# Geant 4

# Low Energy Electromagnetic Physics Working Group


Maria Grazia Pia

INFN Genova

*on behalf of the Low Energy Electromagnetic WG*


Geant4 Review

CERN, 18-22 June 2001

http://www.ge.infn.it/lowE/

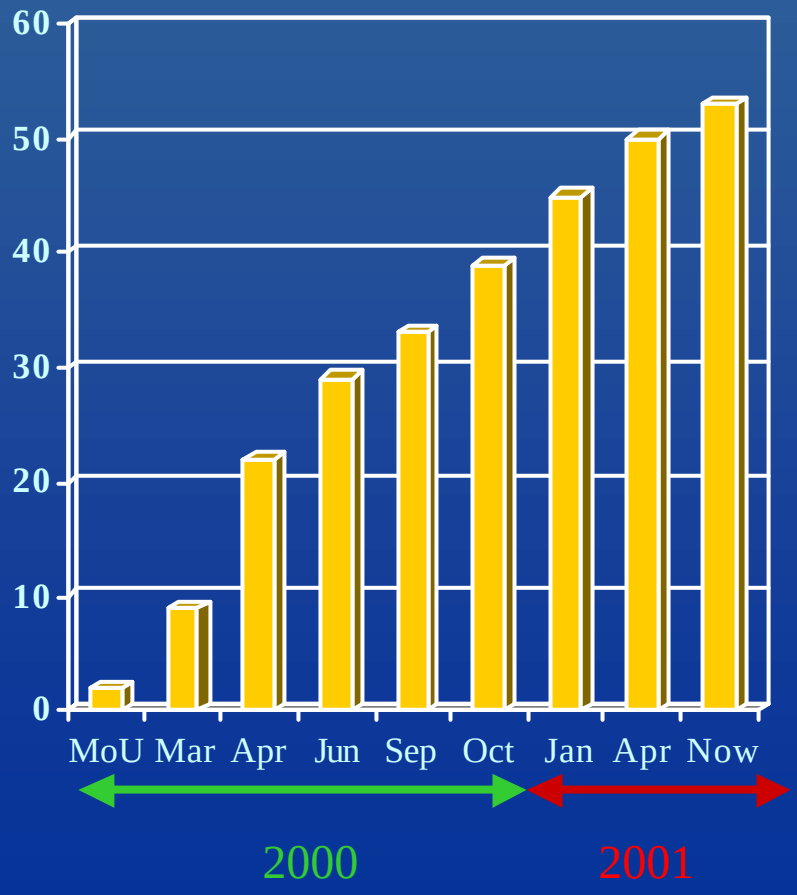
# The youngest Geant4 Working Group

- The activity on LowE electromagnetic physics started informally in October 1998
  - Part of the RD44 electromagnetic category, 1 ESA contractor
  - Continued as a subset of Geant4 general Electromagnetic Working Group (2 people)
  - Initially meant to be one of the "ESA modules" for space radiation background studies, limited to electrons and photons
- The scope of the activity extended soon
  - Physics: also hadrons and ions
  - User communities: also HEP, astroparticle, astrophysics, medical…
  - Developers: several people contributing, not limited to ESA contractor
- Applied to the CB in April 2000 to create a new WG

# A growing Working Group

- 2 collaborators working on LowE e.m. physics in January 1999
- 9 members at the time of the creation of the WG
  - 3 of the initial members lost
  - *including holder of full time ESA contract*
- 53 members now
- Contacts in progress with new people interested to join

## LowE e.m. WG members



# How we operate

Characterized by
- Goal-directed project management
- Rigorous approach to software engineering
- High dynamism and creativity

Wide spectrum of development:
- Physics
- Applications

**Team**
- Regular Working Group meetings
- Emphasis on training of all group members

**Collaboration**
- Promotion of cross-WG activities
- Close relationship with user communities

**Outreach**
- Active strategy of talks and publications
  - for promotion of Geant4 and our own products
  - as an incentive and reward for group members

# Objectives and Projects

- Documented in public planning document every year
- Achievements documented to the Geant4 Collaboration

27 March, 2000
*Version 8*

2000

## LOW ENERGY ELECTROMAGNETIC PHYSICS

Working Group milestones for year 2000

Petteri Nieminen and Maria Grazia Pia

### INTRODUCTION

The Low Energy Electromagnetic Physics domain has been recognised the status of Working Group in March 2000. A substantial effort will be invested into the reorganisation of its activity during year 2000.

### DEFINITION OF OBJECTIVES

#### Physics

The physics developments of the Low Energy Electromagnetic Physics group are driven by user requirements. An updated version of the Low Energy Electromagnetic Physics User Requirement Document is available from the group web page at http://www.ge.infn.it/geant4/lowE/

The main physics goals for year 2000 are listed below, in order of priorities:

1. Assessment and improvements of the current physics implementation *(mandatory)*
2. Implementation of the Auger effect *(mandatory)*
3. Low energy extensions for positrons *(mandatory)*
4. Extensions to lower energies of protons and ions and simulation of straggling *(mandatory)*
5. Extension to lower energies of antiprotons *(mandatory)*
6. Low energy extensions for negative ions *(desirable)*
7. Extensions to lower energies of electrons and photons *(optional)*

#### Software

A major investment is planned to review and substantially improve the current status of the Low Energy Electromagnetic software and software process. Such a substantial effort is required to achieve an Object Oriented, modular, maintainable, reliable code. A very high Quality Assurance level is especially required by some sensitive applications of the Low Energy Electromagnetic Physics code, such as treatment of cancer patients and space missions.

The main software goals of the Low Energy Electromagnetic Physics Working Group for year 2000 are listed below:

1. Explicit definition and documentation of procedures *(mandatory)*
2. Major improvement of the design *(mandatory)*
3. Major improvement of the software quality *(desirable)*



20 March 2001
*Version 3*

2001

## LOW ENERGY ELECTROMAGNETIC PHYSICS

Working Group objectives, 2001

Petteri Nieminen[1] and Maria Grazia Pia
*(for the Low Energy Electromagnetic Physics Working Group)*

### INTRODUCTION

This document summarises the objectives and the projects of the Low Energy Electromagnetic Physics Working Group for the year 2001. They span the domains of physics, design and code quality improvement, software process improvement, user support and development of application examples, publications and presentations.

### DEFINITION OF OBJECTIVES

#### Physics

The physics developments of the Low Energy Electromagnetic Physics group are driven by user requirements. An updated version of the Low Energy Electromagnetic Physics User Requirement Document is available from the group web page at http://www.ge.infn.it/geant4/lowE/

The main physics goals for year 2001 are listed below, in order of priorities:

1. Implementation of proton-induced fluorescence
2. Implementation of the Auger effect
3. Alternative models for Compton scattering (also including polarisation)
4. Polarised Rayleigh scattering
5. Polarised $\gamma$ conversion
6. Low energy extension for positrons
7. Low energy extensions for negative ions
8. Assessment of the quality of the extension of electron and photon processes to energies below 250 eV, based on the Livermore database

#### Software

A major investment is planned to review and substantially improve the current status of the Low Energy Electromagnetic software and software process. Such a substantial effort is required to achieve an Object Oriented, modular, maintainable, reliable code. A very high Quality Assurance level is especially required by some sensitive applications of the Low Energy Electromagnetic Physics code, such as treatment of cancer patients and space missions.

