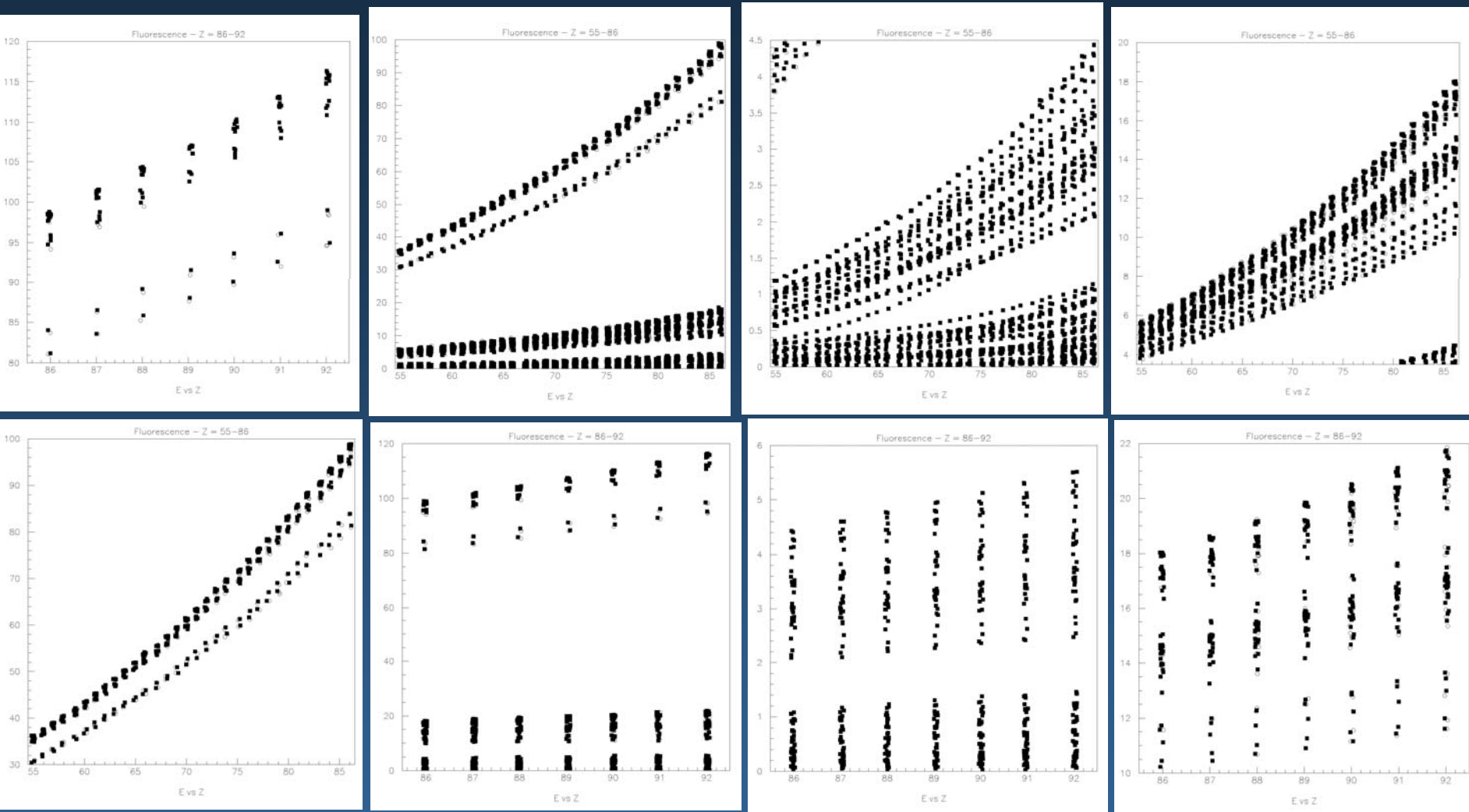
## ● Presentation at IEEE NSS, 1-4 November 2006

## ● Valentina Zampichelli's thesis, 6 December 2006

## ● Publication



Sample results  
(fluorescence)



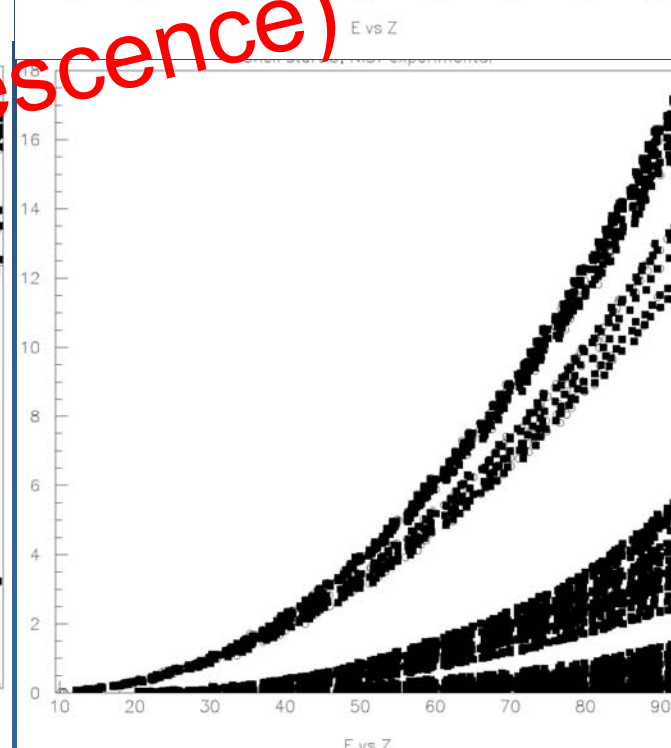
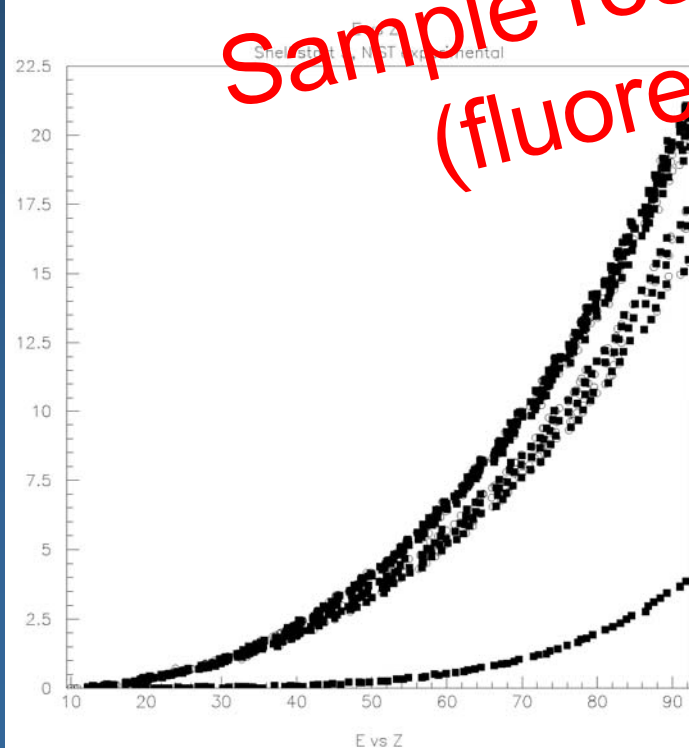
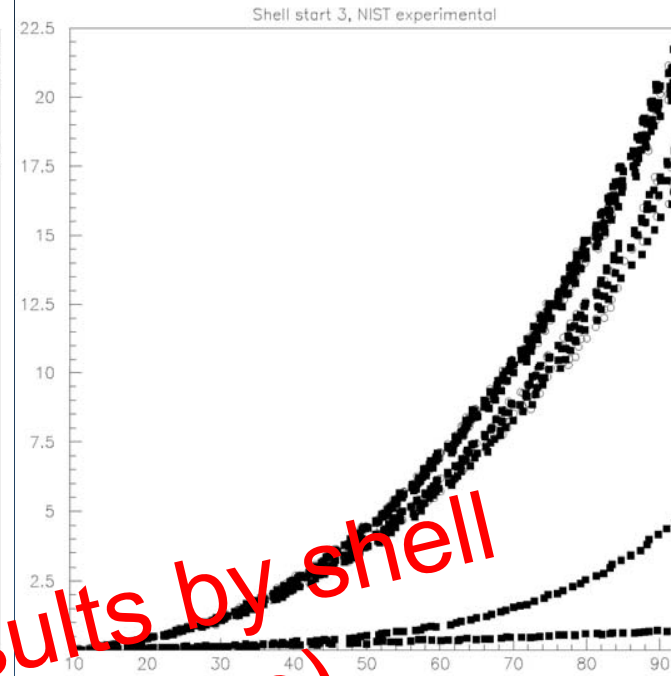
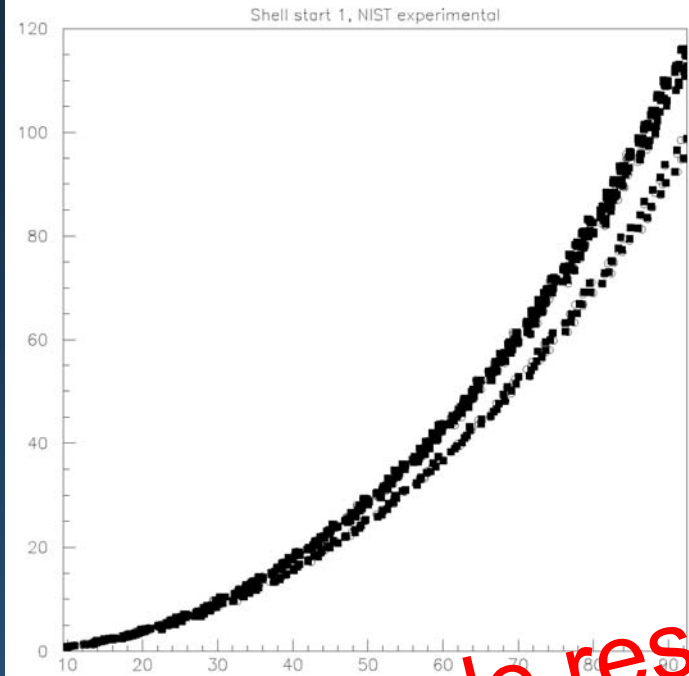
## Preliminary qualitative evaluation:

Good agreement between Geant4 and reference experimental data

Geant4 predicts lower energy transitions not present in the reference data

Maria Grazia Pia, *INFN Genova*





Sample results by shell  
(fluorescence)

Preliminary qualitative evaluation:

Good agreement between Geant4 and reference experimental data confirmed in detailed results shell-by-shell

**Outlook**

Quantitative analysis

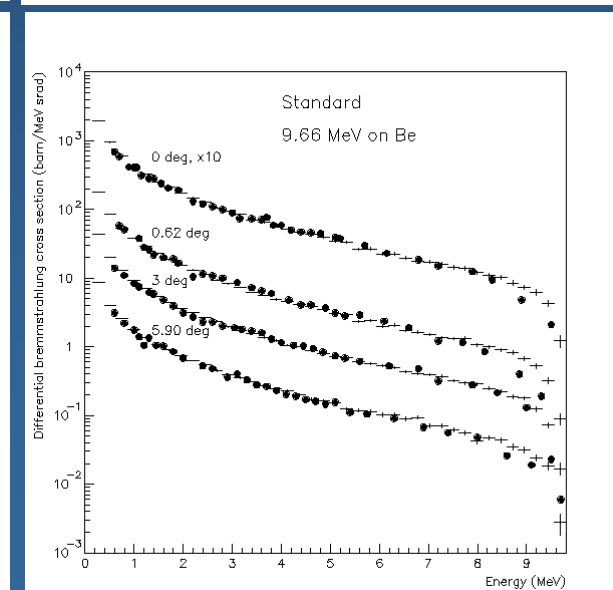
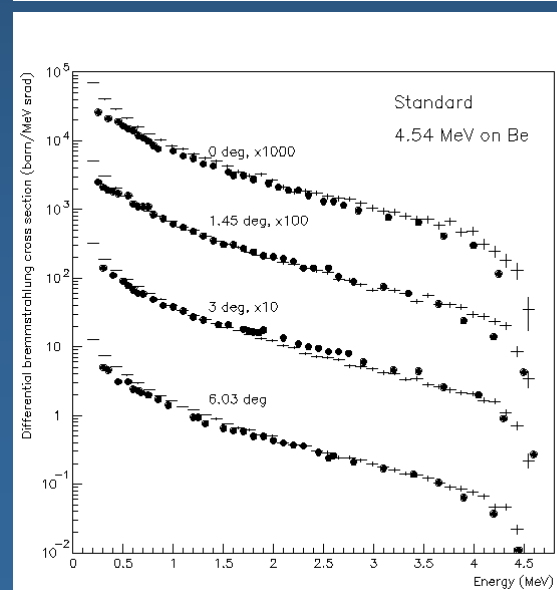
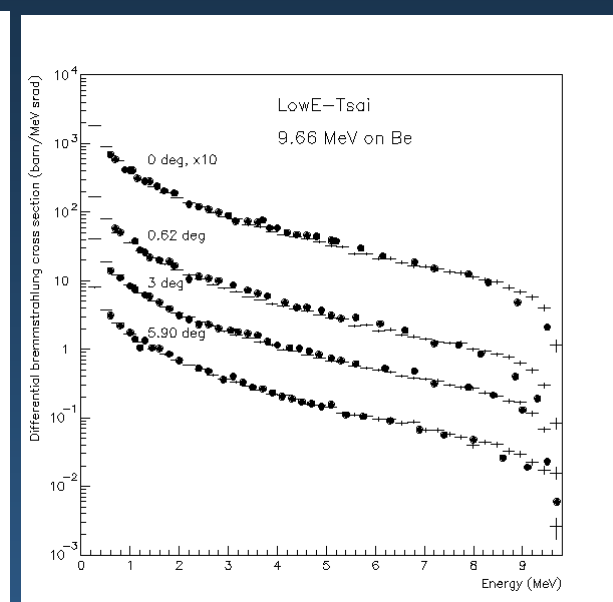
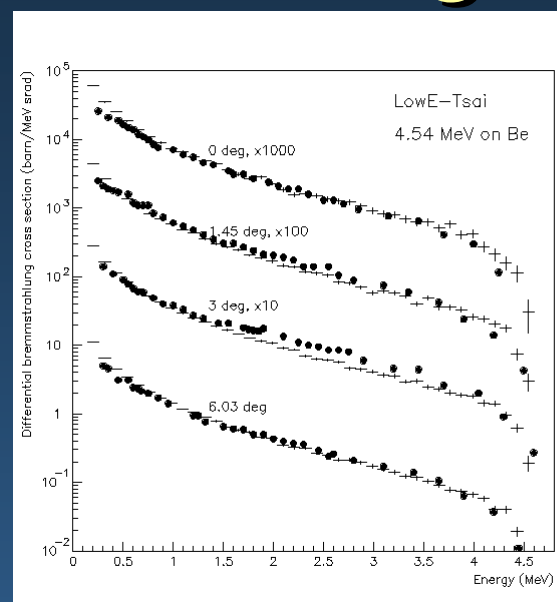
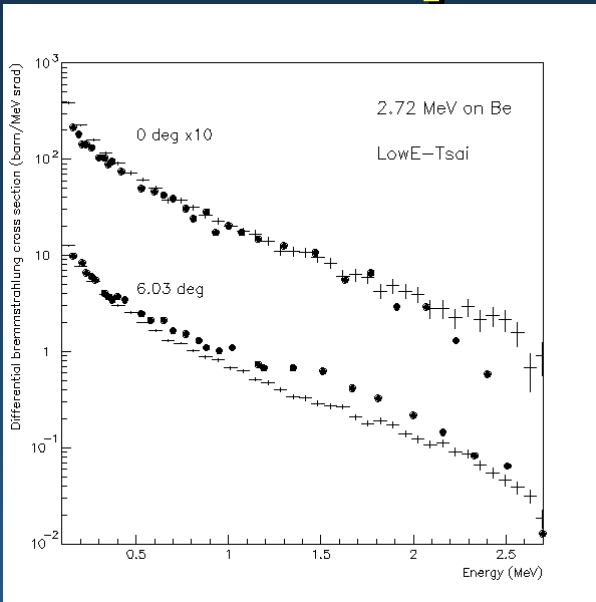
Publication