[1] Document still subject to the approval by P. Nieminen

# Physics developments

- Before the creation of the WG
  - First implementation of e/photon models based on LLNL libraries (shell effects)
  - First implementation of models for hadrons and ions
- Since the creation of the WG
  - New model for positive charged hadrons (Ziegler 1985)
  - Improvements on straggling (hadrons and ions)
  - Dynamic dependence on effective charge in the range calculation
  - Improvements in the validity range of δ ray production
  - New models for ion energy loss fluctuations
  - New model for negative charged hadrons
  - New model for polarised Compton
  - Other physics extensions in progress

# Software Process

## A rigorous approach to software engineering

- Huge effort invested into SPI
  - *started from level 1 (CMM)*
  - *chaotic, left to heroic improvisation*
- Current status
  - *public URD*
  - *full traceability through UR/OOD/implementation/test in CVS repository*
  - *testing suite and testing process*
  - *public documentation of procedures*
  - …

A sample of the improvements:

- establishment *(1999)* and management of User Requirements Document
- establishment and documentation of procedures
- design before coding
- designs and testing under configuration management
- separation of examples from tests
- identification of tasks and responsibilities
- traceability process

*...too long to list all of them*



*more this afternoon...*

# Internal training

- Substantial investment in the internal training in the WG
  - guided readings
  - code reviews
  - mentoring
  - introduction to basic concepts in software process and OO methodologies
- Visible effects on the quality of the software and of the process
- Great interest among the WG members
  - who demand more of it

# Design

Initial situation at the time of the creation of the WG:

- *no architectural nor detailed design*
- *no design process*

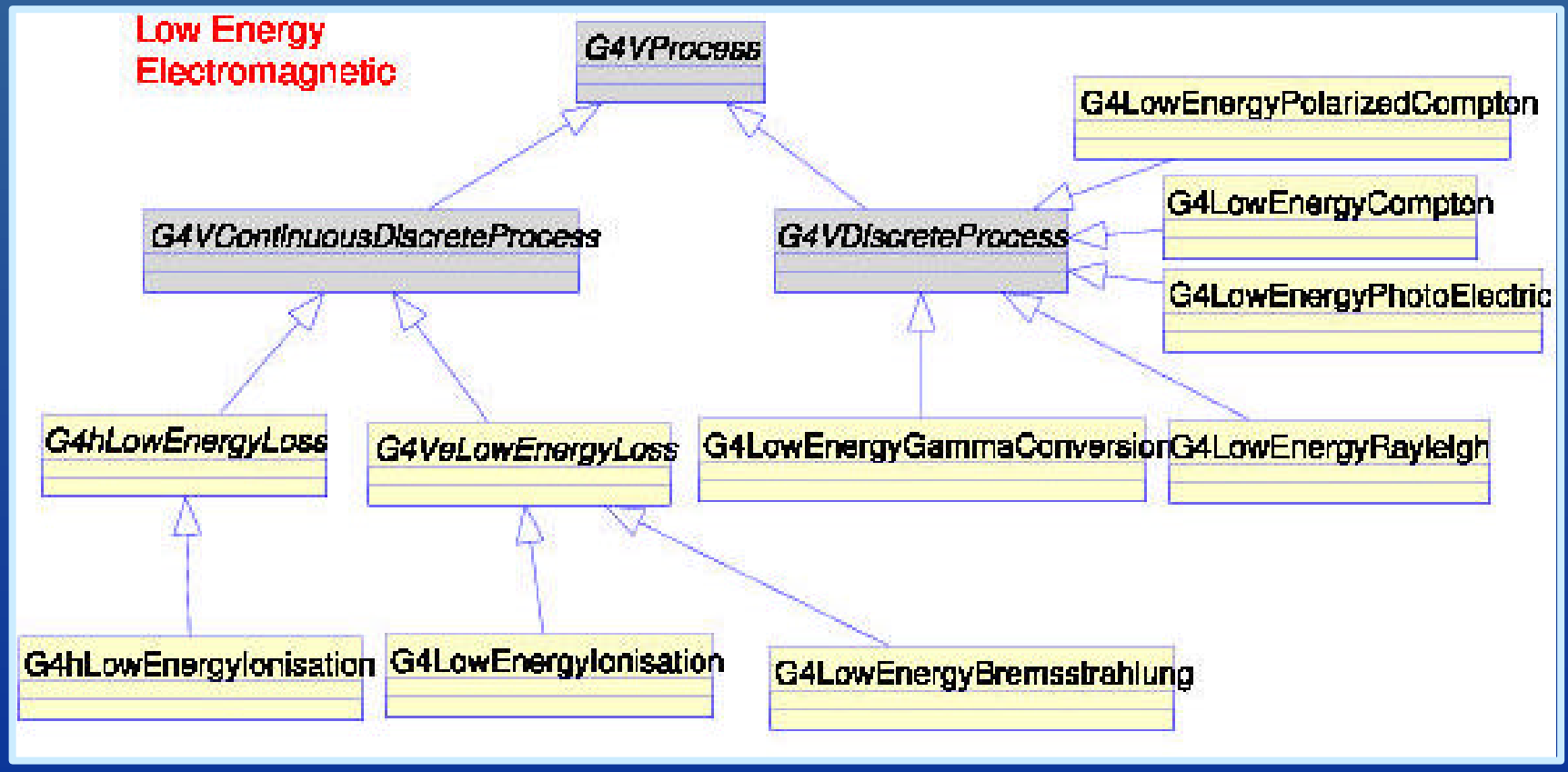
*Why?*
*The initial team did not include any OO nor sw process expert*

Significant improvement of the design and design process needed

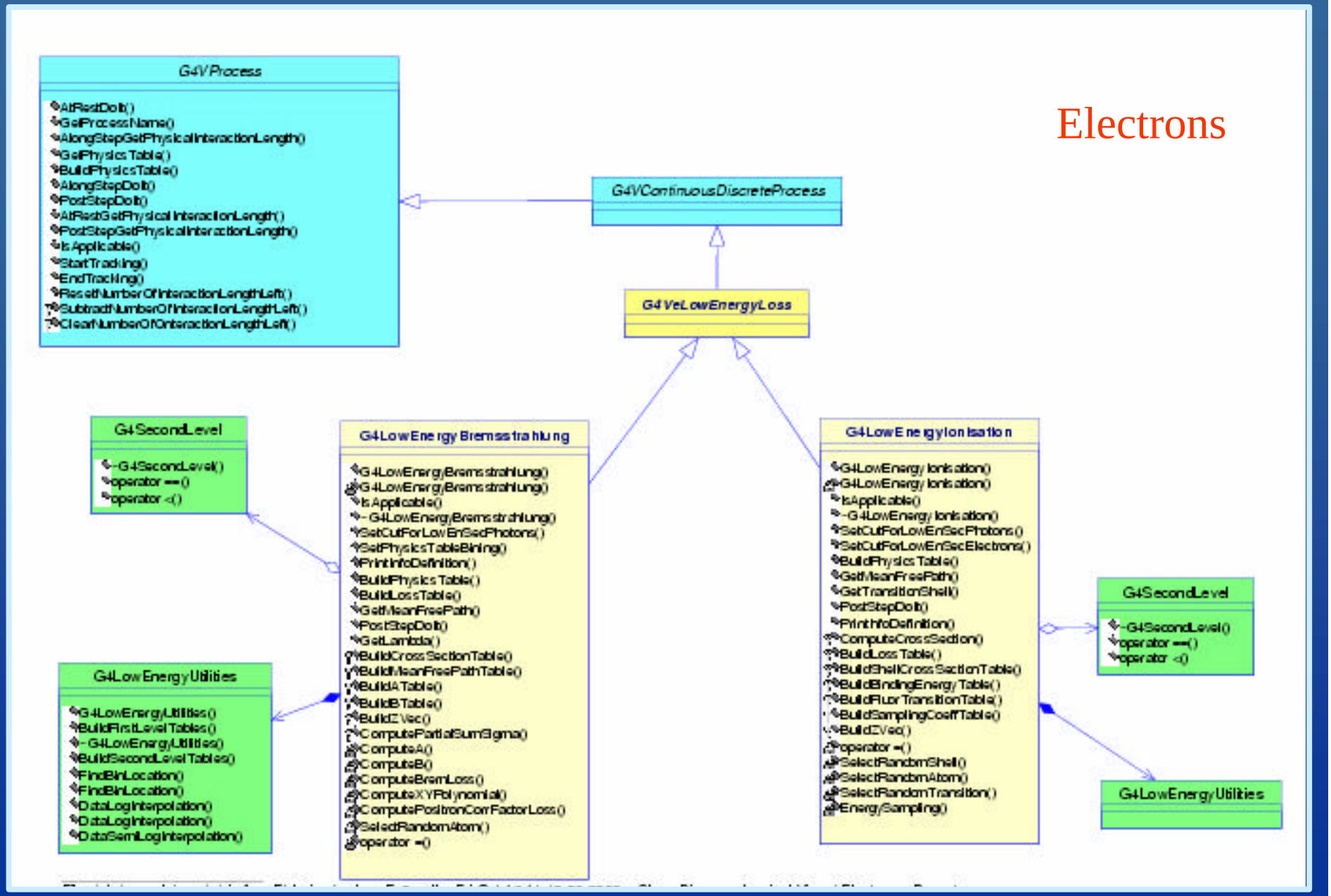
- ➔ *spiral process*
- ➔ *series of design iterations*
- ➔ *design documentation*

- Started with reverse engineering of existing classes
- *Education to design and design process in the WG*

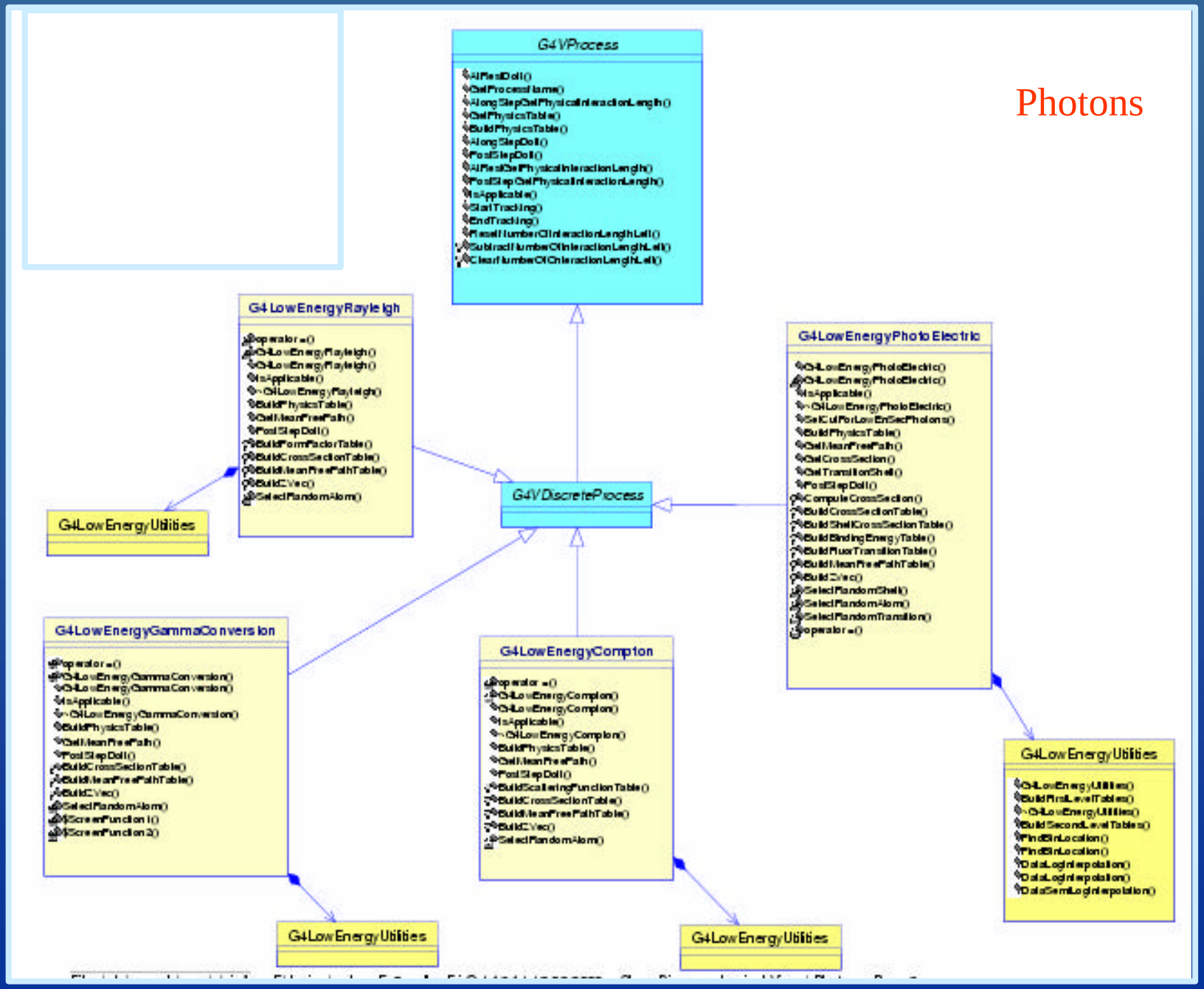
# Top level class diagram



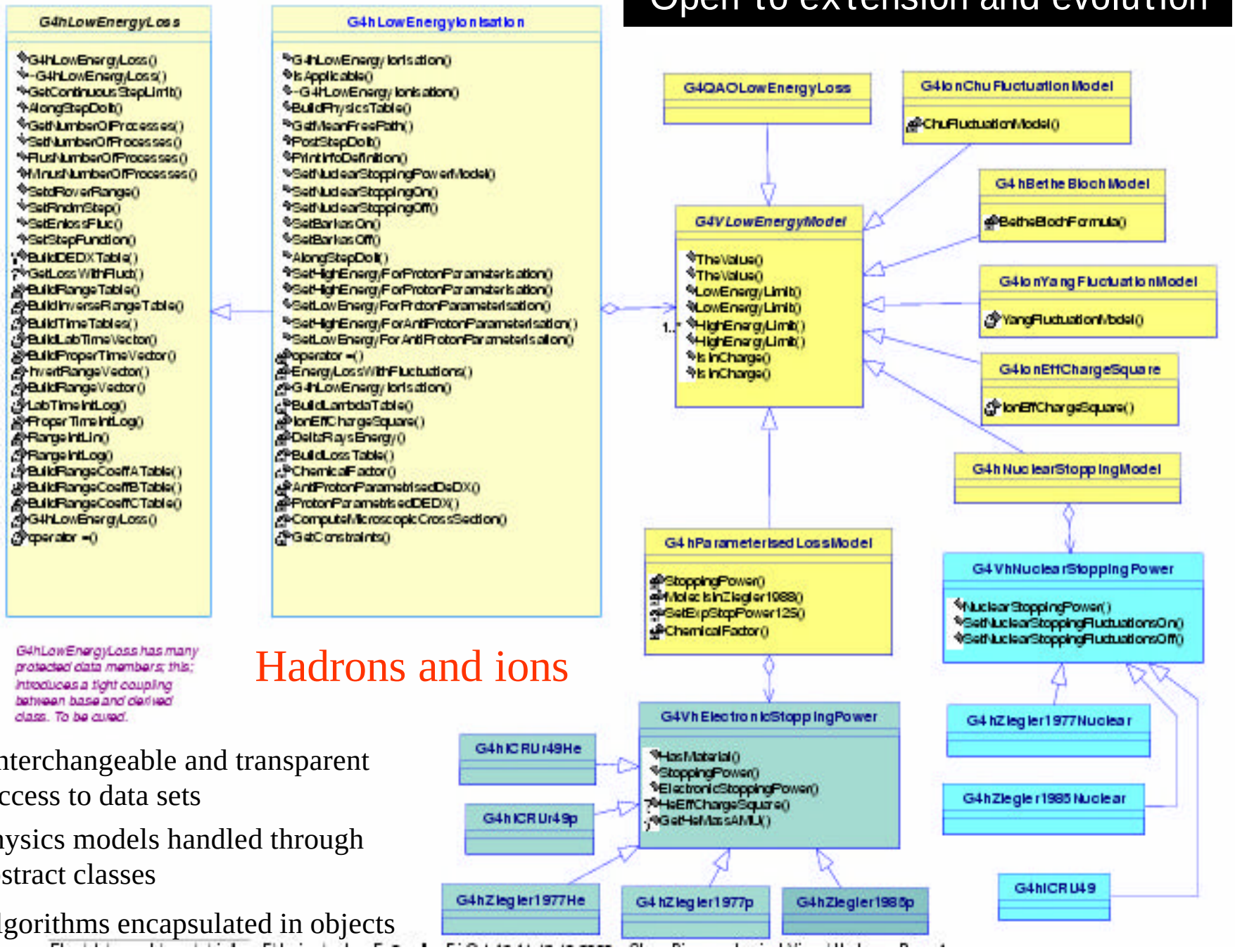
# Electrons


G4VProcess
AtRestDoIt()
GetProcessName()
AlongStepGetPhysicalInteractionLength()
GetPhysicsTable()
BuildPhysicsTable()
AlongStepDoIt()
PostStepDoIt()
AtRestGetPhysicalInteractionLength()
PostStepGetPhysicalInteractionLength()
IsApplicable()
StartTracking()
EndTracking()
ResetNumberOfInteractionLengthLeft()
SubtractNumberOfInteractionLengthLeft()
ClearNumberOfInteractionLengthLeft()
G4VContinuousDiscreteProcess
G4VeLowEnergyLoss
G4SecondLevel
~G4SecondLevel()
operator ==()
operator <()
G4LowEnergyBremsstrahlung
G4LowEnergyBremsstrahlung()
G4LowEnergyBremsstrahlung()
IsApplicable()
~G4LowEnergyBremsstrahlung()
SetCutForLowEnSecPhotons()
SetPhysicsTableBining()
PrintInfoDefinition()
BuildPhysicsTable()
BuildLossTable()
GetMeanFreePath()
PostStepDoIt()
GetLambda()
BuildCrossSectionTable()
BuildMeanFreePathTable()
BuildATable()
BuildBTable()
BuildZVec()
ComputePartialSumSigma()
ComputeA()
ComputeB()
ComputeBremLoss()
ComputeXYPolynomial()
ComputePositronCorrFactorLoss()
SelectRandomAtom()
operator =()
G4LowEnergyIonisation
G4LowEnergyIonisation()
G4LowEnergyIonisation()
IsApplicable()
~G4LowEnergyIonisation()
SetCutForLowEnSecPhotons()
SetCutForLowEnSecElectrons()
BuildPhysicsTable()
GetMeanFreePath()
GetTransitionShell()
PostStepDoIt()
PrintInfoDefinition()
ComputeCrossSection()
BuildLossTable()
BuildShellCrossSectionTable()
BuildBindingEnergyTable()
BuildFluorTransitionTable()
BuildSamplingCoeffTable()
BuildZVec()
operator =()
SelectRandomShell()
SelectRandomAtom()
SelectRandomTransition()
EnergySampling()
G4SecondLevel
~G4SecondLevel()
operator ==()
operator <()
G4LowEnergyUtilities
G4LowEnergyUtilities()
BuildFirstLevelTables()
~G4LowEnergyUtilities()
BuildSecondLevelTables()
FindBinLocation()
FindBinLocation()
DataLogInterpolation()
DataLogInterpolation()
DataSemiLogInterpolation()
G4LowEnergyUtilities

# Photons


G4VProcess
G4LowEnergyRayleigh
G4VDiscreteProcess
G4LowEnergyPhotoElectric
G4LowEnergyUtilities
G4LowEnergyGammaConversion
G4LowEnergyCompton
G4LowEnergyUtilities
G4LowEnergyUtilities
G4LowEnergyUtilities

# Open to extension and evolution




Interchangeable and transparent access to data sets

Physics models handled through abstract classes

Algorithms encapsulated in objects

Version 2

27 May 2001