# Bremsstrahlung

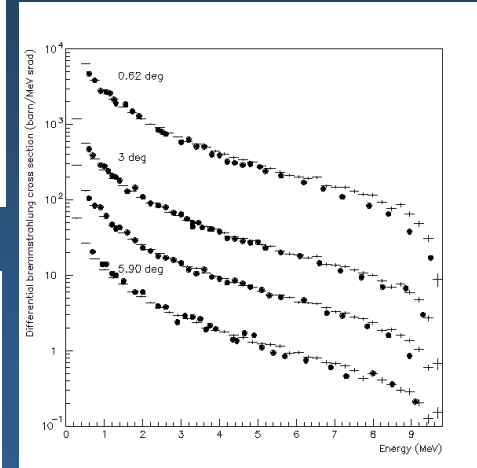
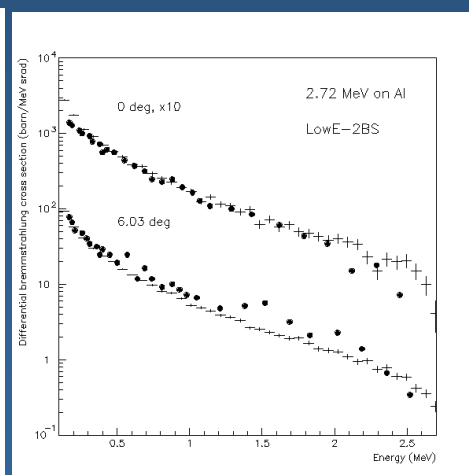
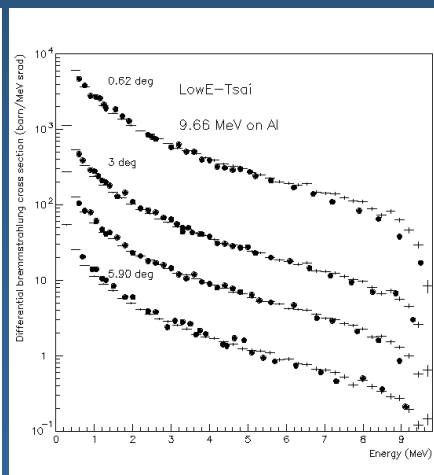
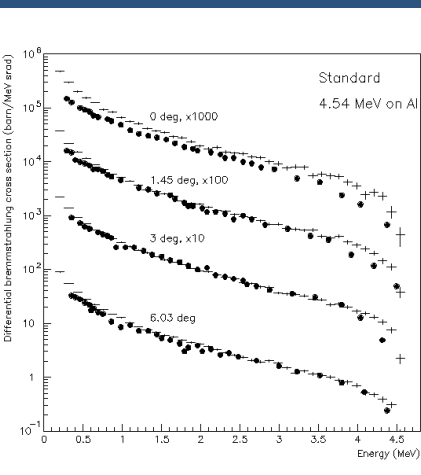
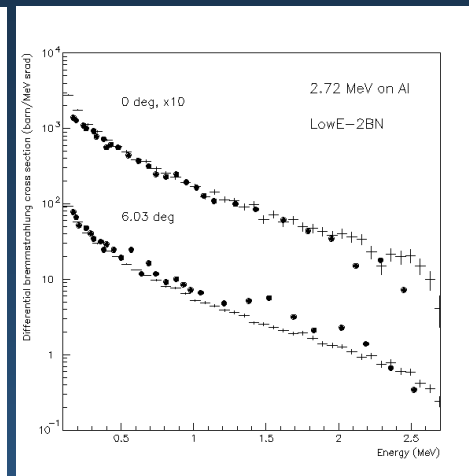
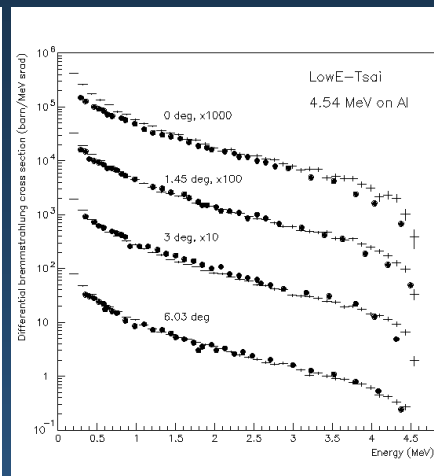
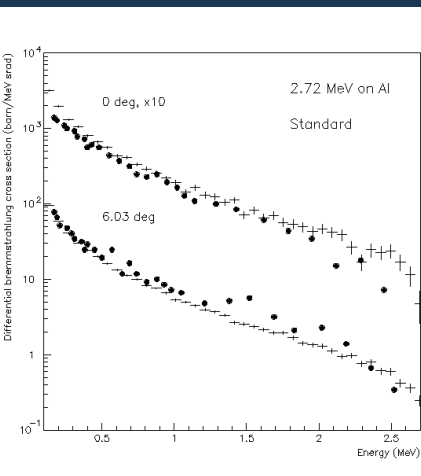
Barbara – Luciano – MG – Susanna