# The Role of Testing in the Software Process of the Geant4 Low-Energy Electromagnetic Physics Working Group

*P. Nieminen and M.G. Pia*

## 1 Introduction

Testing forms a vital part of the software process in developments as advanced and complex as those currently in progress in the Geant4 Low-Energy e-m physics Working Group. The purpose of this document is to outline the procedures to be followed regarding testing both during development of new software, and during updates and corrections to existing code.

## 2 Testing objectives and goals

The objective of testing is to ensure the new, or updated, code performs as intended. Testing should reveal any potential deviancies from expected behaviour of the code both from physics and performance point of view. The goal is high-quality code ready for public release, ultimately leading to easier maintenance and substantial timesaving for developers in the course of the software lifecycle.

## 3 Test designs and testing schedules

### 3.1 Test requirements

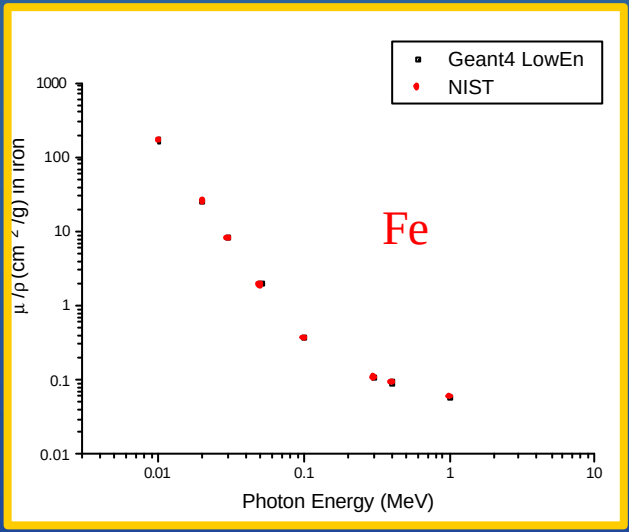
1. Testing should be performed according to agreed and documented procedures.
2. Traceability through requirements -design-implementation-tests should be implemented.
3. The design should be tested for satisfying the user requirements.
4. The code implementation should be tested for compliance with the design.
5. The code should be tested for correct functionality.
6. The code should be tested for compliance with Geant4 coding guidelines.
7. The code should be tested for satisfactory quality, clarity and readability.
8. Every class of the lowenergy category shall be exercised in an appropriate system test (directly or indirectly).
9. The code should be tested on all Geant4 supported platforms.
10. The code shall be submitted to the entire set of tests above to be considered for release.
11. Tests and test tools should be documented.
12. The test code should be kept under configuration management (in Geant4 CVS repository).
13. Reference outputs, data sets for validation tests etc. should be kept in appropriate agreed locations, accessible to the whole WG.
14. Test tools should be maintained.
15. Modifications of the tests (including test tools, reference outputs, data sets etc.) should be performed according to agreed and documented procedures.
16. The most recent test results should be made available to WG coordinators for code to be included in a monthly global tag or in a Geant4 public release, according to the guidelines described in the "Testing process" section.

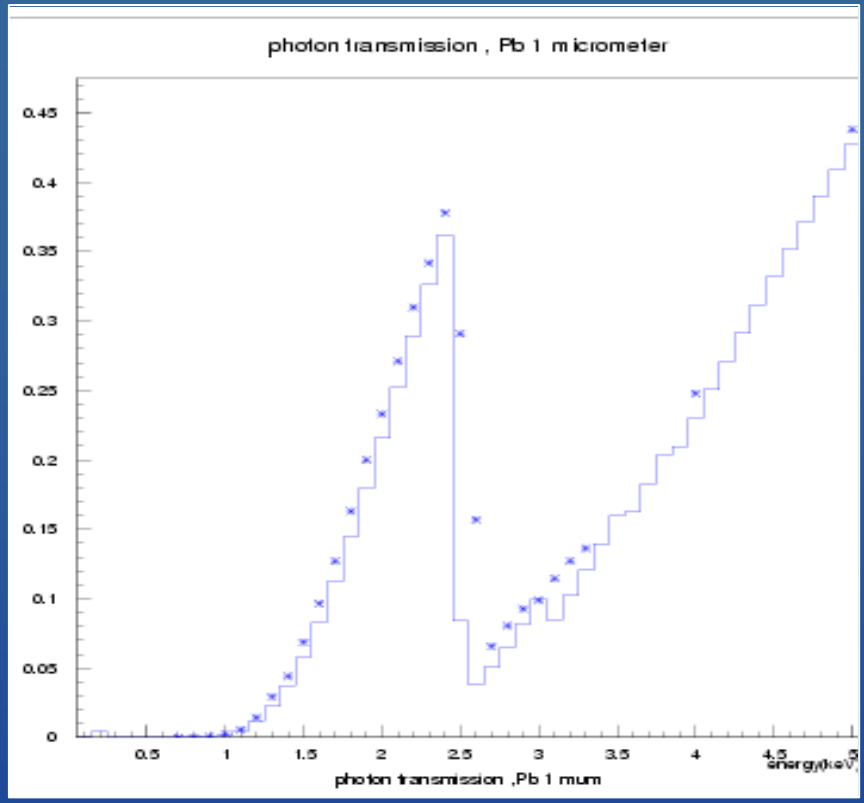
# Testing

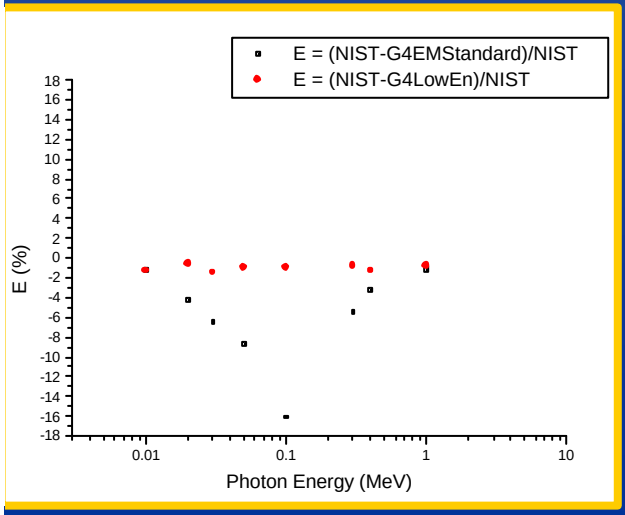
- Suite of unit tests
- 3 system tests
- Suite of physics tests
  *(in progress with publications)*
- Regression testing
- Testing requirements
- Testing procedures
- Physics validation
- Testing integrated with development