- Reference: experimental data in various journal publications
  - Often old, with unclear systematics
- Simulation: all Geant4 Bremsstrahlung flavours
  - Standard, LowE-Livermore (Tsai, 2BN, 2BS), LowE-Penelope
- **Huge effort invested by the Geant4-INFN team**
  - Production at Gran Sasso Laboratory
  - Experimental data acquisition from reference publications
  - Major analysis effort still required

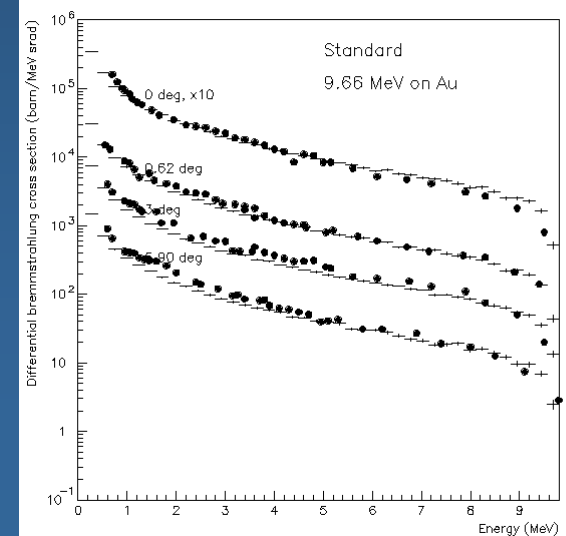
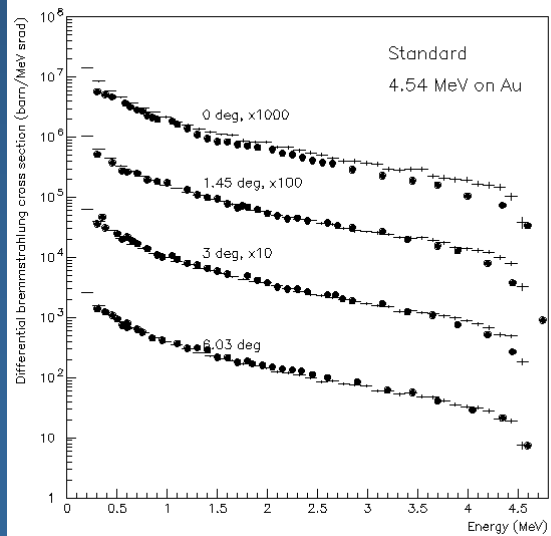
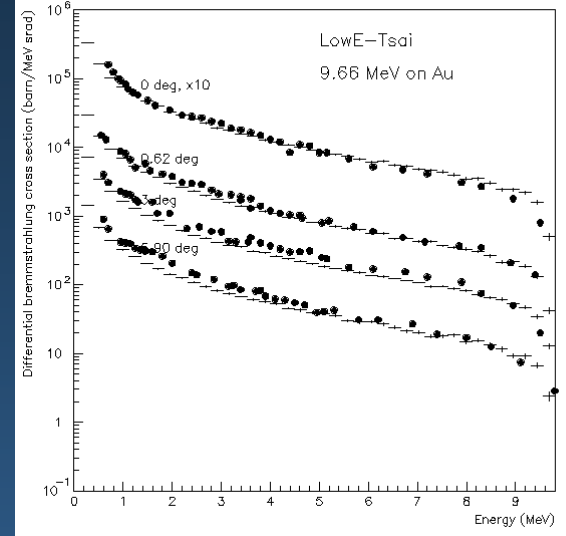
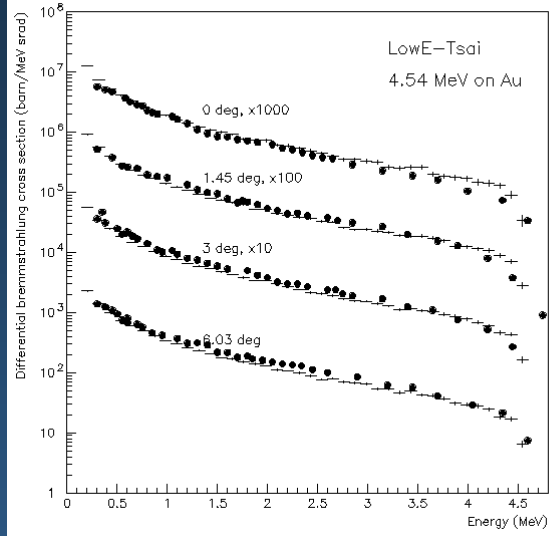
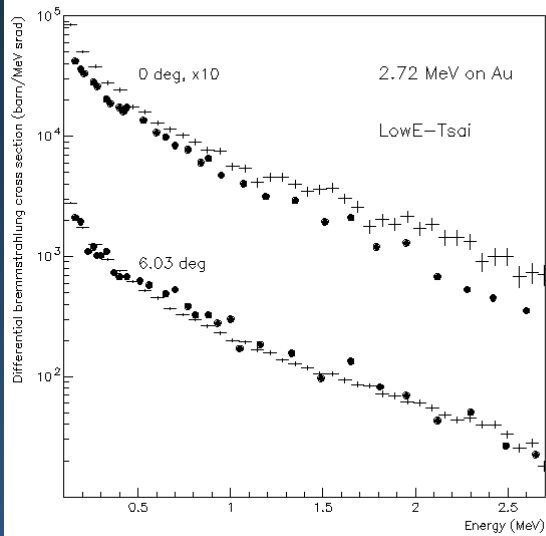
# Some preliminary results: Be



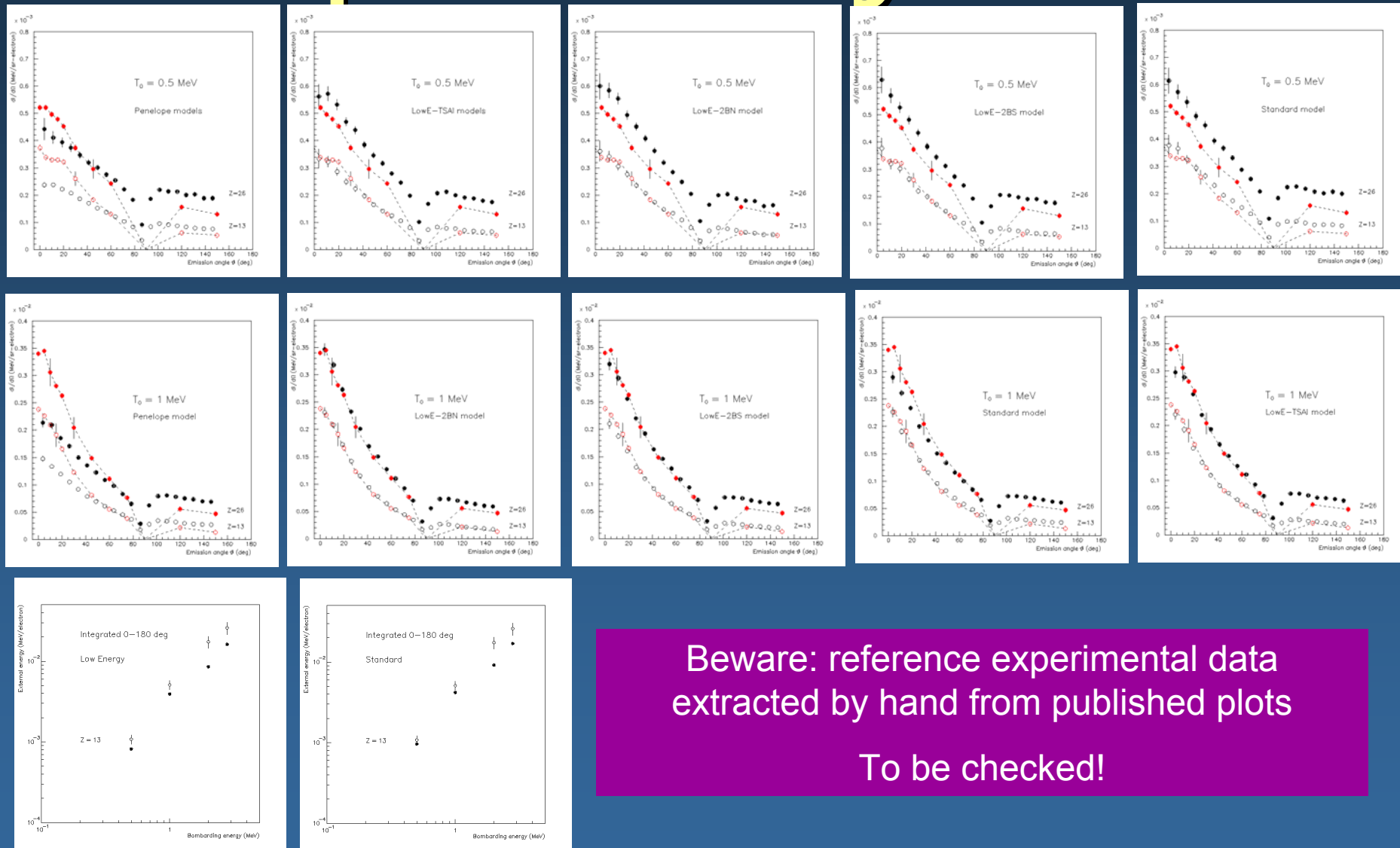
# Some preliminary results: Al



# Some preliminary results: Au



# Some preliminary results



Beware: reference experimental data extracted by hand from published plots  
To be checked!

# Bragg peak

Barbara – Francesco – Giorgio – MG – Pablo – Susanna

- See talk on Advanced Examples

# Other validation activities

Alfonso – Barbara – MG – Michela – Susanna

- See talk on Advanced Examples

**Geant4 Physics Book project**



# Statistical Toolkit

- 2<sup>nd</sup> development cycle
  - Released April 2006
- What's new
  - New tests
  - ROOT User Layer
  - New installation tools
  - Performance analysis

<b>Goodness-of-fit tests for binned distributions</b>	<i>Chi-squared (new implementation)</i> <i>Chi-squared, approximated algorithm</i> Chi-squared (old implementation) Fisz-Cramér-von Mises Anderson-Darling Tiku <i>Anderson-Darling, approximated algorithm</i>
<b>Goodness-of-fit tests for unbinned distributions</b>	Kolmogorov-Smirnov Goodman Fisz-Cramér-von Mises Anderson-Darling Kuiper Watson Tiku <i>Weighted Kolmogorov-Smirnov (AD)</i> <i>Weighted Kolmogorov-Smirnov (Binning)</i> <i>Weighted Cramér-von Mises</i> Gironè Gorla <i>Anderson-Darling approximated</i>

## New developments of the Goodness-of-Fit Statistical Toolkit

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### IEEE Trans. Nucl. Sci., December 2006

**Abstract**—The Statistical Toolkit is an ongoing project for the development of open source software tools for statistical data analysis in experimental particle and nuclear physics. The second development cycle encompassed an extension of the software functionality and new tools to facilitate its usage in experimental particle and nuclear physics. The new developments include additional goodness-of-fit tests, new implementations of existing tests to improve their statistical precision or computational performance, a new component to extend the usability of the toolkit with other data analysis systems, and new tools for an easier configuration and build of the system in the user's computing environment.

**Index Terms**—Software, Data Analysis, Data comparison, Goodness-of-Fit Testing, Statistical Toolkit.