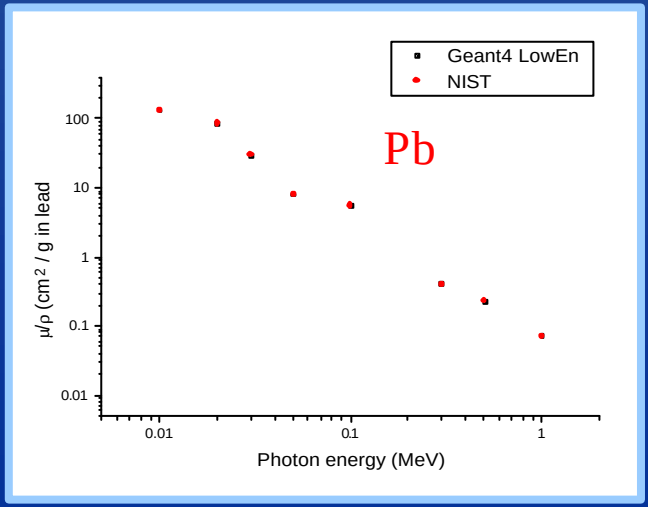
*more this afternoon...*

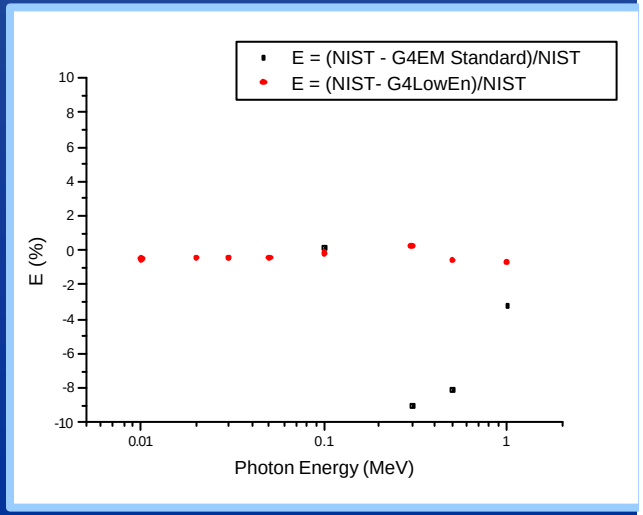
# Results, photons



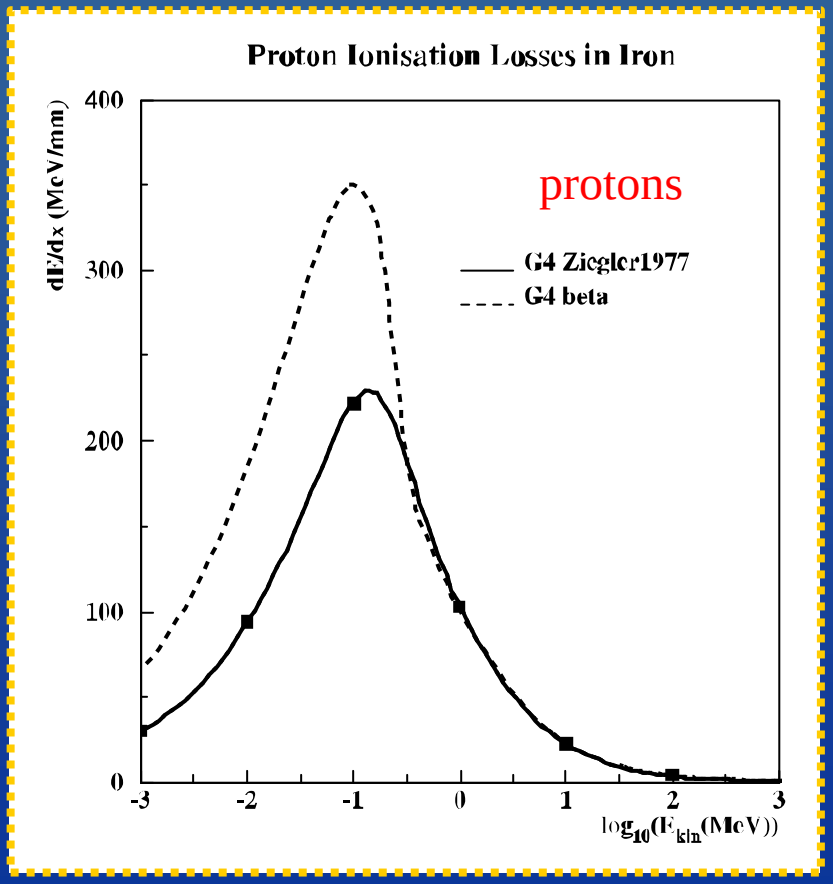



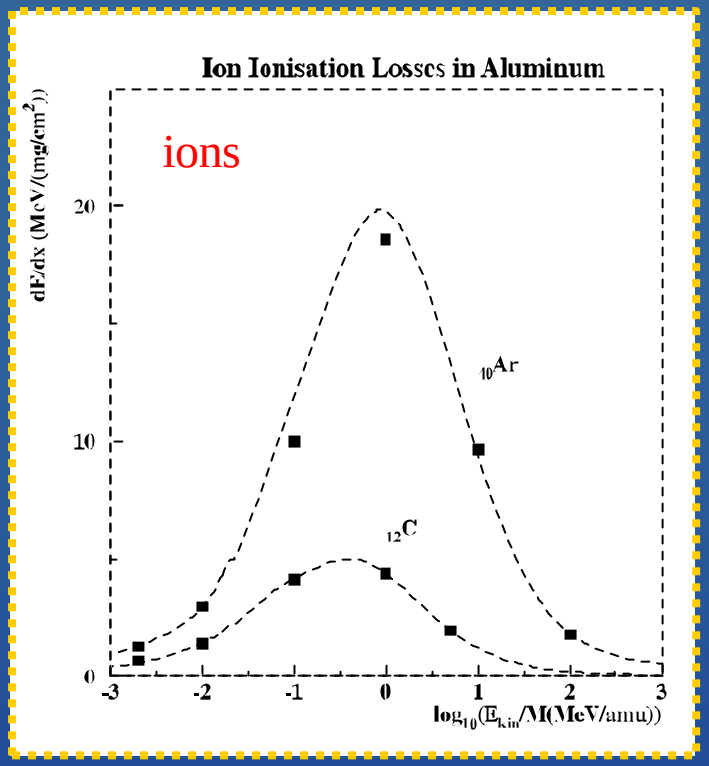



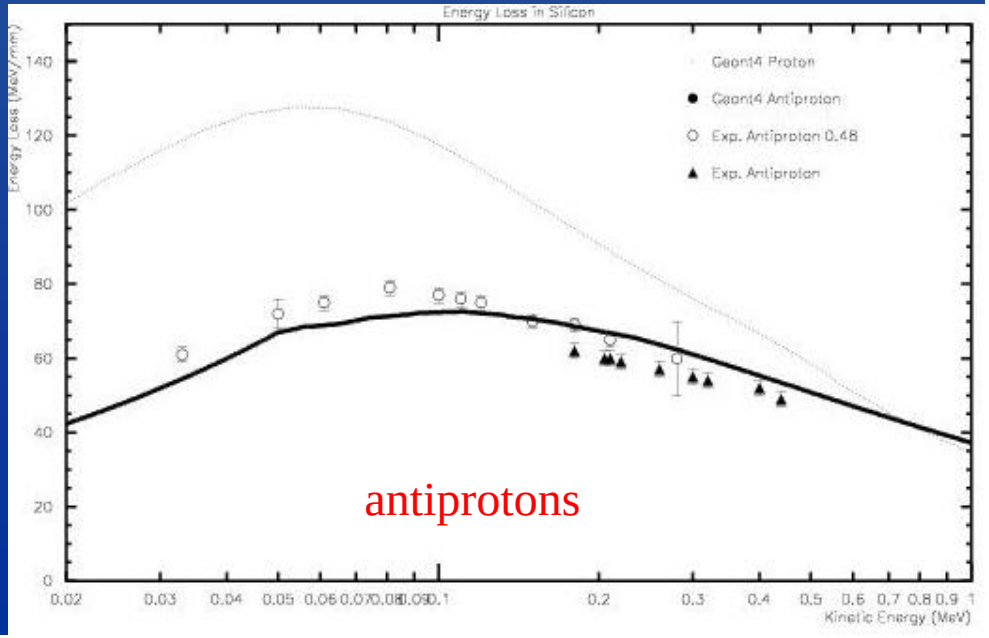



# Results, hadrons and ions



# Documentation

## User Documentation

- Included LowE documentation in Application Developer Guide
- Expanded LowE documentation in Physics Reference Manual
- Added LowE documentation in Toolkit Developer Guide
- Full coverage of all LowE classes in Software Reference Manual

## Web site

http://www.ge.infn.it/lowE/

## Internal documentation

- procedures
- URD
- design documents
- tests
- traceability map

All regularly updated

- Geant4 homepage
- RD44

- Source code
- User documentation

- User Requirements
- OOAD
- Documents
- Group meetings

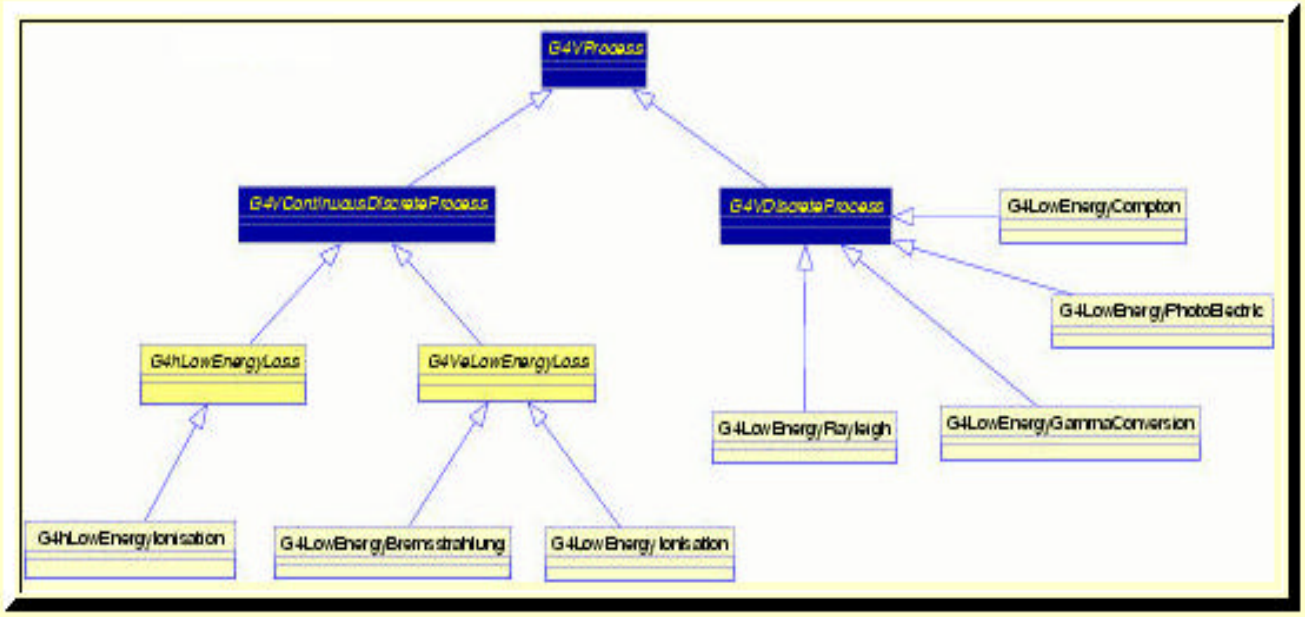
- Contact us
- How to join the Group

- User Support
- Training

Applications
- Space science
- Astrophysics
- Medical physics

- Geant4-DNA

## Low Energy Electromagnetic Processes




A set of models are available in the Geant4 Simulation Toolkit to describe the interactions of photons, electrons, hadrons and ions with matter down to low energies. These models are implemented in the toolkit to extend the coverage of electromagnetic interactions of photons and electrons down to 250 eV, and of protons, ions and antiprotons down to 1 keV range.
Applications of such models range from space and astrophysics to medical field and to fundamental physics.

*Last modified 2 December 2000*
*Petteri Nieminen Maria Grazia Pia*

# Presentations 2000-2001

**2000**

- CHEP 2000 (2) — *Padova, February*
- ESA-CERN Workshop on Fundamental Physics — *CERN, April*
- PTCOG Workshop — *Uppsala, April*
- ICCR — *Heidelberg, May*
- Workshop on Space Radiation Research — *Arona, May*
- ESTRO Congress — *Istanbul, September*
- Calor 2000 — *Annecy, October*
- MC 2000 (3) — *Lisbon, October*
- AIRO — *Pisa, October*

**2001**

- Spacecraft Charging Technology Conference — *ESTEC, May*
- ESTRO Congress — *Stresa, June*
- IFM Congress — *Brescia, June*
- Round Table on Monte Carlo methods for space applications (7) *ESTEC, June*
- CHEP 2001 (4 accepted) — *Bejing, September*

+ several general Geant4 & applications talks by WG members

Seminars *(Bologna, DESY, Frascati, Genova, Roma, Stockholm, Udine…)*

# Publications

The following publications on refereed journals are planned in the short term:

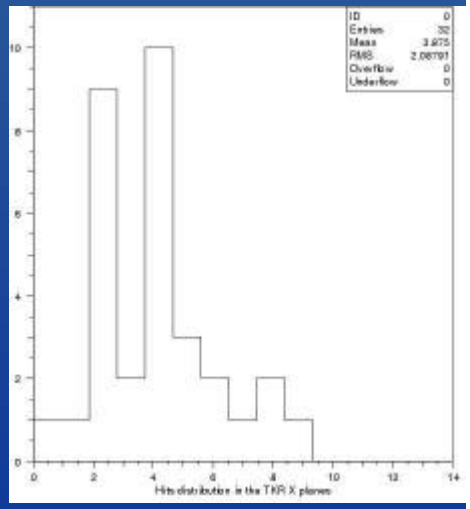
- General LowE paper
- Electrons and photons
- Positive hadrons
- Ions
- Antiprotons
- Microdosimetry
- Space telescope general facility
- Brachytherapy general facility
- Collaboration of frameworks
- Design of the LowE package

*Drafts already available for some of them*

# Other activities

- Close interaction and collaboration with the Standard Electromagnetic WG
  - design iteration in progress in the energy loss domain
  - cross-checks, testing
- Collaboration with AIDA Analysis Tools group and Lizard
  - requirements, playground for prototyping and testing
  - user support
- Collaboration with other WGs: UI/GUI, Visualisation...

*LIZARD histogram*



→ Common paper on "Collaboration of frameworks" in progress

- Advanced examples

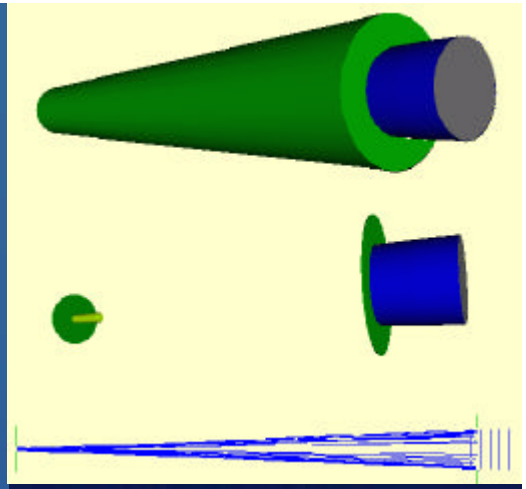
# Advanced examples

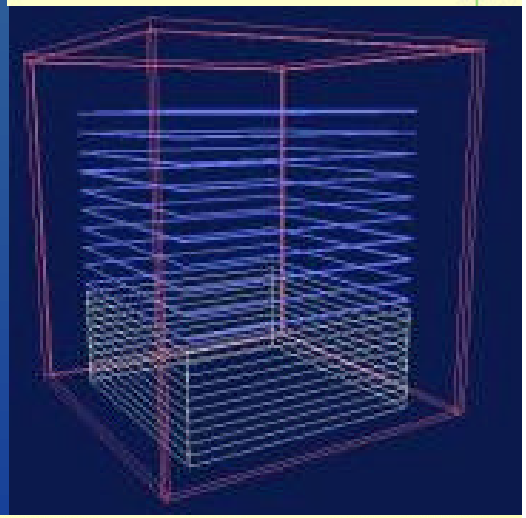
- Three advanced examples developed by the LowE WG
  - X-ray telescope
  - γ-ray telescope
  - brachytherapy

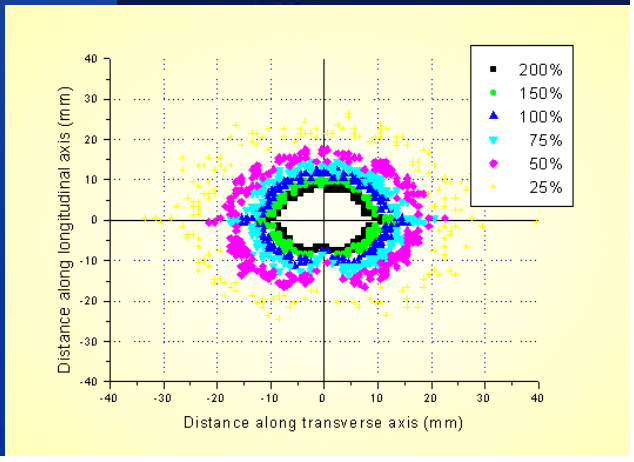
  released in December 2000
  *(first Geant4 advanced examples)*