#### I. INTRODUCTION

THE comparison of data distributions with respect to other reference data or functions is a common problem in experimental physics: some typical cases are the validation of simulation results against experimental data, the evaluation of physical quantities reconstructed by the experiment's software against theoretically expected ones, or monitoring the behaviour of a particle detector with respect to its normal operation reference. Moreover, the regression testing of an experiment's software usually involves some comparisons of data distributions to control the software stability or to verify its evolution.

A recent project, named the Statistical Toolkit [1], undertook the development of an open source software system for the comparison of data distributions, especially addressed to applications in particle and nuclear physics. This project is characterized by an iterative and incremental software process, according to established best practices in software development [2]; the first development cycle is documented in [1].

This paper describes the new developments and improvements of the Statistical Toolkit, which have been released for public usage in version 2. The new features available respond to experimental user requirements.

Several goodness-of-fit tests have been added to the already extensive collection available in the first released version (listed in Table I); some of them introduce new weighted formulations of established tests, for the first time available in a software tool

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for data analysis. To the authors' knowledge, the new version of the Statistical Toolkit implements all the goodness-of-fit tests based on the empirical distribution function (*edf*) known in statistical science. Other tests have been significantly improved, either in their mathematical algorithms or in their computational performance. New developments in the architectural user layer have extended the usability of the Statistical Toolkit together with other widely used software systems for data analysis. A significant redesign of the supporting software tools package facilitates the configuration of the system in the user's own computing environment.