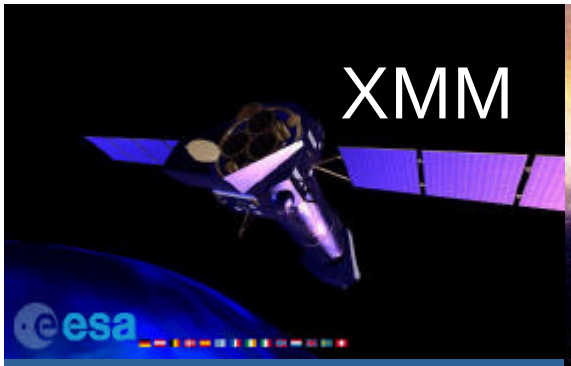
Full scale applications showing physics setting guidelines and advanced interactive facilities in real-life set-ups

- More in progress
  - X-ray fluorescence and PIXE
  - underground physics and radiation environment

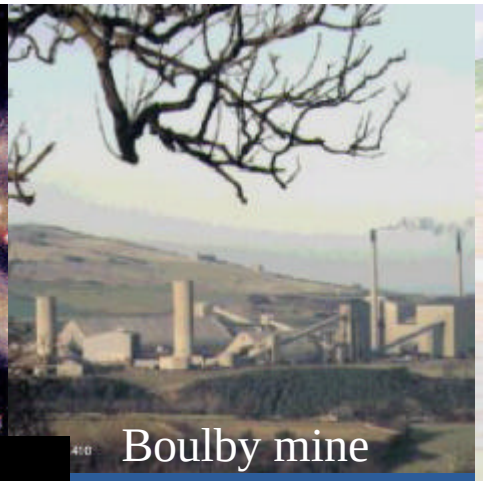


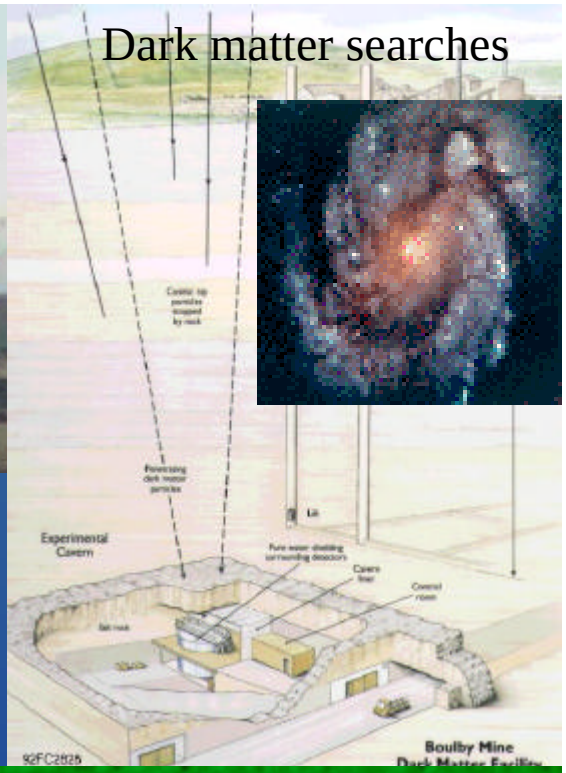


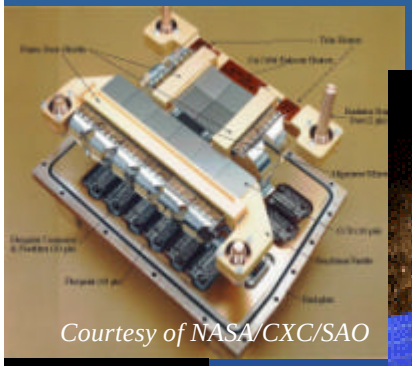


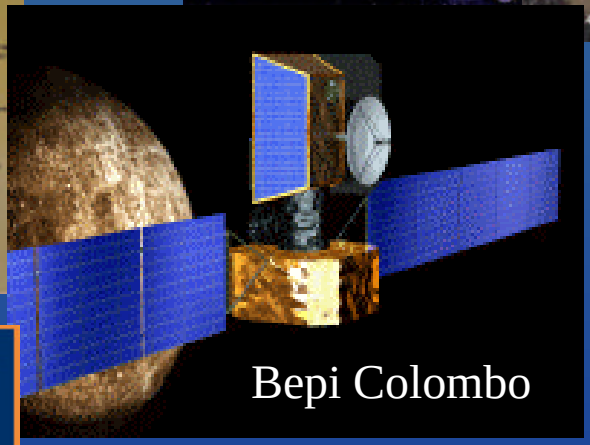






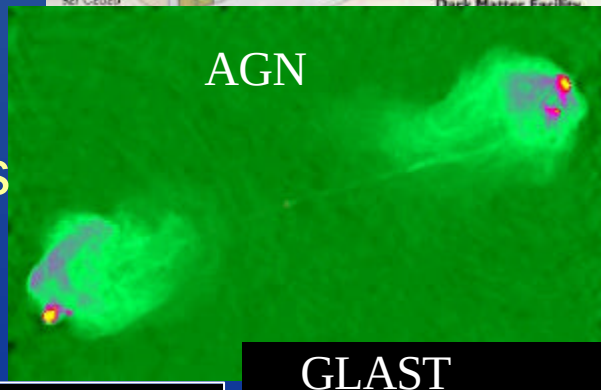



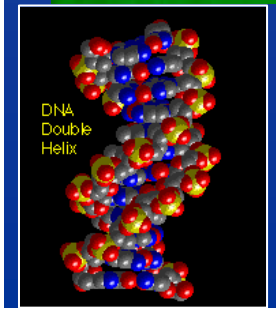




From deep underground to galaxies


From crystals to human beings






# The user community

- The WG promotes close contacts with its users
- Large user community, in expansion
  - excellent relationships with our users
  - users often contact us directly
  - the promotion through conferences, seminars, and web pages plays a fundamental role in the contacts with user communities
- URD created, maintained and regularly updated
- Fruitful collaboration with users on testing → *this afternoon*

# User support

A 

a day keeps the doctor away

This is the average frequency of users contacting us

- *Consultancy*
- *Wishing to join the activity*
- *Providing results*
- *Problem reports (very few!)*

*Excerpts of communications with users on Problem Reports:*

*"I really appreciate your support and I know you are doing your best. If you need any additional information, do not hesitate to contact me."*

*"Thank you very much for pointing out the pertinent parameters.*
*I truly appreciate the time and effort you put into answering my questions."*

# Technology transfer

- Hospitals
  - Italian National Institute for Cancer Research
  - AIRCC
  - University Hospital of Montreal
  - Massachussets General Hospital
  - Coimbra Delegation of Portuguese Oncology Institute
  - Hospital of Savona
  - Frederic Joliot Hospital
  - ...
- Companies
  - From General Electric to RXTEC...

Strategically important for political and financial implications

*Our sister activity*

# Simulation of Interactions of Radiation with Biological Systems at the Cellular and DNA Level

Based on

Geant 4

Sponsored by

esa

Activity of

INFN
ISTITUTO NAZIONALE DI FISICA NUCLEARE

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

*S. Agostinelli, S. Chauvie,, G. Cosmo, R. Corvó, N. Crompton D. Emfietzoglou, J.M. Fernandez Varea, F. Foppiano, S. Garelli, M. Krengli, F. Marchetto, P. Nieminen, M.G. Pia, V. Rolando, A. Solano, G. Sanguineti*

# Conclusions

A highly dynamic Working Group

- New physics domain in Geant4
- A wealth of new physics models
- New fields of application
- Wide interest in the user community
- A rigorous approach to software engineering
- Many results of application

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