The paper also reports a comparative analysis of the computing performance of all the algorithms implemented: these results provide useful guidance to experimental users. A comparative study of the statistical performance of the various goodness-of-fit tests is the object of current research activity [3]- [4]; it will be documented in two dedicated papers currently in preparation, which will analyse the power of the various tests for unbinned and binned distributions respectively.

#### II. OVERVIEW OF THE GOODNESS-OF-FIT STATISTICAL TOOLKIT

The Statistical Toolkit is a software system for statistical data analysis; it is especially targeted to common applications in experimental nuclear and particle science. It exploits the object oriented technology and generic programming techniques; it is implemented in C++. Its life-cycle is based on the iterative-incremental model of the Unified Process [2]; the process framework adopted emphasizes the role of the software architecture and the relevance of use cases in the software development.

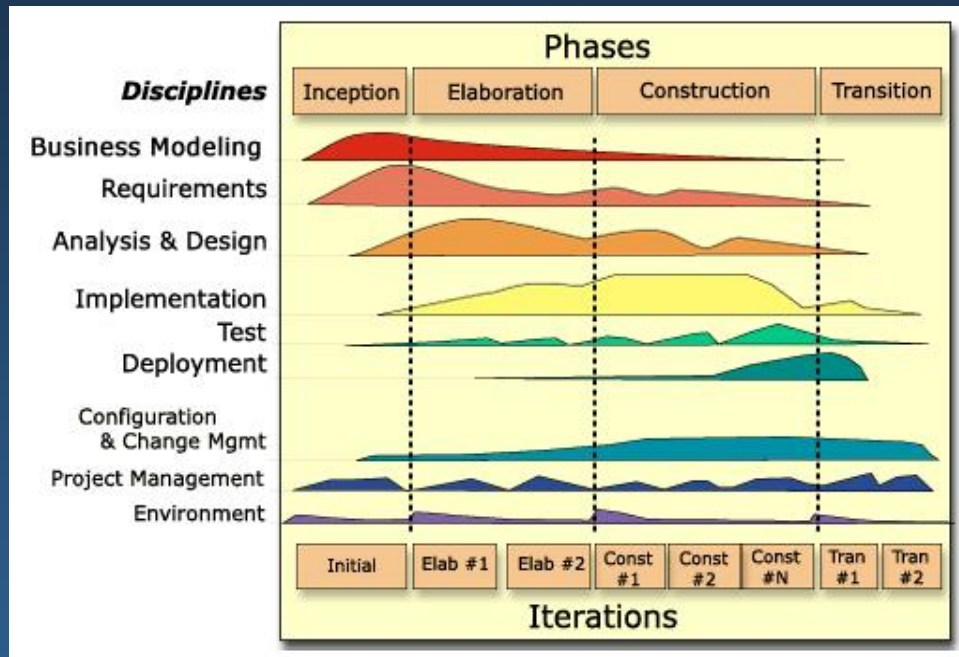
The Statistical Toolkit adopts a component-based architecture, which facilitates its usage in association with other data analysis software systems widely used in particle physics experiments; its sound object oriented design makes it open to extension and evolution.

##### A. Statistical background

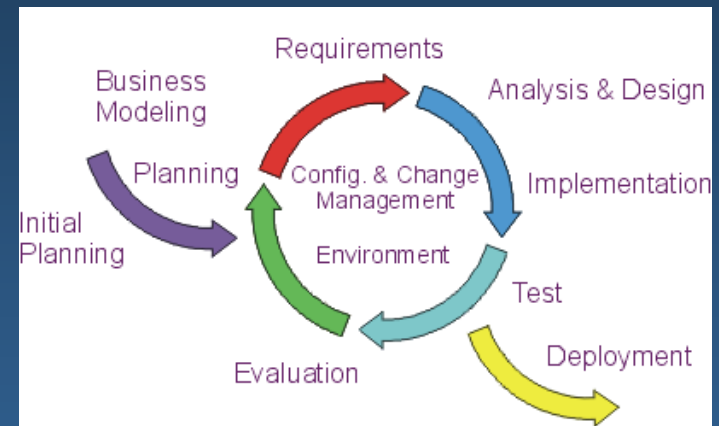
Goodness-of-fit testing provides the mathematical foundation for a rigorous, quantitative evaluation of the compatibility of two data samples, or of a data sample against a reference function.

Let  $X$  and  $Y$  be two real-valued random variables, and let  $(x_1, \dots, x_n)$  and  $(y_1, \dots, y_m)$  be, respectively, two samples of independent and identically distributed observations with

# ...and behind everything



## Unified Process



## A rigorous software process

Incremental and iterative lifecycle

RUP™ as process framework, tailored to the specific project

Mapped onto ISO 15504

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# Our young collaborators

Bright, enthusiastic, hard-working

Most group members:

- age < 35
- temporary positions
- low (or zero) salary

**These young colleagues invest  
their hopes for their future careers in  
Geant 4**

**We should feel our responsibility towards  
our younger colleagues**

High scientific and technical profile of the Collaboration  
Serene, collaborative work environment  
Education to sound research methods  
Publications for their CVs  
Opportunities for conference presentations  
Support to their activities

